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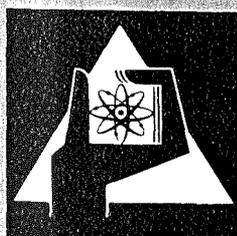
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**Interactive computer graphic methods for the  
direct determination of the phonon frequency  
spectrum by inelastic scattering of neutrons  
from polycrystalline samples**

W. Abel



**GESELLSCHAFT  
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KARLSRUHE

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Interactive computer graphic methods for the direct determination  
of the phonon frequency spectrum by inelastic scattering of  
neutrons from polycrystalline samples

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## Abstract

An on-line graphic display facility has been employed for the determination of the phonon frequency spectrum from inelastic coherent or incoherent scattering data of polycrystalline samples. One of the present interactive graphic programs is based on Egelstaff's method allowing to analyze the experimentally observed scattering law  $S(\alpha, \beta)$ . An interactive version of the LEAP computer code is used to improve the frequency spectrum iteratively. A second program is described which may be applied to analyze the inelastic coherent scattering data from polycrystalline samples using Bredov's method of averaging. Corrections for multi-phonon contributions are calculated, using the conventional phonon expansion in the incoherent approximation. A detailed description of the program operations is given. The programs are written in FORTRAN IV and use an IBM/2250-1 graphic display unit.

## Résumé

Nous avons introduit des méthodes interactives graphiques pour déterminer la densité d'états des phonons obtenue des spectres de temps de vol de neutrons diffusés inélastiquement par des échantillons polycristallins. Dans le cas de diffusion dominante incohérente le programme rapporté premièrement utilise la méthode d'extrapolation proposée par Egelstaff pour analyser des données de la loi de diffusion  $S(\alpha, \beta)$ . Une version modifiée du programme LEAP est utilisée pour arriver à une solution prouvée après des extrapolations reiterées. Dans le cas de diffusion cohérente un deuxième programme applique la méthode de Bredov. La contribution de la diffusion par des phonons multiples est traitée dans l'approximation incohérente. Nous présentons une description détaillée du dialogue entre l'ordinateur et l'utilisateur. Les programmes sont programmés en FORTRAN IV et se servent d'un IBM/2250-1.

Interaktive graphische Methoden zur direkten Bestimmung des  
Phononenfrequenzspektrums mit Hilfe der inelastischen  
Neutronenstreuung an polykristallinen Proben

Kurzfassung

Es wird die Anwendung eines Computer-Display Systems zur Bestimmung des Phononenfrequenzspektrums aus Messdaten der kohärenten oder inkohärenten inelastischen Streuung von Neutronen an polykristallinen Proben beschrieben. Ausgehend von dem experimentell ermittelten Streugesetz  $S(\alpha, \beta)$  wird ein interaktives graphisches Programm zur Bestimmung der Phononenfrequenzverteilung nach der Egelstaff'schen Extrapolationsmethode beschrieben. Zur iterativen Verbesserung des Frequenzspektrums wird eine interaktive Version des Programms LEAP verwendet. Die zweite beschriebene Methode beruht auf der Analyse der kohärenten inelastischen Streudaten polykristalliner Proben mit Hilfe des Bredov'schen Mittelungsverfahrens. Vielphononenkorrekturen werden in inkohärenter Näherung berücksichtigt. Der Dialog zwischen dem Benutzer und dem Rechner wird ausführlich dargestellt. Die Programme sind in FORTRAN IV programmiert und benutzen die graphische Bildschirm-einheit IBM/2250-1.

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Appendix

## 1. Introduction

The inelastic scattering of slow neutrons by condensed matter is a useful tool to provide detailed information about the lattice dynamics of solids such as the vibrational frequency spectrum, the phonon dispersion curves and the polarization vectors, by analysing incoherent or coherent scattering. In order to calculate the frequency spectrum from experimental data on polycrystals, some aspects of an investigation of coherent and incoherent scattering are outlined first.

Information about the phonon dispersion relations and polarization vectors has been obtained from measurements of inelastic coherent neutron cross sections of single crystal samples. From these dispersion relations one can, in principle, deduce the frequency distribution by use of the sampling method, if (i) a theoretical model of the lattice vibrations is available, and (ii) the dispersion curves are measured for a sufficiently large number of directions in the crystal. Establishing the frequency spectrum from experimental dispersion relations, in general, requires very complicated measurements and laborious calculations. Additionally, there are many cases where no single crystals are available or the single crystals are not large enough to yield reasonable counting rates.

On the other hand, the frequency spectrum can be directly obtained for cubic crystals from completely incoherent scattering. Unfortunately, these direct measurements can only be made on few solids because in most cases the basic contribution to scattering is due to coherent scattering and no isolation of the incoherent component is possible by preparing the targets or by developing

special methods of measurement and analysis of scattering data, as mentioned below.

Since for a number of problems arising in solid state physics, only knowledge of the frequency spectrum of the normal modes or the positions of its singular points is of interest, one can avoid the difficulties indicated by determination of the frequency distribution from inelastic scattering experiments on polycrystals, which are not completely incoherent scatterers and for which coherent scattering predominates, respectively. The frequency distribution can, generally, be calculated from experimental data on inelastic coherent one-phonon scattering, if the measurements are performed over quite a wide range of momentum transfers where incoherent approximation is valid, so that an extrapolation of the scattering law data of  $S(\alpha, \beta)/\alpha$  will be applied, using Egelstaff's method /1/. If this region of momentum transfers is not reached in the experiment, the frequency spectrum can be deduced from inelastic coherent scattering data of polycrystalline samples, using Bredov's method /2/. By averaging over a sufficiently large region of the momentum transfers and polarization vectors the frequency distribution is then, under certain experimental conditions, directly related to the (average) coherent one-phonon cross section.

The measurements are conveniently carried out in TDF-spectrometers to determine the energy distributions of the scattered neutrons for a series of different scattering angles. The analysis of the time-of-flight data and conversion to the scattering law is easily achieved, using the TIFLIS code /19/. However, the amount of data produced is quite considerable and

could be extremely cumbersome, also requiring complicated and laborious calculations, unless a rapid and efficient method of analysis is used. Accordingly, there is a continuing interest in the development of on-line interactive graphic computer programs which provide an immediate and interactive access to the data. In sections 3, 4 of this report two interactive graphic computer programs are described, which are based on the methods mentioned above. They serve for the direct determination of the frequency spectrum by analysis of coherent inelastic scattering /3/ and incoherent (predominantly incoherent) inelastic scattering /4/, respectively, and have been used extensively at our Institute for some years. The problem is to investigate how some experimental uncertainties, background, multiple scattering or multi-phonon contributions are reflected in the calculated frequency distribution. Evidently, compared to the conventional batch processing methods the presentation on the screen of the computed results and the interactive control of the evaluation steps enable the user to arrive at a most acceptable solution by observing the changes in various parameters of the physical system and, therefore, to avoid as much as possible an inadequate analysis of the scattering data. On the other hand, the implementation of these facilities can also play a contributory role in the experimental planning of inelastic scattering experiments, because the time for solving particular problems has been considerably reduced.

To process the graphical information, an IBM/2250-1 display unit is used. The programs are written in FORTRAN IV and use the Graphic subroutine Package (GSP) of IBM/5/. More details about

the features of the display unit are given in /6/. However, the user should be familiar with the cursor, light pen and keyboard features of the display unit, which are provided and allow the user to communicate with the program during execution. A simple calling procedure has been written to facilitate the using of the programs in one session. The user may easily select the program which is most suitable for analysing his data. A description of the calling sequence is given in section 5. In section 6 some remarks are given on the current computer implementation of the interactive graphic computer codes.

## 2. Multi-phonon Cross Sections

The interaction of a slow neutron with the crystal lattice can conveniently be described by processes involving the creation or annihilation of one or more phonons. In the harmonic approximation the lattice vibrations can always be considered to give a non-interacting phonon system. Therefore, the scattering cross section may be represented by a superposition of the cross sections of the different phonon processes, the so-called phonon expansion of the differential scattering cross section. If one calculates the estimates of the relative probabilities of phonon processes, for example one-phonon and two-phonon incoherent processes (in the Debye approximation), it can be demonstrated /7/ that for moderate specimen temperatures and low incident neutron energies the main contribution to inelastic scattering is due to one-phonon scattering.

For multi-phonon processes, coherent as well as incoherent, the relation between neutron scattering and dynamic properties of the crystal is much more complicated. However, in the analysis of inelastic scattering experiments high-order processes may often be considered as background scattering. Multi-phonon scattering tends to be a smoothly varying function of the incident energy and scattering angle, and to be very similar to Gaussian functions, so that the more interesting part of the scattering process can be isolated. Therefore, it should be possible to deduce the multi-phonon terms without detailed information about the crystal properties by direct numerical computation. Accordingly, the conventional multi-phonon expansion will be applied to correct the differential cross section in the incoherent

approximation. Note that higher-order processes become more and more significant with increasing incident neutron energy or increasing temperatures. Multi-phonon processes in slow neutron scattering are discussed in more detail in /8/.

### 3. Frequency Spectrum from Inelastic Incoherent Scattering

#### 3.1 General Remarks

To analyze the experimental data on inelastic incoherent scattering from polycrystals, an approach based on the scattering law will be described. This method was originally introduced by Eggestaff for investigation of the dynamics of liquids. Since for a liquid phonons are not so well defined as in the solid state, it is convenient to use the basic correlation functions so that in a more general way the differential cross section can be expressed in terms of the self-correlation functions of van Hove/9/, i.e. the van Hove correlation function formalism is used to establish a direct relationship between the differential scattering cross section and the symmetrized scattering law of the target and the space-time correlation functions, respectively. The scattering law depends only on the properties of the scatterer and describes the structure and the dynamical behaviour of many particle systems, such as simple liquids, molecular systems or solids. An important quantity is the generalized frequency distribution  $p(\beta)$  which is closely related to the physical nature of the system and which can be directly deduced from experimental data on neutron inelastic scattering. The incoherent approximation is always used in the analysis. It will be briefly outlined in the next section that it is sufficient within the framework of the Gaussian approximation/10/ to find the limit of  $S_2(\alpha, \beta)/\alpha$  for a fixed  $\beta$  and different values of  $\alpha$ , extrapolated to zero  $\alpha$ , where  $\alpha$  and  $\beta$  are related to the momentum and energy transfers of the neutron, respectively, to give the

frequency spectrum  $p(\beta)$ . In the third part of this section a detailed description will be given of the modes of interaction between the computer and the user.

### 3.2 Egelstaff's Method of Extrapolation

On the basis of van Hove's formalism the intermediate scattering function  $F(\alpha, t)$ , which is the space transform of the self-correlation function  $G(\underline{p}, t)$ , can be written for monatomic systems as an exponential /11/ :

$$F(\alpha, t) = \exp \left[ \sum_{n=1}^{\infty} (-\alpha)^n w_n(t) \right]$$

where the functions  $w_n(t)$  are related to the velocity-velocity correlation functions. The first term in the series gives the Gaussian approximation mentioned above. Using this approximation it is possible to evaluate exactly incoherent scattering for a perfect (monatomic) gas, a diffusing atom, and a harmonic oscillator. In liquids, on the other hand, the interpretation of scattering requires more or less drastic approximations to obtain simple expressions for the cross section for scattering with energy and momentum transfers. Although this approximation is not in general valid for very large values of  $\alpha$ , one can expect the corrections to be very small if anharmonic effects are not too large. On the other hand, the Gaussian approximation is better for small  $\alpha$ , because the first non-Gaussian term which can be simply derived from the above expression is of the order of  $\alpha^2$ . In practice, assuming a Gaussian for the intermediate scattering function applicable to any scattering system, one should obtain

a good first approximation.

The scattering law  $S_s(\alpha, \beta)$  is the Fourier transform of the intermediate scattering function  $F(\alpha, t)$ , hence with  $w(t) = w_1(t)$

$$S_s(\alpha, \beta) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \exp[-\alpha w(t) + i\beta t] dt$$

where  $t$  is a dimensionless time variable and is measured in units of  $\hbar/kT$ . The dimensionless quantities  $\alpha$  and  $\beta$  are related to the squared momentum transfer  $Q^2$  and the energy transfer  $\hbar\omega$  of the neutron by the following expressions:

$$\alpha = \frac{\hbar^2 Q^2}{2 M kT}$$

$$\beta = \frac{\hbar\omega}{kT}$$

$M$  is the mass of the atom,  $T$  is the temperature of the system.

The conventional phonon expansion can be obtained from the expression above for  $S_s(\alpha, \beta)$  by first isolating the Debye-Waller factor and then expanding in powers of  $\alpha$ . The function  $w(t)$  is proportional to the mean square displacement of the atom after the time  $t$  and by an analytical expression it is directly related to the required  $p(\beta)$ . In practice, the scattering law can be measured over a limited range of energy and momentum transfers in one experiment only. Then the determination of  $w(t)$  from the measured data leads to the mathematical difficulty of carrying out accurately the Fourier transform. To avoid these uncertainties Egelstaff's method of extrapolation is used. Without the Fourier transform the generalized frequency distribution  $p(\beta)$  can be obtained from the expression above for the scattering law

$S(\alpha, \beta)$  if one integrates twice by parts and divides by  $\alpha$ . For the limit  $\alpha \rightarrow 0$  one gets

$$p(\beta) = \beta^2 \lim_{\alpha \rightarrow 0} \alpha^{-1} S(\alpha, \beta)$$

The so defined function  $p(\beta)$  is in the case of a harmonic solid directly related to the phonon density of states  $\rho(\beta)$  by

$$\rho(\beta) = 2 p(\beta) \frac{\sinh(\beta/2)}{\beta}$$

On the other hand, having obtained  $p(\beta)$  experimentally, one can recalculate the scattering law  $S(\alpha, \beta)$  in the harmonic approximation from  $w(t)$  for all values of  $\alpha$  and  $\beta$  which involves simple integrals of about  $p(\beta)$  only. Using the methods proposed by Egelstaff and Schofield/13/ a modified version of the LEAP code/12/ is incorporated in the interactive program so that a more accurate generalized frequency distribution can be obtained when a method of successive approximations is applied by comparison of the calculated results with the experimental data. As already mentioned earlier, the extrapolation can be made when, in favorable cases, scattering may be treated by the incoherent approximation even if there is a large coherent component in scattering. Coherent scattering is important for small values of  $\alpha$  and  $\beta$  and decreases rapidly when  $\alpha$  increases and becomes large compared to the inverse square of the interatomic distances. The same result holds in general for large values of  $\beta$ . Thus, the frequency distribution can be determined quite accurately, if  $\alpha$  is still small enough, so that  $\ln S(\alpha, \beta)/\alpha$  remains a linear

function in  $\alpha$ . However, the main problem arises from the fact that for large momentum transfers, where the incoherent approximation should be valid, multi-phonon contributions must be carefully taken into account. Moreover, in the interpretation of the experimental scattering data the method described here offers the advantage that the graphical representation of the data on the screen allows the user to observe immediately how the rise of data for small  $x$  is affected by increased coherent contributions, by an imperfect primary or secondary energy resolution of the experimental equipment, or by multiple scattering effects, if some are suggested at all. In addition, due to the poorer resolution for large  $\beta$ , care must be taken to obtain improved data in the high-frequency range.

### 3.3 General Description of Program Operation

This section describes the use of the interactive graphic computer program PBETA250 allowing to evaluate the frequency spectrum from experimental scattering law data, as has been mentioned previously. Before discussing the program operation in detail, the basic facilities provided should be briefly indicated. First, to get a rough estimation of the frequency spectrum, the experimental data are extrapolated by fitting these data to a straight line. By stepwise variation of the line parameters by function key attentions a better match of the straight line to the experimental data should be achieved. Second, an improved frequency spectrum may be established using the LEAP code. Each calculation is associated with a succeeding extrapolation which can be performed in different ways. After an extrapolation run has been completed, the resulting frequency spectrum can be examined by its correction at several points, as will be explained later. With respect to the evaluation steps the user is able, at various points during processing, to direct the mode of operation by a choice of several options; one of them must be selected by a light pen detect, or by entering particular information to be supplied in response to a displayed request from the alphanumeric keyboard. A survey of the function keys used here is given in Table 1. Several messages inform the 2250 user about the next action taken by the program. Thus, the experimenter is provided with the means that place him inside the processing loop by giving him a 'conversational' mode of operation. The program may be called by using the calling sequence described

TABLE 1

Key No.	Function†
1	NO for questions
2	YES for questions or continue processing
4	Correction of the extrapolation by moving the line
5	No correction of the displayed line
5	Take the old frequency value
7	Repeat the extrapolation with an another normalization
10	Parallel displacement of the line in upward direction
11	Parallel displacement of the line in downward direction
13	Keyboard entry of the shift increment, if desired
14	Increase shift increment by factor 2
15	Decrease shift increment by factor 2
16	Clockwise rotation of the straight line
17	Anti-clockwise rotation of the straight line
19	Keyboard entry of the increment for rotation steps
20	Increase rotation increment
21	Decrease rotation increment
22	Display of the frequency spectrum extrapolated before
28	Equivalent to the END key for keyboard input
30	EXIT or end of program

† Notice that these keys are not always active though the lights are switched on. To use these keys correctly, the user is referred to the description given below.

below in section 5. After selection a title frame identifying the procedure is displayed. The user is requested to select the input mode of the scattering law data (Fig.1).

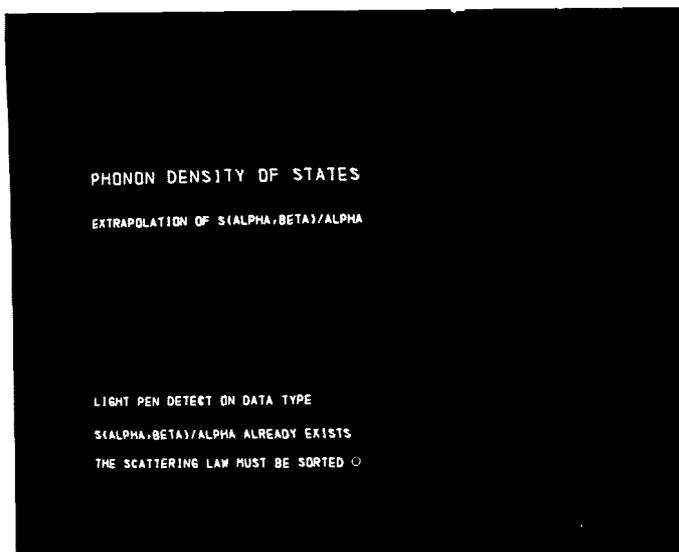


Fig. 1: Title frame and selection of input mode of  $S_s(\alpha, \beta)/\alpha$

The user must now identify his data set to be evaluated by entering the first name in the qualified data set name from the keyboard. After completing the user must perform the END function with depressing of key 28 or the END key on the keyboard. Through it, the user indicates, in every input request, that he has finished entering information. This name is then used by a special program to locate the data set and make it available for processing. If the data set cannot be found on a specific volume, the user may reenter a new name or cancel the run by depressing key 30 resulting in a return to the calling program:

```
DATA SET TOF.IAK352 NOT FOUND
```

```
ENTER NEW NAME OR CANCEL
```

```
DATA NAME _
```

If no errors have been detected, a title now appears on the screen. The cursor indicates that the user may accomplish, if desired, the title with any information identifying his problem. During the input operation the message READ INPUT SPECTRA is displayed on the lower part of the screen. The input whose formatting must be identical to that of the TIFLIS program/19/ may contain either the scattering law data arranged for several  $\beta$  values and a series of  $\alpha$  values or the scattering law data for each detector. In the latter case the user is requested to enter the one-phonon limit and the energy interval from the keyboard. These data are used to calculate the appropriate  $\beta$ -mesh for the sort program which is then called to interpolate the scattering law for constant energy transfer. However, a sufficient range of energy transfers should be given in the input data set allowing the user to evaluate his data for energy gain or energy loss, if desired. It is to be emphasized that this facility provided additionally is a time-consuming process. The response time to this operation may amount to 5 minutes or more. With respect to the LEAP code the  $\beta$  values must be positive, equally spaced, and arranged in a decreasing order. The maximum number of the  $\alpha$ -values is limited to 50, whereas the energy scale may consist of up to 80  $\beta$ -values. Thus, the data must be rearranged to be retrieved as they are needed for an evaluation of the data obtained from spectra either for energy gain or energy loss. Hence, a subprogram is included to establish properly the relationship between the experimental data and the recalculated data using a direct addressing technique before passing to the LEAP code or returning to the user. After the input operation has been com-

pleted, the message above is removed from the screen. At this point, before starting the extrapolation loop, the user must decide whether a hard copy plot of the experimental scattering law data together with the 'fitted' extrapolation line is required or not. If yes, a plot title will be expected to be entered from the alphanumeric keyboard. The beginning of the textual information is indicated by the initially positioned cursor, the length of the text is limited by a displayed asterisk at the right of this line where the incident energy of the neutrons and the temperature of the evaluated sample are displayed simultaneously. Typing errors can be easily corrected by repositioning the cursor using the BACKSPACE key and retyping the new character.

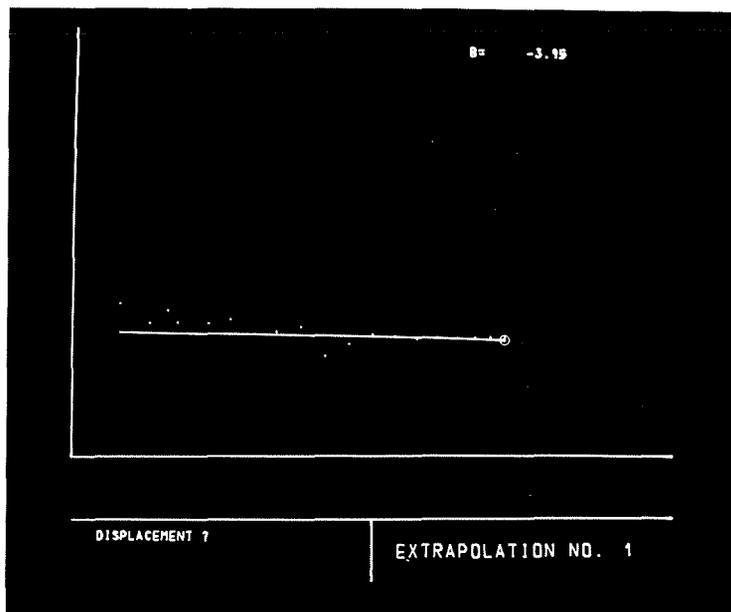


Fig. 2: The display shows an extrapolation for one  $\beta$

When displaying the scattering law data for the first  $\beta$ , the message RANGE OF EXTRAPOLATION indicates that two points are to be selected by light pen detects to perform a first extrapolation.

tion. In this case and also in many other situations, the supplemental message (BY) LIGHT PEN DETECT is displayed on the screen to help the user to answer the request. In the following processing the slope determined initially of the straight line will be taken as constant as long as possible, because the slope of the line is a sensitive parameter in the interpretation of data /14/. After the selection of the end points of the interval has been completed, the program asks the user whether the points are determined accurately or not. By answering RANGE OK. and depression of key 1 the region can be chosen again. Depression of key 2 results in the display of the extrapolation line whose parameters are calculated by a least-squares method. In all other cases, CURVE THROUGH POINT mentions that a reference point must be determined through which the line will then be drawn. However, the parameters of the straight line may be changed by answering DISPLACEMENT with depressing key 4 (Fig.2). To obtain a reasonable good 'fit' of the line drawn to the experimental data, the user may move the straight line over the screen in suitable constant steps, using the function keys given in Table 1. Using key 5 or key 2 does not result in corrections and gives rise to the calculation of the required frequency value and the display of the scattering law data for the next  $\beta$ , and so on.

When all extrapolations have been completed, the frequency spectrum  $\rho(\beta)$  will be displayed on the screen (Fig.3). In the lower part of the screen the message CORRECTION OF  $\rho(\beta)$  indicates that the frequency spectrum can be inspected by testing several extrapolations with light pen detects on any point which is verified by the display of an 'X' symbol at this location.

Depressing key 2 results in the display of the experimental scattering law data together with the extrapolation line so that an examination of the appropriate extrapolation will be possible.

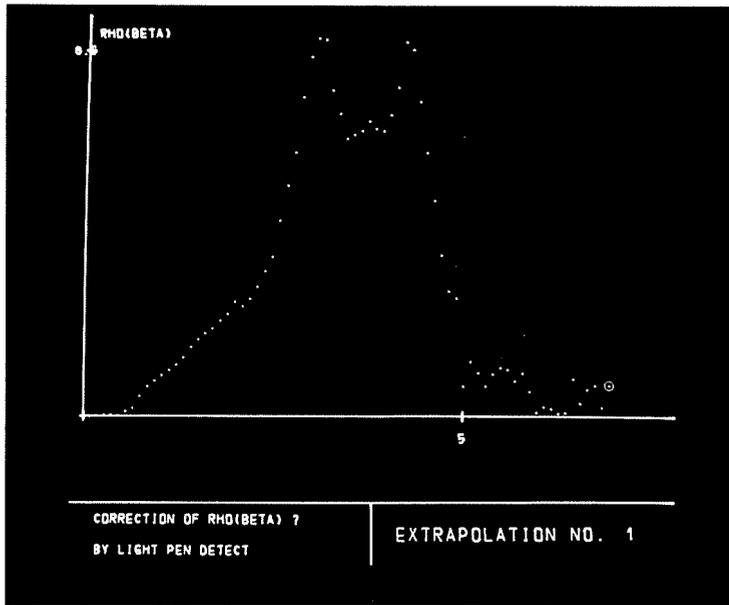


Fig. 3: Frequency spectrum  $\rho(\beta)$  which may be examined

On the other hand, using key 7 enables the user to correct the frequency spectrum directly without being forced to repeat completely the extrapolation for the distinct  $\beta$ . To do this, the new point must be selected on a vertical line which is displayed at this position by relating the correlation value of the line element detected to the number of the scaled segments of the vertical line. This procedure can be repeated as often as desired because the request SELECT NEW POINT is automatically recalled. The correction loop can be terminated when this request is answered by depressing key 1. At this point, the frequency spectrum will be put out as a printer plot and in a tabular form. Additionally, a card output or a hard copy plot can be produced by pointing either at the PUNCH or PLOT option. If no such output

is needed, depressing key 2 removes the frequency spectrum from the screen and continues processing.

If no further refinement of the first estimation of the frequency spectrum will be required, the END option causes a return to the calling procedure. After touching RESTART with the light pen, the user may repeat the same loop again. Otherwise, a light pen detect on CONTINUE means that the extrapolation will now be performed using the recalculated data with a slightly modified version of the LEAP code. A list of self-explanatory option messages displayed simultaneously allows the user to direct the input to the LEAP program by touching one or more of the information requests with the light pen in any order. The end of a selection must be signaled by depression of key 2 or through touching any portion of the last line of Fig.4.

```
RECALCULATION OF THE SCATTERING LAW
FROM P(BETA)

RD(BETA) TO P(BETA)
NEW TEMPERATURE ?
DIFFUSION ?
SMOOTHING OF P(BETA) ?
SCT-APPROXIMATION ?
PRINT OUT PHONON TERMS
PRINT OUT S(A,B) A=CONST.
PRINT OUT S(A,B)/A B=CONST.
END OF INPUT OR CHANGING
```

Fig. 4: Input to the LEAP code by selection of options

Next, the user is requested to type in from the alphanumeric keyboard the PNDRM normalization constant of the frequency

spectrum and the number of MAXT phonon terms used in the calculation. Depending on the stage of calculation, the messages

PHONON EXPANSION

and

SCATTERING LAW  $S(\text{ALPHA}, \text{BETA})/\text{ALPHA}$

are displayed one after the other. The manner by which LEAP reproduces the scattering law is not described here. For further details see Ref./13/. When recalculation of the scattering law is completed, the program returns to a similar extrapolation loop as described above. To facilitate the extrapolation using the model calculation, the user has three possibilities; one of which is to be chosen by light pen detects or by depressing key 2 (Fig.5).

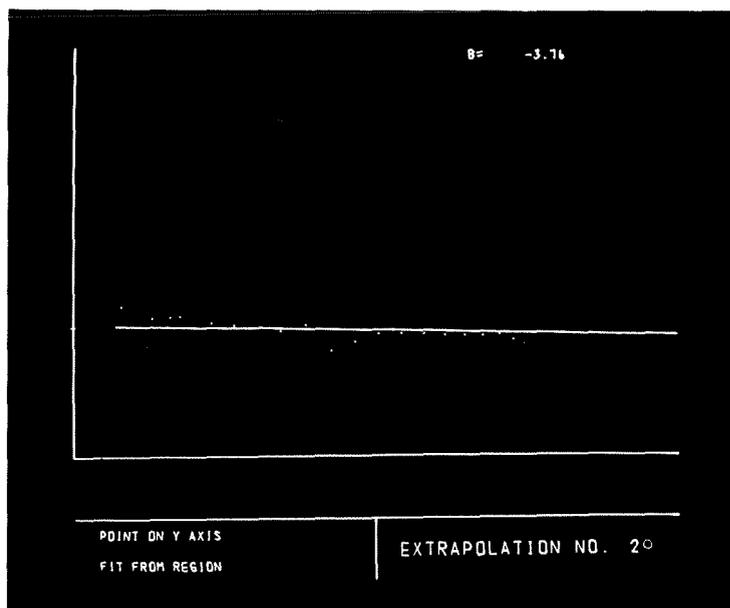


Fig. 5: The user is requested to select the extrapolation mode

First, a direct determination of the extrapolated frequency value on the y axis is possible in response to the requests POINT ON Y-AXIS, CURVE THROUGH POINT and the repeated request POINT ON

Y-AXIS. On the other hand, if the recalculated data are linear enough for large  $x$ , after touching FIT FROM REGION, the user is requested to enter via light pen detects the region he wants to use in fitting of the data to a straight line. The range selected can be redefined after depressing key 1, if necessary. Third, if all data show a sufficiently good linear behaviour, depressing key 2 causes a fit through all experimental points. Note that the slope of the fitted curve may, in this case, strongly differ from that of the input data, even if only few points are outside the statistics so that the last feature does not seem to be very suitable to arrive at an acceptable extrapolation. During the DISPLACEMENT phase only the constant parameter of the straight line may be altered, i.e. the computed slope will be taken as constant.

If the process already converges quite well for distinct values of  $\beta$ , depressing key 6 enables the user to accept the value of the frequency spectrum extrapolated before without changing. In order to repeat the same calculation with another normalization, one must depress key 1.

At the end of this extrapolation run the user may examine the frequency spectrum in the same way as described above. Moreover, depressing key 22 allows the user to inspect the previously extrapolated frequency spectrum at the same time. This display must be removed from the screen by a second depression of the same function key. If a correction of the frequency spectrum at several points is needed, the curve originally computed by LEAP will be shown so that the whole extrapolation must be repeated for these points.

If no such corrections are desired, the user may use the options, which are displayed on the lower part of the screen(Fig.6), to choose the next program action. The run may be canceled by touching the END option with the light pen. At this point, the NEXTDD option also allows the user to define another data set he wants to process, if desired. In order to repeat the extrapolation run with the same data set, the user must select the RESTART option with the light pen. On the other hand, to improve the frequency spectrum, the extrapolation loop can in turn be continued using the CONTINUE option.

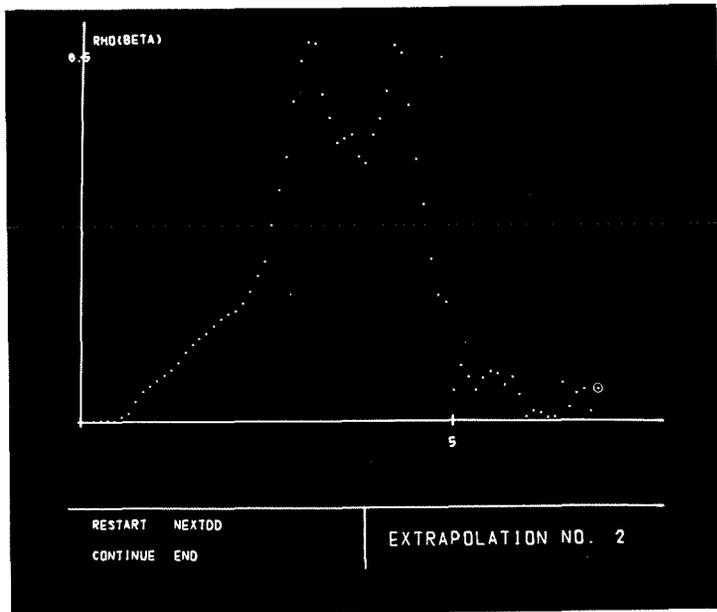


Fig. 6: Frequency spectrum with program options

## 4. Frequency Spectrum from Inelastic Coherent Scattering

### 4.1 General Remarks

In a wide range of solid crystals coherent inelastic scattering of slow neutrons on single-crystal samples is used to determine the dispersion relations  $\omega = \omega_j(\underline{q})$  (for a wave vector  $\underline{q}$  and the  $j$ th branch or polarization index of the normal mode) by measuring the angular and energy distributions of the scattered neutrons with respect to the orientation of the crystal. Evidently, the frequency distribution of the normal modes may be directly deduced from the experimental dispersion curves using the sampling method, but this procedure requires the measurement of the dispersion relations for a large number of phonon wave-vector directions. Therefore, the dispersion relations, which are measured for a few number of highly symmetric directions in the reciprocal lattice only, are conveniently analyzed in terms of a suitable model of (harmonic) lattice dynamics by fitting the model parameters to the experimental data. For example, the dispersion curves are used to verify the Born-von Kármán model using a nearest-neighbour approximation for the atom-atom interaction. The frequencies are then obtained by diagonalizing the dynamical matrix. In order to determine the over-all frequency distribution by reasonable good sampling, a large number of matrix diagonalizations must be performed in the irreducible part of the Brillouin zone for as many independent wave vectors as possible. Moreover, the interpolation of the correct frequencies in the off-symmetry directions depends on the validity of the theoretical model to describe the dynamical

properties of the crystal. Another way of calculating the frequency distribution is the 'extrapolation method' introduced by Gilat and Dolling/15/. This method offers the advantage that the number of diagonalizations can be significantly reduced, also requiring less computing time, even in cases where there is more than one atom in the unit cell. Although the resolution in frequency is remarkably improved, care must be taken to consider possible degeneracies in the eigenfrequencies. However, if no single crystals of the matter being studied are available, the determination of the dispersion relations from measurements of the coherent scattering of polycrystalline samples will be hardly successful, as the measured distribution represents an average over distributions of the neutrons scattered on a large number of single-crystal grains. Then the coherent peaks overlap each other and are broadened so that it should be possible to determine with a sufficiently good accuracy the dispersion relations for distinct values of the wave vector. Many improvements have been made on the sampling method, but investigations showed that uncertainties in the fit of model parameters to the experimental data may lead to appreciable errors in the frequency spectrum, i.e. the position, size and shape of the peaks in the frequency distribution depend sensibly upon the lattice model employed. For this reason and from the point of view of a rapid and efficient data analysis, Bredov's method of analyzing the inelastic coherent scattering cross section from polycrystalline samples, which corresponds to an 'experimental sampling', has been found to be a suitable procedure/16/.

#### 4.2 Bredov's Method of Averaging

It is well known that the energy distributions measured on a polycrystalline sample in an ordinary TOF-experiment contains but partial information about the frequencies of the lattice vibrations, if inelastic scattering is completely governed by coherent effects. To obtain the complete frequency spectrum, inelastic scattering experiments must be performed in these cases under distinct experimental conditions implying averaging of the coherent one-phonon scattering cross section over a sufficiently large region of momentum transfer, so that for an arbitrary wave vector and any polarization the measured distribution of the neutrons scattered into a solid angle depends only on the energy transfer. These conditions can be ensured, if the scattering vectors fill almost uniformly and completely the Brillouin zone. A detailed investigation of the validity and applicability of this method is given, for example, in /17/. Establishment of the direct relationship between the average one-phonon coherent cross section and the frequency spectrum requires some important assumptions which will now be summarized. First, the Debye-Waller factor for a given energy transfer is assumed in most cases to be not much dependent on the momentum transfer. Second, the 'active' sampling volume contributing to the average should be large compared to the volume of the Brillouin zone, i.e. the success of this average process depends strongly on the uniform distribution of the ends of scattering vectors inside a spherical region which is determined by the minimum and maximum scattering angles given in the experiment. Third, the average value of the inner product between the momentum transfer and the polarization vector, i.e.

$\langle |q \cdot \sigma_j|^2 \rangle$ , required in the coherent one-phonon cross section can be replaced for a cubic crystal by  $Q^2/3$  where  $Q^2$  has the same meaning as in section 3.2. To obtain an estimation of the frequency spectrum, the so-called 'experimental' averaging mentioned above can be realized in the experiment, using the 'inner' or 'outer' method of averaging. The interactive procedure described uses 'outer' averaging in which for a fixed direction of the incident neutrons the scattered neutrons are observed for a set of equally spaced scattering angles, i.e. the sum is taken over the TOF-spectra measured at different scattering angles and weighted by the sine of the scattering angle. This reflects the fact that the Q-steps are not equally spaced in the experiment. The computational part of the interactive graphic program is based on a computer program written by Reichardt et al./18/.

#### 4.3 General Description of Program Operation

As already mentioned, the interactive graphic program MUPH0250 is, basically, an outgrowth of the program MUPHUCOR, originally written by Reichardt et al./18/. The manner by which the program derives the frequency spectrum from the experimental TOF-data is not described in detail here. It is sufficient to state that the program is versatile to allow for a variety of constraints to be applied to the evaluation process. By inclusion of the graphical representation of the computed results the experimenter arrives at a most acceptable solution when he observes the consequences of changes in relevant variable parameters he wants to adjust, which are summarized below.

1. Determination of the range of evaluation in the TOF-spectra.
2. Choice of the range of detectors for integration over the region of the scattering angles.
3. Correction for time-dependent background.
4. Correction for constant background.
5. Variation of the mass of the scattering system.
6. Two iteration methods can be used alternatively.
7. Variation of the upper limit of the frequency spectrum.
8. Correction for experimental resolution.
9. Iteration of the Debye-Waller factor.

After initiation of the program by a light pen detect on the appropriate line of the SELECT frame, a title is displayed (Fig.7). There are two possibilities of evaluating the TOF-data. Therefore, this frame asks the user of which type are the given input data.

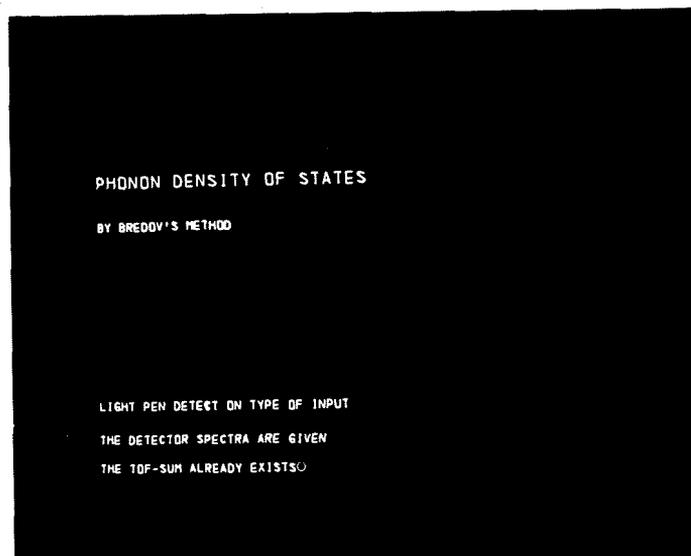


Fig. 7: Title frame and selection of TOF-data input mode

After selection the screen goes blank and the program begins processing. If the detector spectra have been saved by the TIFLIS

program, the user is now requested to identify his data set by entering the data name from the keyboard.

DATA NAME \_

If the data set does not exist, the user is then requested to type in the name of another data set being evaluated or to cancel the session by depressing key 30.

On the other hand, if THE TOF-SUM ALREADY EXISTS, the data must be supplied from cards. For processing more than one TOF-sum of several sample measurements the card sets may follow each other. In both cases, the session may be canceled using key 30, whereas depressing key 2 starts processing.

Depending on the selected input mode, the data are read in from a system device (tape or disk) or from cards as described below. If the detector spectra are given, the message READ INPUT SPECTRA is displayed on the lower area of the screen while the time-of-flight data are transferred. Formatting of this input must be identical to that of the TIFLIS program/19/. If the TOF-data reside on cards, the user is first requested to define the length of the sum-spectrum by a light pen detect on the appropriate option message in the next frame. If ALL CHANNELS are given, the number of channels must be entered from the alphanumeric keyboard as indicated by the cursor. In this case, a variation of the range of channels will be possible in order to adjust the sum spectrum. A light pen detect on FIXED REGION invokes the requests of the FIRST CHANNEL and LAST CHANNEL. Then the message READ INPUT TOF-SUM appears on the screen during input operation. Next, some experimental parameters are expected to be entered from the

alphanumeric keyboard together with additional parameters for the sum spectrum as specified from external programs generating the sum-spectrum.

After the input of the TOF-data has been completed, a list of some relevant experimental parameters will be displayed (Fig.8). In the lower area of the screen the cursor indicates that the user is requested to accomplish a title, identifying the particular run with relevant details. The length of this additional information is also restricted by an asterisk displayed to avoid an overwriting of the subsequent information in the same line.

```
EXPERIMENTAL CONSTANTS :  
  
INCIDENT NEUTRON ENERGY      45.0  
FLIGHT PATH (SECONDARY)     301.00  
CHANNEL WIDTH                 8.0  
MASS OF THE SCATTERER       50.15  
TEMPERATURE                  11.00  
  
TITLE: VANADIUM_             * E0=45.0 T= 11.000
```

Fig. 8: Display of experimental constants; a title is requested.

The next frame (Fig.9), which may be recalled as often as necessary during an evaluation run, contains a cumulative list of the variable parameters involved in the calculation of the multi-phonon contributions and the in averaging over the TOF-data. As explained later, a choice of a symbolic textual element allows the user to change one or more of these parameters

he wants to adjust. To specify an initial choice of the parameters, the appropriate line will be displayed at the bottom of the screen, requesting the user to enter the data from the keyboard.

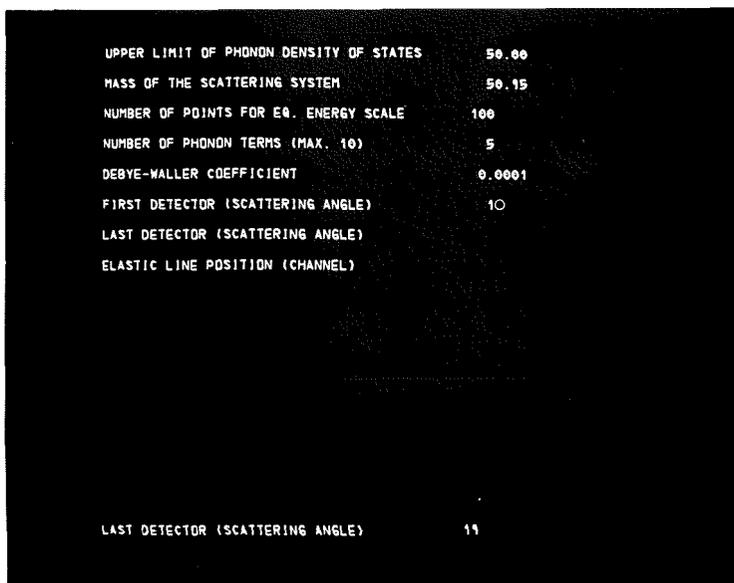


Fig. 9: Parameter frame during input request

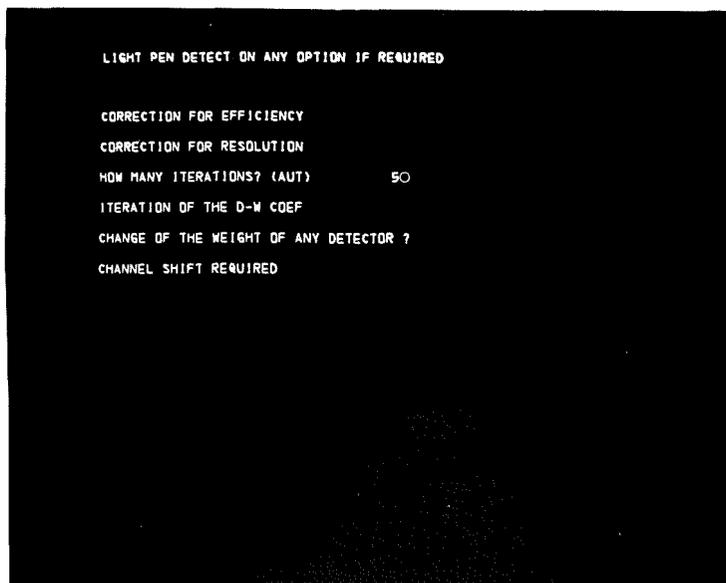


Fig. 10: Program options to be selected

The input values will then be displayed in a column at the right of the actual parameter line. When the list has been completed, depressing key 1 enables the user to change an incorrect value by a light pen detect on the appropriate text as indicated by the

heading information message LIGHT PEN DETECT ON THE REQUIRED ELEMENT. Finally, key 2 must be depressed to proceed with the evaluation. Next, the user is requested to select some of the program options with the light pen (Fig.10), if desired. The number of iterations automatically performed is initialized by 5 and can be altered after selection by subsequent read-in from the alphameric keyboard; after the iterations have been processed, the program stops and displays the frequency spectrum as described below. The end of a choice must be signaled by depressing key 2.

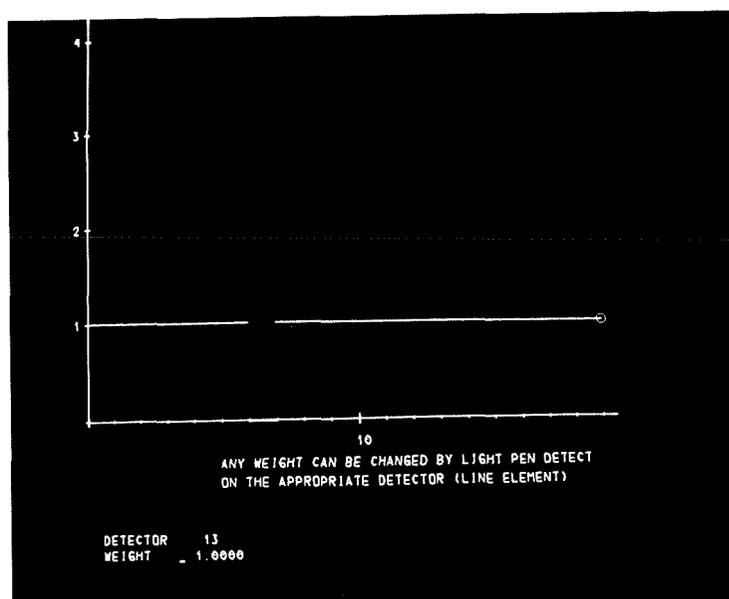


Fig. 11: Changing the weight of any detector

If the last option in Fig.10 has been selected, the user is now able to change the weight of several detectors. After selection of a line element representing the number of the detector, the user is requested to enter the new value from the keyboard (Fig.11) and a redisplay of this 'histogram' is initiated. To terminate this procedure and to continue processing, the user must depress the function key 2. If the sum spectrum exists for

all channels, the user can now inspect the whole spectrum on the screen. Scaling of the vertical axis is performed by depressing key 26 or key 27 to expand or contract vertically (suppression of the elastic line). The request SELECT END POINTS OF ENERGY RANGE indicates that two points must be touched with the light pen. After selection the channel numbers and the related energy transfers are displayed in the lower area of the screen (Fig.12). Answering RANGE O.K. with key 1, a new range can be determined. After depressing key 2 an enlarged display of the selected range of the TOF-spectrum is invoked. A hard copy plot of the whole TOF-spectrum similar to the actual display will then be produced automatically.

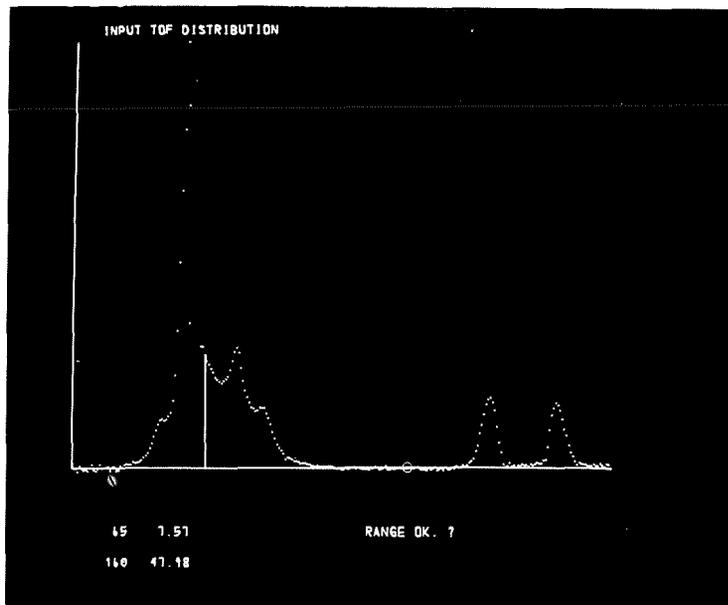


Fig. 12: TOF-spectrum with the selected range of evaluation

The next stage of evaluation is the correction for the background, time-dependent as well as constant. If no correction whatsoever is desired processing continues by depressing key 2 and will be carried on with the resolution run, if selected earlier, or the iteration run. Otherwise, the user is requested

to select either of the options given below:

LIGHT PEN DETECT ON THE TYPE OF BACKGROUND  
TIME-DEPENDENT      CONSTANT

In the case of a time-dependent background, a correction for the constant background is initiated automatically. However, only a short description of this procedure will be given here. Nevertheless, there are few operations which are applicable. The data for the time-dependent background must be supplied from cards or can, in principle, be generated using the correction option (key 19). The time factor can be entered from the keyboard after depressing key 21. Smoothing by polynomials is included optionally and will be processed after depressing key 20. In many cases, the most important correction which must be applied to the data is the correction for constant background.

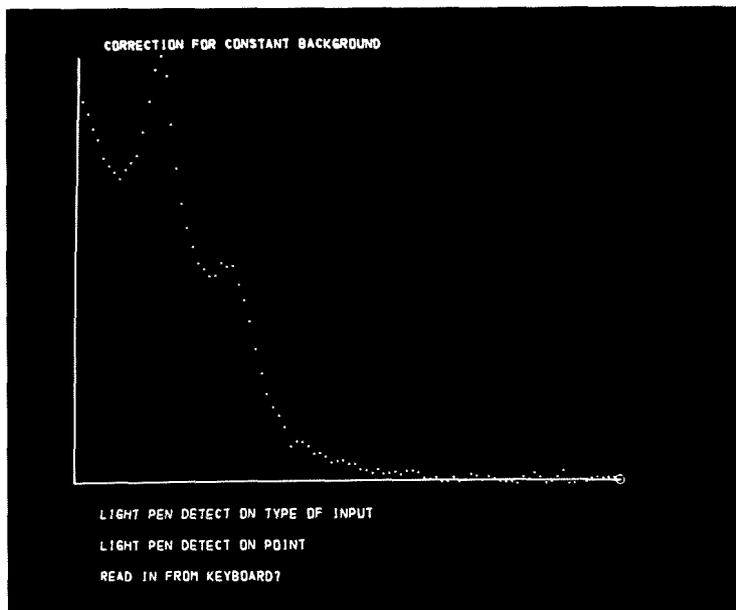


Fig. 13: Initial correction for constant background

During this correction a title is displayed on the top of the screen which is removed at the end of this procedure. A constant

background can be defined initially by a light pen detect on either of the options listed in the lower area of Fig.13. However, without answering one of the requests in Fig.13 the constant background may be directly determined by touching with the light pen a representative point in the spectrum. Then, a line is drawn according to the selection. Depressing key 1 causes the removal of this line, indicating that the selection may be repeated. It is not necessary to do this, because the initial value can be changed by function key attentions as described below. Depressing key 2 causes display of the corrected spectrum on the screen as a first estimation. At this point, the user has several function key options at his disposal, to adjust the correction for constant background. They are given in Table 2.

TABLE 2

Key No.	Function
1	Repeat the correction
2	End of correction, continue the evaluation run
14	Change the T <sub>JF</sub> -sum by parameter variation
15	Smoothing of the spectrum will be initiated
25	Enter the keyboard factor (initially specified by 10%)
26	Decrease constant background
27	Increase constant background

As shown in Table 2 repeated depression of key 26 or key 27 increases or decreases by 10% of the initial value the value of

the constant background and results in the redisplay of the corrected spectrum. Also an information message is issued which contains the current value of the constant background.

However, correction or 'smoothing' of the spectrum may sometimes be desirable. Thus, depressing key 15 invokes a display of two further options. First, by pointing at POINTS, individual channel contents can be replaced by new values after the selection of a relevant point in response to LIGHT PEN DETECT CN POINT. The new value can be entered by light pen selections as already described earlier. Since the request is repeated automatically, the user must stop this loop by depressing key 1, whenever desired. If, on the other hand, the over-all display should be changed, the selection of SMOOTHING BY LINE ELEMENTS invokes the request of a starting point where smoothing would begin. By indicating the END POINT OF NEW LINE ELEMENT on the vertical line displayed at the identified position, several line elements will be created to represent the new curve. Depressing key 8 allows to the user backward erasion, element by element, of line elements just generated. Since more than one channel usually fall into a line element, those channels are interpolated linearly. This loop must also be terminated by depressing key 1.

In both cases, if no further corrections or graphical smoothing are needed, depressing key 9 results in the termination of this operation.

The end of the data reduction run as described above must be signaled by depressing key 2. At the next stage of evaluation one could attempt to correct the spectrum for experimental

resolution, if the appropriate option had been detected earlier. To indicate this, the message CORRECTION FOR RESOLUTION will be issued at the top of the screen followed by a request to the user to enter initial specifications of the parameters which are involved in the resolution run. This is shown in the lower part of Fig.14.

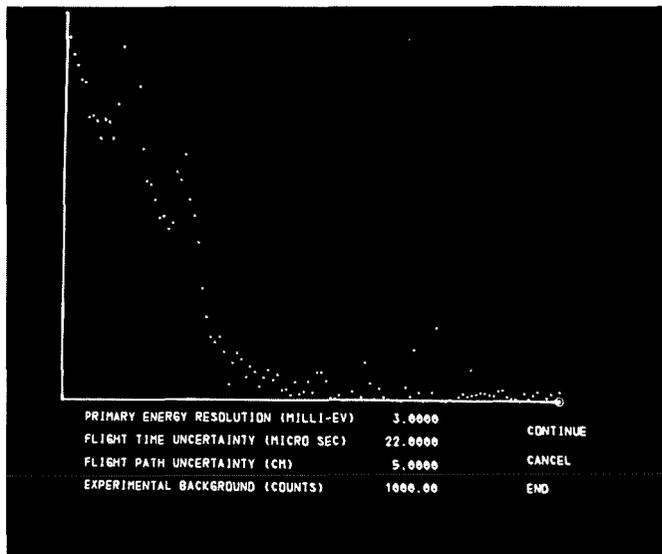


Fig. 14: Correction for experimental resolution

Further parameters which must be typed in are the number of convolutions performed automatically and the number of smoothing processes, if desired. The last request invokes the input of the range of channels being smoothed. After the list has been completed the corrected spectrum will be displayed following the number of convolutions defined above. In the lower area right of the screen three options are displayed which enable the user to perform another iteration, CONTINUE, or to terminate the resolution run, END, if it was successful. The CANCEL option can be used to finish this correction, if the process does not converge. Then, the no resolution corrected spectrum is used in

the subsequent evaluation process. Many attempts can be made to arrive at a most acceptable result by changing one or more of the relevant parameters by light pen detects on the appropriate parameter lines. Then, the cursor appears in the entry area at the right, indicating that a new value can be typed in from the keyboard. The CONTINUE option must be used to signify the completion of a parameter choice for a new run.

In cases where no correction for resolution would be applied to the data, the next main task in program operation is the evaluation of the frequency spectrum. Now, a first estimation of the frequency spectrum is calculated from the corrected TGF-data converted to the double differential cross section. In addition to this, the Debye-Waller factor is assumed to be small and then may be taken into account iteratively. For the smallest energy transfers the values of the frequency spectrum will be inserted using the Debye approximation as extrapolated from the first three points of the experimental distribution function. Before starting the iteration loop, the user is requested to decide whether the DIFFERENCE method or the QUOTIENT method is used to examine how good the calculated frequency spectrum matches the input distribution after a distinct number of iterations, supposing the same normalization. Upon subtracting the calculated multi-phonon contributions and normalization in this way, a better guess of the frequency spectrum is obtained. Once the iteration loop has been completed, the frequency spectrum is displayed on the screen. At this point, the user is faced with a choice of many options as shown in Fig.15. He may change, for

example, one or more parameters related to the averaging process of the TOF-data, change the parameters involved in the phonon expansion, initiate a display of numerical information, or produce hard copy output of the frequency spectrum. The functions of these options are explained in more detail in Table 3. The selection of one of the options invokes redisplay of the frequency spectrum after the program operation specified has been completed. To decide whether the new run led to an improved result, depressing key 4 causes the frequency spectrum as determined with the previous set of parameters to be displayed simultaneously on the screen. In the case of a combined evaluation of the energy gain and energy loss spectra the energy gain spectrum will then be issued to allow direct comparison.

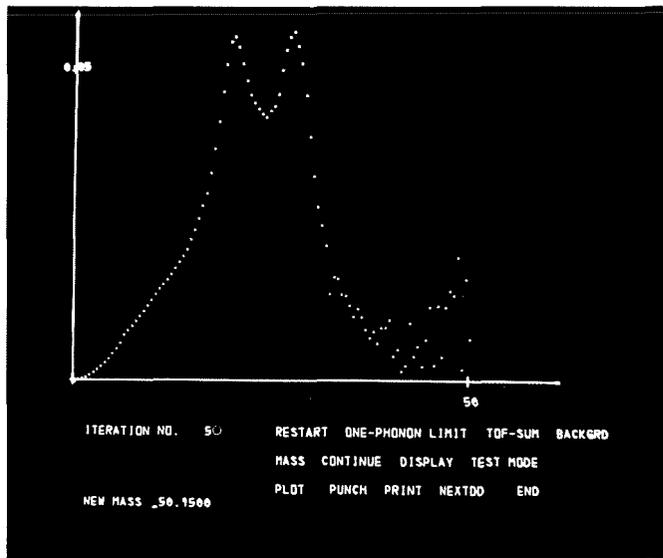


Fig. 15: Display of the frequency spectrum after 5 iterations. The MASS option has been selected in order to change the reference mass of the scattering system.

TABLE 3

Option	Function
RESTART	At this point the user has the option to return to a read-in of the problem parameters and of the input spectra. RESTART is also useful when a user wants to run a job again that has just been finished, with or without alteration. After selection the user is able to perform an evaluation of the spectrum either for energy gain and energy loss in the same run. Additionally, the user is requested to decide whether he wants to analyze the spectrum for energy loss using the energy gain spectrum, if just evaluated, for normalizations and multi-phonon corrections.
PHONON-LIMIT	This alters the related parameters describing the energy scale and the one-phonon limit representing the upper tail of the acoustic part of the frequency spectrum in order to calculate a new estimation of the frequency spectrum without changing the TOF-sum spectrum.
TOF-SUM	This option allows the user to change the sum spectrum and to repeat the data reduction.
END	End of the current run.
NEXTDD	The user may designate a new data set for evaluation.
MASS	The reference mass of the scattering system may be altered. If the Debye-Waller coefficient were not iterated, this factor would be displayed and the new value corresponding to the new mass can be entered from the keyboard.
CONTINUE	Execute the next iteration without changing any parameters
DISPLAY	Here, the user has a lot of information at his disposal which may be called in any order by depressing several function keys:  Key 16 input distribution of $G(\omega)$ from TOF-data Key 17 input distribution from multi-phonon terms Key 18 $\int G(\omega) d\omega$ (TOF-sum from iterated $G(\omega)$ ) Key 22 convergence test (multi-phonon correction) Key 23 Debye temperature vs $\omega$ (renormalized $G(\omega)$ ) Key 24 - moments from -3 to +7  To return to the calling program, the user must depress key 1. The quantities written in brackets are displayed whenever a combined evaluation of the

TABLE 3 (continued)

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	energy spectra for energy gain and energy loss has been performed.
TEST-MODE	This option allows the user to repeat the same iteration loop with the other convergence test mode.
PLJT	The PLOT option is used to produce a hard copy plot of the frequency spectrum.
PUNCH	This option is used to produce a punching output of the frequency spectrum.
PRINT	The PRINT option produces a print-out of the frequency spectrum in tables and as a printer plot both for the equidistant energy scale and for the time-constant scale.
BACKGRD	This option may be used to repeat the correction for constant background.

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### 5. Description of the Calling Procedure

With respect to an efficient application of the two computer codes an interactive graphic main routine has been developed which directs the loading of the major links represented by the programs. At the beginning of the session an overall title (Fig.16) is displayed on the screen, which must be removed from the screen by depressing key 2 to start processing. First, a SELECT frame appears on the screen and asks the user which one of the programs is suitable to be used for processing his data (Fig.17).

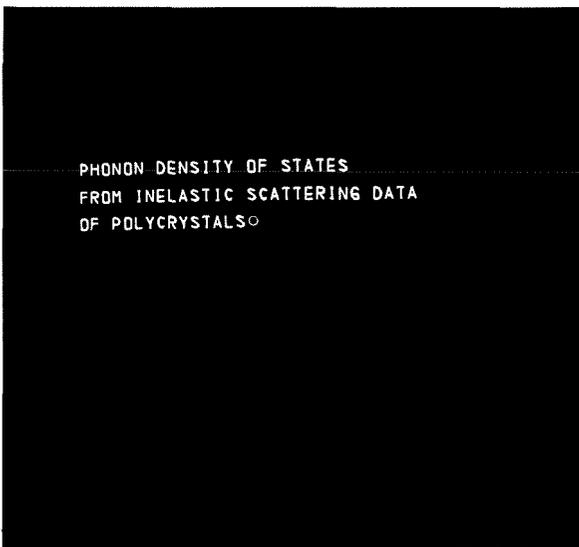


Fig. 16: Title after job start

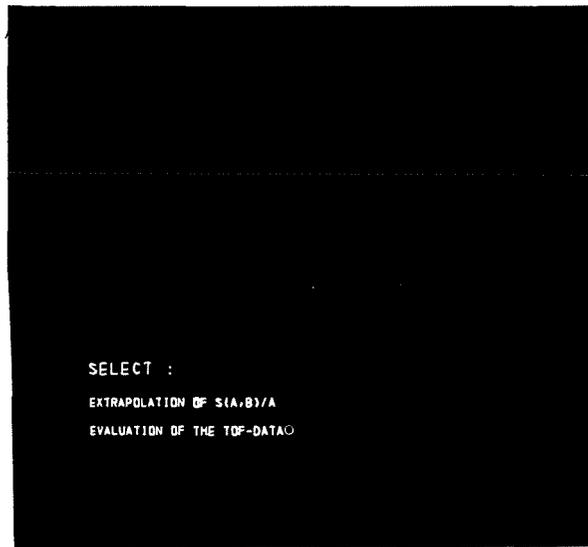


Fig. 17: SELECT frame

When a program has completed processing as indicated by the user having selected the END option at the end of a particular run, another select frame is displayed together with a history of the current 'job' just run as a reminder (Fig.18). Since the user had only one job to process, he selects CANCEL JOB. If he wants to perform further evaluations with or without different data sets, the user must select the RECALL operation from the select frame

to continue the session. A recall frame now appears on the screen (Fig.19). After touching the MODIFY option the new procedure may be selected from the redisplayed select frame. Selecting of the program just run results in the same operation as initiated by the NEXTDD program option. If the user has been selected the ACCEPT operation, the same job may be called again. At this level, the last operation is equivalent to the RESTART option.

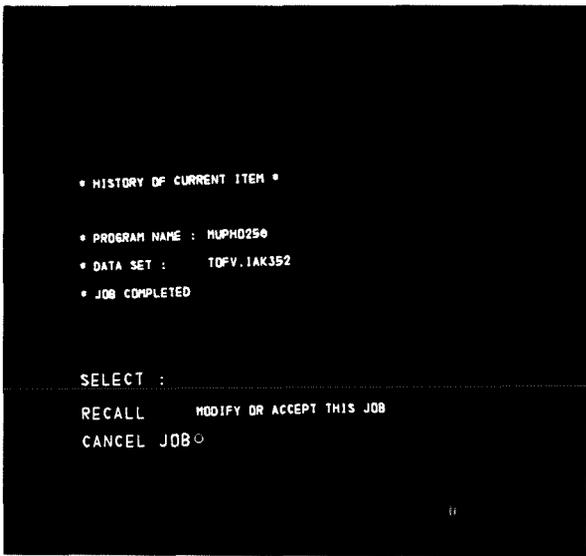


Fig. 18: SELECT frame, when a run has completed processing

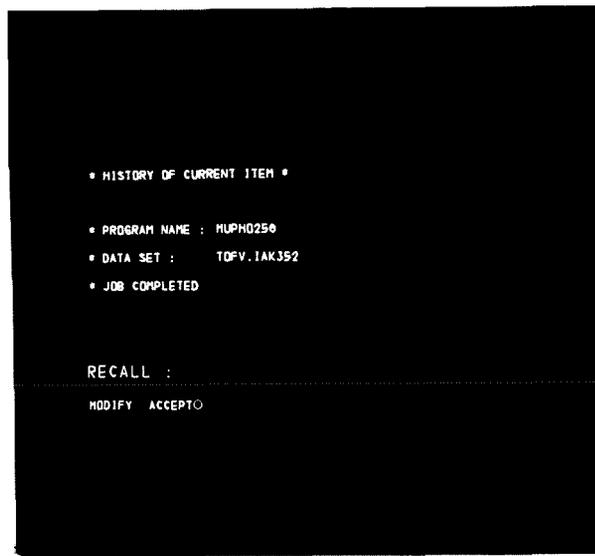


Fig. 19: RECALL frame for defining another run

## 6. Computer Implementations

The program system is currently implemented on the IBM/370-168 configuration at the Karlsruhe Nuclear Research Center (GfK). The programs are written in FORTRAN IV and the IBM GSP package is used for all display management functions. The limit on the array size for formatting the displays is primarily imposed by the display capabilities of the 2250 unit, but also by the wish to minimize the core store requirement. Especially, a substantial fraction of the core requirement is caused by GSP and amounts to about 60K bytes. Therefore, the programs are organized into an overlay structure. However, the size of the complete executable load module (largest path + buffer areas) amounts to around 300K bytes. The CPU time depends upon the number of extrapolations (LEAP calculations) or the number of iterations and multi-phonon terms, respectively. A solution is obtained in less than 2 minutes of CPU time at the most, whilst the total session time is typically no more than 30 minutes. Under normal operating conditions in a multiprogramming environment the response time to most actions initiated by the user is of the order of 1 second. Although large-scale calculations, such as multi-phonon calculations, are included, the on-line participation ensures an efficient performance of such calculations for which the computing time is not too large compared with the normal human conversational times because of the implementation of the programs on a high-speed computer.

### Acknowledgement

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Appendix 1 : Overlay Tree for the graphic program system

```
INCLUDE Ljad( INGRID )
INCLUDE SYSLIB( IHCGSP03 )
INCLUDE Ljad( PRINTP$, GDR250, INITDA, CRDD250 )
OVERLAY ALPHA
INSERT MAIN1
INSERT SCALS, PARM, WERTE, IKENN, PRINT, FREQ, INPUT, SETGD1
OVERLAY BETA
INSERT SORTSG
INSERT SORTPC, SORTA, WTDISK, SUCH, SELECT, SCA, SORTIN
INSERT CS1, CDAT, SORT, SKIP, DBINT
OVERLAY BETA
INSERT PBGX, FITG
OVERLAY BETA
INSERT LEAP
INSERT LP, CONVOL, P, SEDGE, SUM
OVERLAY GAMMA
INSERT LPO
OVERLAY GAMMA
INSERT LP1, RONAPE, TAEND
OVERLAY GAMMA
INSERT LP2, EDGE
OVERLAY GAMMA
INSERT LP3, BESK1, SBFILL, SCT, SERIES, SPOOK
OVERLAY GAMMA
INSERT SURTB
OVERLAY ALPHA
INSERT MAIN2
INSERT SETGD2
INSERT MUPHC, MUPHV, MUDPT, MUPH1, MUPH2, MUPH3, DISPV, FNLAST, WGH
INSERT RDVAR, CHVAR, PRVAR, CHOPT, DISP4, DISPE, DISPE, CHGFK, DISP
INSERT DISP3, BNESC, BEQSC, FPXB, PIDIS
OVERLAY BETA
INSERT READIN
OVERLAY BETA
INSERT CHFZS
INSERT WEIGHT, CHNSH
OVERLAY BETA
INSERT RESOL
OVERLAY BETA
INSERT PO
INSERT BEQSC
OVERLAY BETA
INSERT P1, MOMENT, DISPP1, VIPHU
INSERT MULTI
OVERLAY BETA
INSERT P2, DISPP2, P2DIS
ENTRY MAIN
```

Appendix 2 : JCL requirements for the program system call

```
//IAK352GD JOB (0352,143,POA5A),ABEL,REGION=290K,CLASS=G,
// TIME=3
/*FORMAT PJ,DDNAME=FT08F001,FORMS=STANZ
// EXEC FGLG,LIB=IAK,PARM.L='LIST,OVLY,MAP,SIZE=(272K,100K)'
//L.SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR
//          DD DSN=GFK.FORTLIB,DISP=SHR
//          DD DSN=LOAD.GSP,DISP=SHR
//          DD DSN=LOAD.CALCOMP,DISP=SHR
//L.SYSIN DD DSN=TS0352.GJOVL.DATA,DISP=SHR
//G.FT10F001 DD UNIT=2250-1
//G.FT01F001 DD DSN= &&B1,SPACE=(2048,(99),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT02F001 DD DSN= &&B2,SPACE=(2048,(99),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT03F001 DD DSN= &&B3,SPACE=(2048,(99),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT20F001 DD DSN= &&TS,SPACE=(2048,(99),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT21F001 DD DSN= &&S1,SPACE=(400,(80),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT22F001 DD DSN= &&S2,SPACE=(400,(80),,CONTIG),
// DCB=BUFNO=1,UNIT=SYSDA
//G.FT25F001 DD UNIT=SYSDA,DSN= &&MPHT,DISP=(NEW,DELETE),
// DCB=(RECFM=VBS,BLKSIZE=3520),SPACE=(TRK,50)
//G.FT30F001 DD UNIT=3330,VOL=SER=TSTLIB,DISP=(OLD,KEEP)
//G.FT40F001 DD DSN= &&SAB,UNIT=SYSDA,DISP=(NEW,DELETE),
// DCB=(RECFM=VBS,BLKSIZE=3520),SPACE=(TRK,10)
//G.FT07F001 DD SYSOUT=P
//G.FT08F001 DD SYSOUT=B,DCB=BLKSIZE=80
//G.SYSIN DD *
```

```
<TOF-sum 1 >
<Time-dependent background>
<TOF-sum 2 >
<Time-dependent background>
<TOF-sum 3 >
...
//
```