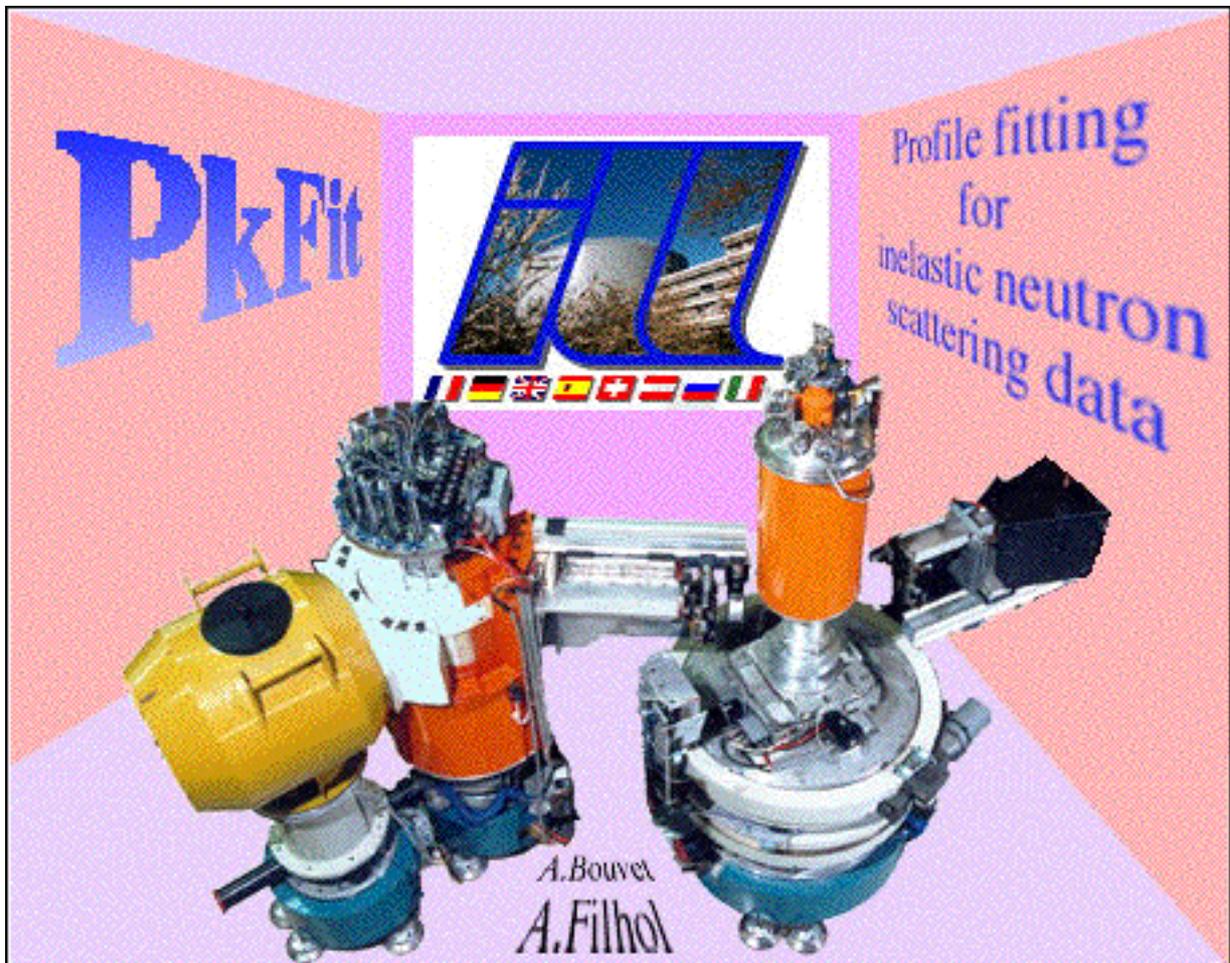


# PkFit

for the MacOS

User's manual



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**PkFit** v2.3  
for **Macintosh**

**User's manual**

**A tool to fit data from neutron three-axis spectrometers**

by

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## 1 - Introduction

**PkFit** [7] is the third of three components in the Institut Laue Langevin (ILL) software package for three-axis spectrometers (TAS) data processing:

**ResCal**    computation of the instrumental resolution function  
**Filing**    data file handling  
**PkFit**     profile fitting

A short description of **ResCal** and **Filing** is given below. However, the installation guides and the tutorials of the TAS software package can be found on the web site:

`<http://www.ill.fr/tas/welcome.html>`

The application can be also downloaded from this site or directly through anonymous ftp from:

`<ftp.ill.fr/pub/tas/pkfit/appl>`

**Filing** - a user friendly software for MacOS, OpenVMS and UNIX computers - is intended for the data file handling of neutron Three-Axis Spectrometers (TAS). It makes it possible:

- to combine (i.e. add or subtract with optional weights) equivalent data files (i.e. files with compatible scan variables and resolution parameters)
- to group scan points
- to change the resolution parameters and save them to a file in the ILL TAS format,
- to concatenate a free format data file and a parameter file into a single file in the ILL TAS format,
- to plot several data files on the same graph,
- etc.

**Rescal** - a user friendly software for the Macintosh - is intended for the calculation of resolution functions, phonon-scan profiles and Bragg widths for neutron three-axis spectrometers (TAS). The resolution function can be calculated by means of two methods: the Cooper-Nathans method [1] and the Popovici method [6]

The Cooper-Nathans method, used in the old version of RESCAL for VAX computer, is a classical method based on rather simplifying assumptions, i.e. gaussian beams, angular collimations. The input parameters are taken either from the data files (TAS formats) or from a resolution parameter file. These parameters can be changed, listed, saved and printed via the appropriate menu items.

The Popovici method, used also in the program RESTRAX for UNIX and VMS workstations, is a more efficient method which permits to take into account focusing monochromators and analyzers as well as spatial beam collimations. The input parameters are taken from three sources:

**PkFit** [7] - a user friendly software for the Macintosh, OpenVMS and UNIX workstations - is intended for the data processing of neutron three-axis spectrometers. Inelastic, quasi-elastic or elastic spectra are fitted by a linear background plus a series of peak functions. The program offers several built-in peak functions but the user may add its own peak shapes through stand-alone code resources. The model can include the Bose factor, the  $k_f$  or  $k_i$  correction, the neutron absorption and the convolution of the signal with a one-dimensional or a four-dimensional resolution function. The latter is calculated from the configuration parameters of the spectrometer through the help of the Cooper-Nathans method [1] or the Popovici method [6]. Fast 4D integration is performed by means of new methods, one based on a Monte-Carlo integration technique and the other based on a Gaussian approximation.

The present report describes only **PkFit** which, however, shares some algorithms with the two others, e.g. the resolution calculation, the file format management, etc. In section 2 the basic features of **PkFit** are explained. After reading it the user will be able to use the program. The definition of the parameters used in the program and in this guide is given in section 3. A description of the readable file formats is given in section 4. A detailed description of each program option is given in sections 5 to 10 while the mathematics of the calculations is given in section 11.

**PkFit** for Macintosh is based on the original code of Peter H.C. Hullah<sup>1</sup> (1979), which have been modified by one of the ILL-chaots in July 1986. The program was installed on the ILL DIVA server in February 1987 by Paul Frings. The authors

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<sup>1</sup> Peter H.C. Hullah, P.C.L., Dept. of Physics, 115, New Cavendish St., London W.1., England.

substantially improved it and introduced new features (1d/4d resolution calculation, user defined peak functions, etc.). The old sources have been converted to FORTRAN 77 and re-organized so as to be more easily adaptable to different computers with the help of the MPW environment<sup>2</sup> and the Language Systems<sup>3</sup> FORTRAN compiler. The Macintosh version uses the Apple's ToolBox for a convivial interactivity and the TSiGraphics<sup>4</sup> library for graphics. An OpenVMS/UNIX version also exists and is based on the freeware library PGPLOT<sup>5</sup> for graphics and for the user interface.

This guide contains a description of the different data files that **PkFit** can read and process, a description of the command corresponding to each item of its menus, the mathematical expressions used and details on how a user can add its own peak functions to the program.

*The authors are not responsible for erroneous results obtained with **PkFit**. This guide can not substitute the lack of knowledge of users on Three-Axis Spectrometer, inelastic neutron scattering and data analysis, above all when using the 4d deconvolution.*

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<sup>2</sup> Macintosh Programming Workshop™ by Apple Computer, Inc.

<sup>3</sup> Language Systems Corporation™, 100 Carpenter Drive Sterling, VA 20164

<sup>4</sup> Techno-Sciences, Inc., 1001 Derekwood Lane, Suite 204, Lanham, Maryland 20706 (Internet [tsigraphics@technosci.com](mailto:tsigraphics@technosci.com))

<sup>5</sup> Tim Pearson, Astronomy Department, Caltech 105-24, Pasadena 91125, USA (internet: [tjp@deimos.caltech.edu](mailto:tjp@deimos.caltech.edu))

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## 2 - Running PkFit

*Note: We assume that the reader is familiar with the use of a Macintosh computer and of a three-axis spectrometer.*

Installing **PkFit** on your Macintosh is very simple, however, you need appropriate hardware and software as explained in section 2.1. You can then launch the program (see section 2.2) and discover its major features (see section 2.3). As a help to new users the basic actions to be performed are given:

- to fit TAS data files with **PkFit** (see section 2.4)
- to calculate, simulate and visualize the resolution function with **PkFit** and **ResCal** (see section 2.5).

### 2.1 - Installing PkFit on your Macintosh

#### What you need

- A Macintosh with 128K ROM or more.
- At least 1.5 Mb of available RAM memory space for each application
- A hard disk drive (preferably) with at least 1.1 Mb of available space for each application.
- Hardware requirements depend on the program version:
  - PkFit68020 and Filing68020 require a Motorola 68020, 68030 or 68040 processor.
  - PkFit68020\_FPU and Filing68020\_FPU require a Motorola 68020, 68030 or 68040 processor plus a floating point unit (FPU), which considerably speeds up the calculations.
  - PkFitPPC and FilingPPC require a PowerPC processor.
- System 7.0 or higher.

## Installing PkFit

The TAS software package can be obtained on request from the authors or can be downloaded from the web site <<http://www.ill.fr/tas/welcome.html>> or through anonymous ftp from <ftp.ill.fr/pub/tas/pkfit>. The following table describes the contents of the ftp server:

Platform	OS	File name	Comments
Macintosh	68k	<a href="#">TAS_prog_68k.sea.hqx</a>	a binhexed file of a self extracting application
	68k with FPU	<a href="#">TAS_prog_68k_FPU.sea.hqx</a>	
	PowerPC	<a href="#">TAS_prog_PPC.sea.hqx</a>	
Dec-alpha	OpenVMS 6.2	<a href="#">TAS_prog_VMS.tar.gz</a>	a gzipped tar archive
HP-9000	UNIX	<a href="#">TAS_prog_HP-UNIX.tar.gz</a>	
Silicon Graphic	IRIX 5.3	<a href="#">TAS_prog_SGI.tar.gz</a>	

Select the package most appropriate to your computer. It is available in the form of a self extracting archive-file compacted by StuffIt and binhexed with Fetch. First unbinhex the file and then double-click its icon to expand it. You will be asked to give the name of the folder in which the following files will be expanded:

- the Filing application
- the PkFit application
- the ResCal application (which is also contained in PkFit)
- the help file "pkf.help"
- the Kaleidagraph documents "PkFitPlotScript.plot" and "PkFitPlotScript"
- the directory "makePlug-ins" and "Plug-ins" where is an example of a PkFit user-function

## 2.2 - Launching PkFit

To launch **PkFit**, simply double-click on its icon. A header window is displayed (see cover figure) and the program waits for either a mouse click in that window (shortcut: press "return" or "enter"). **PkFit** checks that the version you are running is compatible with the system and the hardware of your Macintosh. In fact, to speed up calculations **PkFit** exists in several versions, each optimized for a specific hardware (e.g., for a MC68020 Motorola processor with/without a Floating Point Unit (FPU) or for a PowerPC processor). If you get an error message at start up, either download a program version compatible with your Macintosh or use an appropriate Macintosh.

If the environment test is satisfied the program then displays a menu bar and a text window (Fig. 1) in which numerical output and error messages will appear. Other windows will also be used by the program when necessary. These windows are described in more details in section 2.3.

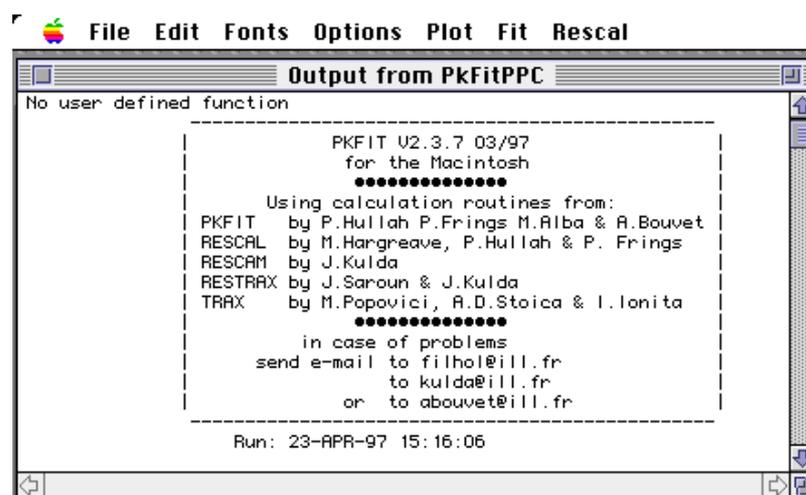


Fig. 1: The menu bar and the output window at startup.

The bases of the use of **PkFit** are given in section 2.4 while a detailed menu-by-menu description of its options is given in sections 5 to 10.

## 2.3 - PkFit windows

**PkFit** uses several kinds of windows:

Header window      This window is shown only once at startup. Click it or press enter or return to continue.

Text window        Displays the history of the session (file contents, some numerical results, error messages, etc.). Its contents have a

limited size but, when the limit is reached, the program automatically saves the text to a file named "output from PkFit". Note that successive run of the program may erase old versions of that file which have not been renamed or moved. If the program fails to create that file the message << Spool file could not be opened >> is written on top of the text window.

Graphic window	Displays results as plots.
Dialogue windows	Allow interactive input or modification of parameters.
Help window	The on-line help tool is described in section 7.12.

As usual with the Macintosh interface, dialogues cannot be moved, resized or printed. In contrast, the graphic and the text windows are resizable (click and drag their bottom right corner), movable (use the drag bar) and printable (item **Print** from the menu **File**). Their contents can be also copied to the clipboard (item **Copy** from the menu **Edit**) or saved in a file (item **Save As** from the menu **File**).

## 2.4 - Basic use of PkFit

**PkFit** may be used in many distinct manners that will become apparent when reading the manual and using the program. As a quick start we give a basic sequence of actions to perform a fit on three-axis spectrometer data but a tutorial is available from the web.

1. Optionally set the preferences parameters (section 7.11)
2. Open a data file (section 5.1)
3. Optionally set
  - the energy unit (section 7.1)
  - the monitor (section 7.2)
  - the axes (section 7.3)
4. Optionally add to the model
  - a temperature factor (section 7.4)
  - the  $k_f$  or  $k_i$  correction (section 7.5)
  - the absorption correction (section 7.6)
5. Optionally choose a resolution calculation method (section 10.1)
6. Optionally set or edit the resolution parameters (section 10.2)
  - or even input a new resolution parameter set from file (section 10.8)
7. Initialize the fit parameters (section 9.1 and 9.3)

- set the peak number  
click the top of the peaks  
set the peak types
8. Optionally add or remove constraints on the fit parameters (section 9.2)
  9. Perform the fit of the model (section 9.5)
  10. Print the current plot / results / data / etc. (section 5.6)
  11. Save to a disk file (section 5.3)
    - the new data set at the ILL data format
    - the plot to a PICT file
    - the log file and resolution parameter file
  12. To treat other data files repeat steps 1 to 11. However, for a series of similar spectra, repeating step 2 and 7-11 is generally enough.
  13. Save a session file before quitting **PkFit** (section 5.9)

Then, with programs such as **Kaleidagraph**<sup>6</sup>, the log files can be read to produce graphs with publication quality (see section 12). The session file also can be read to obtain the variation of the fit parameters for the different data files (i.e., for dispersion curves, temperature dependencies,...).

## 2.5 - Using resolution calculation

In **PkFit** and **ResCal** for the MacOS, the resolution function can be calculated by means of two methods:

- the Cooper-Nathans method [1]
- the Popovici method [6].

The Cooper-Nathans method, used in the old version of RESCAL for VAX computer, is a classical method based on rather simplifying assumptions, i.e. Gaussian beams, angular collimations. The input parameters are taken either from the data files (TAS formats) or from a resolution parameter file. These parameters can be changed, listed, saved and printed via the appropriate menu items.

The Popovici method, used also in the program RESTRAX for UNIX and VMS workstations, is a more efficient method which permits to take into account focusing

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<sup>6</sup> Kaleidagraph™ is a product of Abelbeck Software.

monochromators and analyzers as well as spatial beam collimations. The input parameters are taken from three sources:

- the RESCAL parameter set, used also in the Cooper-Nathans method, are taken either from the data files (TAS formats) or from a resolution parameter file (see section 4.2).
- the focalization parameter set: the monochromator and analyzer curvatures, the sample diameter and height, must be given by the user. They can be edited in the **Focalization parameter** dialogue (see section 10.2 and Fig. 44).
- additional parameters describing the dimensions of the TAS elements and their distances, are taken either from the built-in parameter set of the ILL TAS-configuration or from a TAS configuration file (see section 4.3).

As a quick start, we list here a set of basic actions:

- 1 Choose the method to calculate the resolution calculation (section 10.1)
- 2 Set the TAS configuration parameters (Popovici method only) either from the popup menu **built-in configuration parameters** of the ILL TAS instrument or from the button **Read** to read them from a file (section 10.1)
- 3 Check the resolution parameters (section 10.2)
- 4 Check the focusing parameters (Popovici method only) by clicking the button **Focusing param** in the dialogue **Set resol. param.** (section 10.2)
- 5 View the resulting resolution function in the form of matrices (section 10.3)
- 6 View the resulting resolution function in the form of ellipsoid cuts and projections in the Cooper-Nathans coordinates (section 10.4)
- 7 View the resulting resolution function in the form of ellipsoid cuts and projections in the dispersion frames (section 10.5)
- 8 View the pseudo Bragg and Vanadium width at the current (Q,En) position (section 10.6)
- 9 Simulate a phonon profile by means of a Monte-Carlo integration technique (section 10.7)
- 10 Read resolution parameters from a file (section 10.8)
- 11 Save current resolution parameters to a file. Check the box **Resol. param.** in the save dialogue (section 5.3)

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## 3 - Definitions and algorithms

### 3.1 - Usual maximum configuration

The values below are only an indication since the authors may decide to change them at any time.

Maximum number of data points: 500  
Maximum number of peaks: 6  
Maximum number of peak parameters: 4 (only 3 are fitted)  
Peak shapes (five built-in, up to 10 defined by the user)

G	Gaussian peak shape
I	incoherent peak in an energy scan
L	Lorentzian peak shape
O	damped harmonic oscillator
B	Bragg peak
D	convolution of a delta function and a 4 <sup>th</sup> dimensional gaussian resolution
X	user defined peak shape (see section 13.1 and reference [5])

### 3.2 - Fit parameters

Background parameters: 2 (linear background)

Peak parameters: 3 per peak (the 4th one is never fitted)

- Each one can be either fitted or kept fixed (see section 9.2).
- Linear constraints can be applied to fit parameters (see sections 9.2)
- In the case of a delta function, the width is not a fitted parameter. It is replaced by one dispersion curve parameter:
  - the slope of the dispersion curve for the local linear or quadratic cases.
  - the gap for the sinusoidal case.

In a future version, it will be possible to choose the dispersion curve parameter to be fitted.

- In the case of a harmonic oscillator function, a constraint of type  $AC^2=Cte$  or  $AC=Cte$  can be applied (see section 9.3)

### 3.3 - Instrument scan and sample parameters

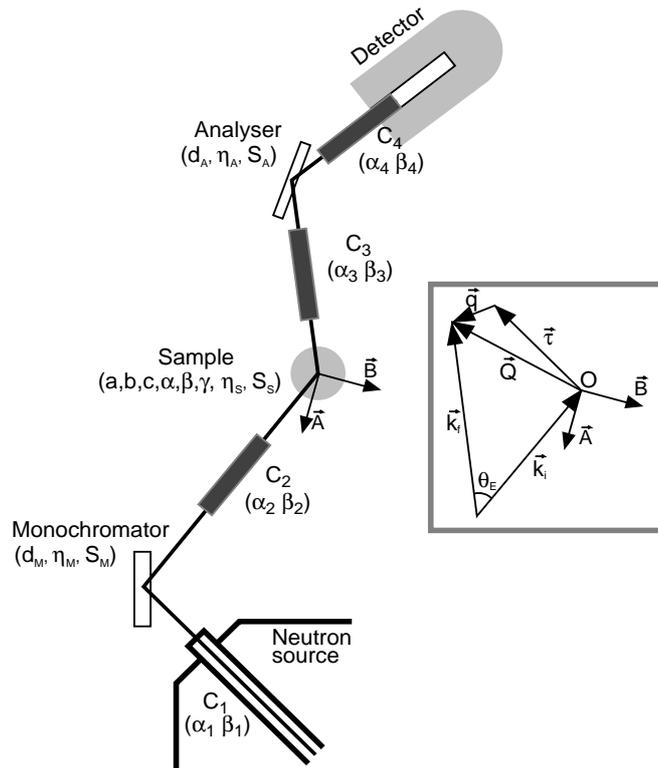
The TAS spectrometer parameters, as used in the following, are defined below and in figure 2 while the vector definition for a TAS experiment is given in the inset of figure 2. The definition of the scattering sense coefficients is shown on figure 3.

#### Instrument parameters

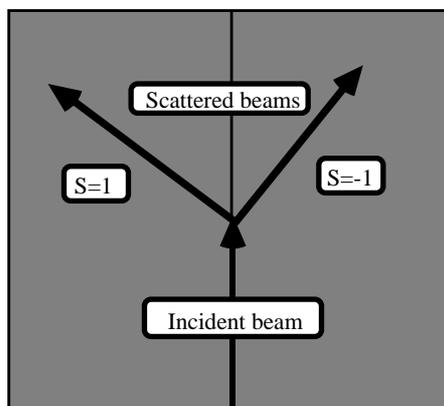
$d_M, d_A$	monochromator and analyzer d-spacing
$\eta_M, \eta_A, \eta_S$	monochromator, analyzer and sample mosaic
$S_M, S_A, S_S$	monochromator, analyzer and sample scattering sense
$\alpha_1, \alpha_2, \alpha_3, \alpha_4$	horizontal collimations
$\beta_1, \beta_2, \beta_3, \beta_4$	vertical collimations
$a, b, c, \alpha, \beta, \gamma$	cell parameters of the sample

#### Vectors of a TAS experiment

$\vec{k}_i$	Incident wave vector
$\vec{k}_f$	Final wave vector
$\vec{A}, \vec{B}$	1 <sup>st</sup> and 2 <sup>nd</sup> horizontal wave vectors defining the scattering plan
$\vec{\tau}$	position of the nearest zone center
$\vec{q}$	Relative wave vector
$\vec{Q}$	Absolute wave vector
$\vec{\theta}_E$	Rotation angle of the sample



**Fig. 2:** Resolution parameters of three-axis spectrometers.  $C_1, C_2, C_3, C_4$  indicates the collimators and the inset recalls the definition of the various vectors used in the following.



**Fig. 3:** Definition of the scattering-sense coefficients

### 3.4 - Resolution function

The instrumental resolution function of three-axis spectrometers implemented in **PkFit** is of the normalized Gaussian type. The resolution function is written in section 11.2. In the case of a constant  $k_i$  scan, the resolution volume is accounted for by the  $k_f^3 \cdot \text{tg}^{-1}(\theta_A)$  correction. In the case of a constant  $k_f$  scan, the resolution volume, when multiplied by the monitor efficiency (in  $1/k_i$ ) and by the term  $k_f/k_i$  of the cross section, is simply a constant.

At present **PkFit** can convolute its own built-in functions but not yet the user-defined functions. The convolution dimension can be 0 (no convolution), 1 (convolution in the scan direction only) or 4. *In the 1D case*, the instrumental resolution function is assumed to be a 1D Gaussian whose width can be set by the user or calculated from the resolution matrix. Two methods are available to perform the convolution. The first uses a numerical integration, which is fast but may need several trials to converge. The second approximates the signal by a sum of Gaussian and then performs an analytic integration (see section 11.7). *In the 4D case*, a "sum of Gaussian" approximation, similar to the one used in the 1D case, also makes it possible to convolute the 4D resolution function with a 4D scattering function (see section 11.7). This is useful, e.g., to study phase transition phenomena (for example see reference [8]). The 4D convolution is also available in the case of undamped and damped dispersive excitations but as explained below this requires special attention.

### 3.5 - Available dispersion curves

Three kinds of dispersion curves (see section 11.4) are implemented in **PkFit**:

- a local linear dispersion curve
- a local quadratic dispersion curve
- a sinusoidal dispersion curve
- user defined curve shapes. Future versions will enable the user to implement his own curve shapes in external code resources (see section 13 and reference [5])

No form-factor or structure-factor effects are included in these model curves yet. This will be done in a future version by means of Monte-Carlo simulations. Also, extra dispersion-curve shapes will probably be added as intrinsic functions or user functions.

### 3.6 - Calculation method

The resolution matrix is calculated either by the Cooper-Nathans method [1] or by the Popovici method [6]. The phonon width is calculated by means of a Monte-Carlo integration technique as described in section 11.3.

The procedure to fit the data is the nonlinear least square algorithm Gauss-Newton (see section 11.5), which minimize the sum-of-squares of the difference of calculated and measured values, weighted by the experimental errors. However this method, as all least square method, suffers disadvantages that the range of convergence is not very great and thus the refinements may converge to local minima.

### 3.7 - Built-in corrections

- Temperature factor

It allows for the excited state populations and is described by the following multiplicative factor:

$$TF(\omega) = \frac{\omega}{1 - \exp(-\hbar\omega / k_B T)}$$

The  $\omega$  factor is introduced here to avoid the divergence at  $\omega=0$ . Indeed, the dynamic structure factor  $S(Q,\omega)$  is the imaginary part of the dynamic susceptibility, which verifies the rule:

$$S(q, -\omega) = e^{-\hbar\omega / k_B T} S(q, \omega)$$

Thus  $S(Q,\omega)$  is an odder function in energy. The different peak shapes available then are even function in energy, i.e., Gaussian, Lorentzian or harmonic oscillator.

- $k_f$  and  $k_i$  correction

It enables to take into account the resolution volume, which depends on the instrument geometry and on the incident neutron beam energy. A theoretical expression is available only in the case of a constant  $k_i$  scan on a three-axis spectrometer. For other cases, the correction can be read from a file (see section 7.5).

- Absorption correction

It can be calculated for the following sample shape:

- Infinite slab
- Finite slab (with faces parallel or perpendicular to the scattering plane)
- Cylinder (with axes perpendicular or in the scattering plane)
- Sphere.

As for the other corrections this term is added to the model as a multiplicative factor. Furthermore, the absorption calculation can be applied to the background. In this case the fitted parameter F0 corresponds to the electronic background, and the absorption dependent background BG0 corresponds to the background from the sample. In future versions it will be possible to choose the background fitted-parameter between F0 and BG0.

Initialization of the absorption coefficients is described in section 7.6, and the mathematical expressions are shown in section 11.6.

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## 4 - File formats

PkFit can read (see section 5.1) or write (see section 5.3) different types of files:

- the data files. They contain the scan variables and can contain the resolution parameters too. The file formats are listed in section 4.1 and are described in appendices A to D.
- the resolution parameters' files. See section 4.2 and a complete description in appendix E.
- the TAS configuration files. See the description in section 4.3.
- a configuration file which sets/saves the current settings of the program (see section 7.11)
- a help file (see section 7.12)
- log files and session files which are very usefull for subsequent processing of the fit results (see section 4.4 and 4.5).

Note that **PkFit**, as **Filing**, saves data sets in the ILL TAS format. However, data are written in the standard free format `WRITE ( LOUT , * )` and the comment "Free format" is written in the Data FORTRAN Format line.

### 4.1 - Data-file formats

**PkFit**, like **Filing** and **ResCal**, can read data from ASCII files in the formats listed below:

#### ILL TAS Format

(see appendix-A)

Files coming directly from an ILL three-axis spectrometer (default format since 1994). Each file contains only one spectrum. This is a unified format [3] for all TAS program at the ILL.

Siloe (see appendix-B)  
Files from instruments DN1 and DN3 at the CENG<sup>7</sup>.

Free Format (see appendix-C)  
A simple format which can be used for the input of data not coming from ILL or CENG instruments. Files are plain ASCII files such as

- those transferred from a UNIX or VMS station.
- documents prepared with a text editor (e.g., **SimpleText**<sup>8</sup>, **BBEdit**<sup>9</sup>, etc.).
- documents prepared with a word processor or a program as **Kaleidagraph**<sup>10</sup> or **Excel**<sup>11</sup> and saved as text documents.

Old ILL TAS Format (see appendix-D)  
Files coming directly from an ILL 3-axis spectrometer and created by the old **TAS** program (default format up to 1992). Each file contains only one spectrum.  
or files created by the old program **Filing** of VAX VMS.

Old ILL Archive File (see appendix-D)  
ASCII files retrieved from the ILL data base with the help of **Spectra** and created by the old **TAS** program (default format up to 1992). Such files may contain more than one spectrum.

INX File (see reference [14])  
ASCII files created by the program INX [14], a program for time-of-flight data reduction (The spectrum abscissa must be the neutron energy transfert in meV).

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<sup>7</sup> Centre d'Etudes Nucléaires de Grenoble, 17 av des Martyrs, 38054 Grenoble Cedex 9, France.

<sup>8</sup> SimpleText™ is a product of Apple Computer, Inc.

<sup>9</sup> BBEEdit™ is a product of Bare Bones Software, Inc.

<sup>10</sup> i.e. select the item **Tab-Delimited Text** from the item **Export** of the menu **File**

<sup>11</sup> Excel™ is product of Microsoft Corporation.

## 4.2 - Resolution-parameter file formats

**PkFit** is able to read two different formats. See appendix-E for the definition of the resolution parameters and section 3.3 for their correspondence to the instrument parameters.

The first format corresponds to that used by the old VAX version of **ResCal**. The parameter values are written in one column in free format in the following order:

```
DM, DA ,
ETAM, ETAA, ETAS ,
SM, SA, SS ,
KFIX, FX ,
ALF1, ALF2, ALF3, ALF4, BET1, BET2, BET3, BET4 ,
AS, BS, CS, AA, BB, CC, AX, AY, AZ, BX, BY, BZ ,
QH, QK, QL, EN, DH, DK, DL, DE
```

In the second format each line also corresponds to one parameter. The line order is not important, but each line is divided in two parts:

- the first 18 characters contain the name and the unit of the parameter
- the following 20 characters contain the parameter value in free format (see example below).

DM	(Å)	=	3.35750007629395
DA	(Å)	=	3.35750007629395
ETAM	(')	=	30.00000000000000
ETAS	(')	=	20.00000000000000
ETAA	(')	=	30.00000000000000
SM		=	1.0000000000000000
SS		=	-1.0000000000000000
SA		=	1.0000000000000000
KFIX	(Å <sup>-1</sup> )	=	2.66199994087219
ALF1	(')	=	60.00000000000000
ALF2	(')	=	20.00000000000000
ALF3	(')	=	40.00000000000000
ALF4	(')	=	60.00000000000000
BET1	(')	=	120.00000000000000
BET2	(')	=	120.00000000000000
BET3	(')	=	120.00000000000000
BET4	(')	=	120.00000000000000
AS	(Å)	=	5.42999982833862
BS	(Å)	=	5.42999982833862
CS	(Å)	=	5.42999982833862
AA	(deg)	=	90.00000000000000
BB	(deg)	=	90.00000000000000
CC	(deg)	=	90.00000000000000
AX	(rlu)	=	1.0000000000000000
AY	(rlu)	=	1.0000000000000000
AZ	(rlu)	=	0.0000000000000000
BX	(rlu)	=	0.0000000000000000
BY	(rlu)	=	0.0000000000000000
BZ	(rlu)	=	1.0000000000000000
QH	(rlu)	=	0.200000002980232
QK	(rlu)	=	0.0000000000000000
QL	(rlu)	=	0.0000000000000000
EN	(meV)	=	57.00000000000000
DH	(rlu)	=	0.0000000000000000
DK	(rlu)	=	0.0000000000000000
DL	(rlu)	=	0.0000000000000000
DE	(meV)	=	0.666999816894531
QH0	(rlu)	=	0.200000002980232
QK0	(rlu)	=	0.0000000000000000
QL0	(rlu)	=	0.0000000000000000
EN0	(meV)	=	57.00000000000000
TAUH	(rlu)	=	0.0000000000000000
TAUK	(rlu)	=	0.0000000000000000
TAUL	(rlu)	=	0.0000000000000000
FX		=	2.0000000000000000

### 4.3 - TAS-configuration file

The TAS configuration file is composed by a succession of two lines: the first line is a comment line which describes the values listed in the second line. All distances and dimensions are in cm.

#### Comments:

- `title` (max.60 characters) :  
This name will appear on the printed output.
- `source` (`shape,diameter,width,height,n-guide,gamma[rad/Å]`) :  
`shape` (0) circular or (1) rectangular  
`diameter` used if `shape=0`  
`width,height` used if `shape=1`  
`n-guide` neutron guide considered (1) or not (0)  
`gamma` if `n-guide=1`, this number is interpreted as the critical angle for 1 Å neutrons. The initial angular distribution of the beam is then a rectangular box with  $FWHM=2*\gamma*\lambda$ .
- `monochromator` (`chi,aniz.,poiss.,thick.,height,length`) :  
`chi` crystal cutting angle, 0 for the symmetric Bragg reflection  
`aniz` ratio btw. the vertical and horizontal mosaicity  
`poiss` Poisson constant for the elastically bent crystals (usually about 0.3)  
`thick.,height,length` crystal dimensions
- `analyzer` (`chi,aniz.,poiss.,thick.,height,length`) :  
the same as for the monochromator
- `detector` (`shape,diameter,width,height`) :  
the same as for the source
- `distances` (`l1,l2,l3,l4`) :  
distances source - monochromator, monochromator - sample, sample - analyzer and analyzer - detector.
- `1st collimator` (`distance,length,hor1,hor2,ver1,ver2`) :  
`distance` measured from the previous element (the source in this case) to the entrance window.  
`hor1,hor2` width of the entrance and exit windows  
`ver1,ver2` height of the entrance and exit windows

and the same for the other three collimators.

### Example: TAS configuration file format

```
title (max.60 characters) :
IN20 - Si/Si - open
source (shape,diameter,width,height,n-guide,gamma[rad/A]):
0 10. 10. 10. 0 0.00167
monochromator (chi,aniz.,poiss.,thick.,height,length):
0.0 1 0.15 0.9 12.0 12.0
analyzer (chi,aniz.,poiss.,thick.,height,length):
0.0 1 0.15 0.9 12.0 12.0
detector (shape,diameter,width,height):
1 4.0 3.0 5.0
distances (l1,l2,l3,l4):
900. 210. 150. 70.
1st collimator (distance,length,hor1,hor2,ver1,ver2):
236. 534. 7.5 5.0 9.0 11.0
2nd collimator (distance,length,hor1,hor2,ver1,ver2):
100. 39. 4. 4. 7. 7.
3rd collimator (distance,length,hor1,hor2,ver1,ver2):
80. 39. 4. 4. 7. 7.
4th collimator (distance,length,hor1,hor2,ver1,ver2):
35. 24. 4. 4. 12. 12.
```

## 4.4 - Log files

Each time you have successfully processed a spectrum it is a good practice to save both the data and the results to a log file. The latter may be understood as an output file which can be used for subsequent post processing with other programs. For example, Kaleidagraph can be used to produce documents with publishing quality from these log files (see section 12).

The log file is a plain text file to which PkFit saves:

- the log-file name and its creation date,
- the data-file contents in the ILL format (including the header),
- the model description and the values of the fit parameters,
- the type and the values of the applied corrections,
- the value of the refinement factor,
- the correction parameters,
- and the fit curves.

## Example of a log file:

```
DisqueDur:TAS_Examples:enscan.LOG Creation date:07-MAR-97 14:24:52
-----
Data
INSIR: 4E2
EXNO:
USER :
LOCAL:
FILE : DisqueDur:TAS_Examples:enscan.LOG
DATE : 07-MAR-97 14:26:33
TITLE: 4f2:enscan.tas:CEB6 AFQ phase
COMM:
COM1 :
FOSCE: QI= 0.0000, QK= -0.7500, QI= 0.0000, EN= 0.993, UN=neV
STEPS: DEN= 0.0830
PARAM: DM= 3.3535, DA= 3.3535, SM= 1., SS=-1., SA= 1., EIPM= 17.0, EIPA= 24.0
PARAM: FX= 0., KFIX= 1.5500
PARAM: ALF1= 80., ALF2= 40., ALF3= 61., ALF4= 61.
PARAM: BET1= 52., BET2= 69., BET3=135., BET4=235.
PARAM: AS= 4.1343, BS= 4.1343, CS= 4.1343
PARAM: AA= 90.000, BB= 90.000, CC= 90.000, EIPAS= 20.0
PARAM: AX= 1.000, AY= -1.000, AZ= 0.000
PARAM: BX= 1.000, BY= 1.000, BZ= 0.000
FORMT: (F9.4 ,1X,F12.2,1X,F12.3,1X,F10.2,1X,I4)
DATA :
  EN      CNTS      DELT      ML      HNT
-0.4140    24.00      4.900  30000.00  1
-0.3310    31.00      5.600  30000.00  2
...

-----
Fit Parameters
BCK = 37.88 (76) + 0.0 (fixed)
Peak , Type , GW ,DimCorv, Hight ,Hight Err., Width ,Width Err., Center ,Cent. Err., Area , Area Err.
 1 , "G" , 0.0 , 0 , 160.4389, 1.753783, .2105637, .0018042, -.017736, .0010128, 715.8035, 7.824565

chi**2 = 5.94

-----
Fit Curves
  EN      KF_cor.  Bose_fac. Absorption  Itotal
-1.00000  1.000  1.000  1.000  37.878
-0.97236  1.000  1.000  1.000  37.878
...
 4.5000  1.000  1.000  1.000  37.878
```

## 4.5 - Session files

A session file contains the final values of the fitted parameters for all the data files which have been processed during the current **PkFit** session. For each data file the corresponding set of parameters is written on the same line. The session file is a plain TEXT file (ASCII file) with a record length of 650, and a coma as column separator (see an example below). It can be imported by applications such as **Excel** or **Kaleidagraph** and is convenient for the study of, e.g., temperature scans or dispersion curves in a series of scans.

### Example of a session file:

```
F91757.LOG DATE:29-APR-97 17:57:58
File Name , FO , FO Err, SO , SO Err, Type , GW , DimCorv, HI , HI Err, WI , WI Err, CI , ...
enscan.tas ,23.38287,2.162169, 0.0 , 0.0 , "I" ,.2164377, 1 ,166.8111,1.817929, .2164377, 0.0 ,-.017221, ...
...
```

---

## 5 - Menu File

### 5.1 - Item Open



Select **Open** from the menu **File** (keyboard shortcut **command-O**). The program then displays a modified Macintosh open-file dialogue (Fig. 4) which allows you to select the data file to be read. Be careful that opening a new file automatically resets the current data and result sets.

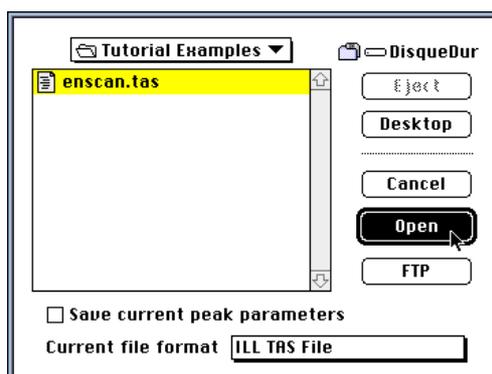


Fig. 4: Opening a data file.

*This standard Macintosh dialogue allows the opening of the desired data file. Select successively the appropriate drive, the folder, the file and then press the button Open.*

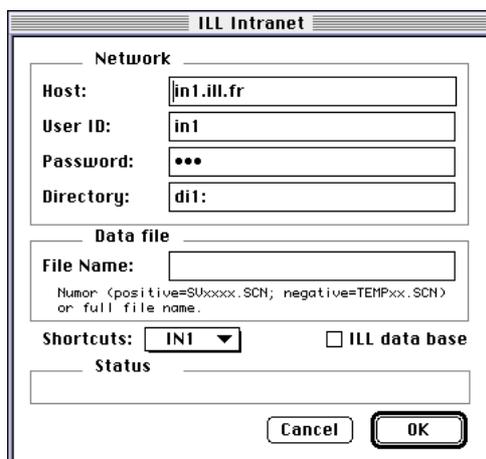
The button **FTP** is for intranet access to data files on a remote computer. When used, a new dialogue (Fig. 5) is shown which makes it possible to set the network parameters and to give the name of the file to be fetched, opened and then automatically deleted from the local computer<sup>12</sup>.

ILL users should note that the popup menu shortcuts (Fig. 5) makes it easy to set parameters of the TAS instruments. If the box "ILL data base" is unchecked, the file is taken from the instrument computer. If the box is checked the data are read from the ILL data base. In that later case the data are assumed to be for the selected instrument and current reactor cycle (e.g. "/usr/illdata/data/in1/"). To access an old cycle, replace

---

<sup>12</sup>The files on the remote computer are never modified or deleted by PkFit.

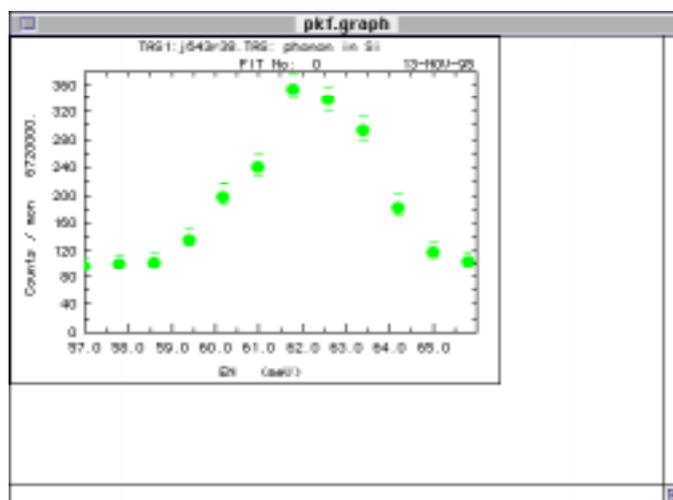
the default cycle directory (i.e. "data") by the wanted cycle number (e.g. "961" for the first cycle of 1996).



*Fig. 5: The ILL intranet dialogue.*

If you do not use the ftp option, select the file name as usual, select the file format (see section 4 and appendices A to D) and then click the button **Open** (Fig. 4).

If the data file has been successfully read, **PkFit** then opens a graphic window (Fig. 6) and displays the spectrum<sup>13</sup>.

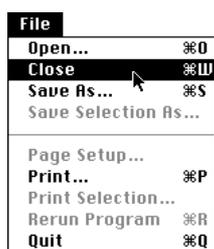


*Fig. 6: The graphic window.*

*It is divided into three parts: the plot region (top left), the message region (bottom) and the parameter region (top right) which are presently empty.*

<sup>13</sup> In the case of a SPECTRA data file, an additional dialogue asks for the number of the spectrum to be selected

## 5.2 - Item Close



Select **Close** from the menu **File** (keyboard shortcut **command-W**) to close the graphic window. Be careful that the current data and result sets are automatically reset and thus must be saved before if necessary.

## 5.3 - Item Save As...



Select **Save As...** from menu **File** (shortcut **command-S**) to save window contents, results and data to disk files.

A dialogue box allows you to select the windows or the files to be saved (Fig. 7). The text window contents is saved as a plain text (ASCII) file. The graphic window is saved as a PICT file. Note that you can also use item **Copy** from the menu **Edit** to copy the contents of the front window to the clipboard.

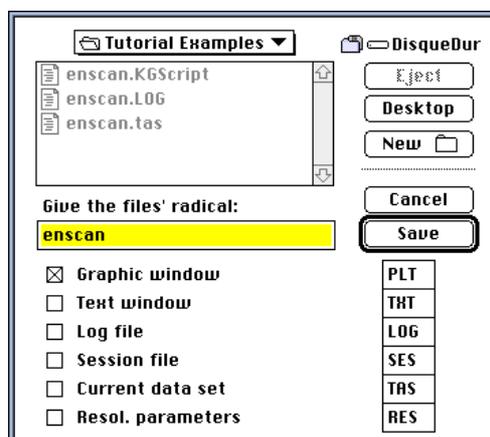


Fig. 7: The graphic window.

Each time you have successfully processed a spectrum it is a good practice to save both the data and the results to a log file (see section 4.4).

## 5.4 - Item Save Selection As...

If the front Window is the text window, this item makes it possible to save the current selection to a TEXT file.

## 5.5 - Page Setup...

Display the standard Macintosh dialogue which allows to select the printing options. Note that the standard dialogue "Page Setup" is *automatically opened the first time the graphic window is printed and that it cannot be changed afterwards in the current session*. However, for other windows or files it can be changed at any time. Be sure to have the text window selected to enable the item **Page Setup...**

## 5.6 - Item Print



Select **Print** from the menu **File** (shortcut **command-P**) to print selected windows and/or files to the default printer<sup>14</sup>. A dialogue box is shown (Fig. 8).

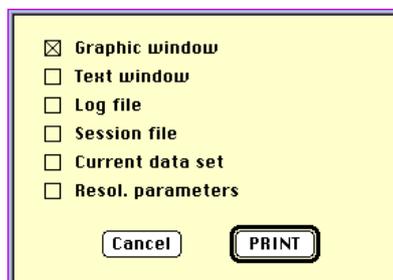


Fig. 8: The print dialogue

Due to a bug in Language Systems FORTRAN compiler, this option is sometimes capricious. If the contents of the text window does not print, use item **Select all** from the menu **Edit** and then item **Print Selection** from the menu **File**.

## 5.7 - Item Print Selection...

If the front Window is the text window, you can print the current selection.

---

<sup>14</sup> You can select the default printer with item **Chooser** of the apple menu (🍏)

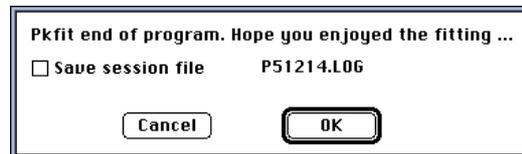
## 5.8 - Item Rerun Program

This item is a built-in feature of the FORTRAN compiler and cannot be removed. Use it with care - it can cause crashes!

## 5.9 - Quitting PkFit



Select **Quit** from the menu **File** (keyboard shortcut **command-Q**). A dialogue box (Fig. 9) allows you to save a session file (see section 4.5).



*Fig. 9: Saving a session file.*

---

## 6 - Menus Edit and Fonts

The menu **Edit** makes it possible to modify the contents of some windows of the program. The menu **Fonts** can be used to change the font of the text window.

### 6.1 - Can't undo / Undo

Not available for commands. Not yet available for text editing but we expect that Language Systems will provide it in future versions of its FORTRAN compiler.

### 6.2 - Cut

If the front window is the text window, you can cut the selected part which is automatically copied to the clipboard.

### 6.3 - Copy

If the front window is the text window, you can copy the selected part to the clipboard. If the front window is the graphic window, its whole contents are copied to the clipboard.

### 6.4 - Paste

If the text window is front most, you can paste the contents of the clipboard (only text) to it. This function is not available for the graphic window.

### 6.5 - Clear window

If the front window is the text window, its contents are erased. This function is useful as the text window contents have a limited size.

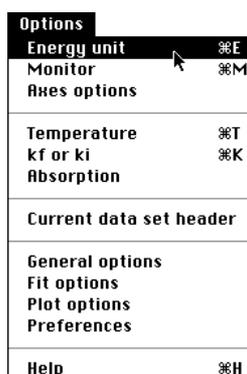
### 6.6 - Fonts

The menu **Fonts** lists the set of fonts currently installed in the system of your Macintosh. Selecting a new font will change the typing of the whole contents of the text window.

---

## 7 - Menu Options

### 7.1 - Energy unit



The energy unit can be chosen at any time. Select **Energy Unit** from the menu **Options** (keyboard shortcut **command-E**). A dialogue (Fig. 10) allows you to set the energy unit of the data set contents and to set the energy unit of the plot.

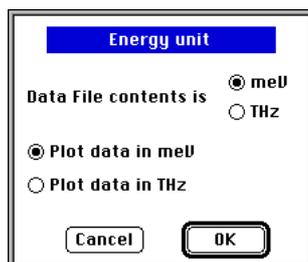


Fig. 10: Set the energy unit for data in file and for the plots.

### 7.2 - Monitor initialization



Select **Monitor** from the menu **Options** (keyboard shortcut **command-M**). A dialogue box (Fig. 11) allows you to select the type of normalization to be applied to the data and to set the corresponding parameter. Note that the program reminds you the monitor value of the first data point. If the "forced monitor" option is set in the preference dialogue (see section 7.11) or in the general dialogue (see section 7.8), the item monitor is disabled.

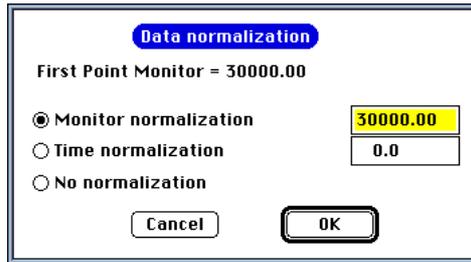


Fig. 11: Set the plot monitor

### 7.3 - Axis options

Options	
Energy unit	⌘E
Monitor	⌘M
<b>Axis options</b>	
Temperature	⌘T
kf or ki	⌘K
Absorption	
Current data set header	
General options	
Fit options	
Plot options	
Preferences	
Help	⌘H

Select **Axis options** from the menu **Options**. A dialogue box (Fig. 12) allows you to select, via popup menus, the variables of the current data set to be associated with the x axis, the y axis and the error bars.

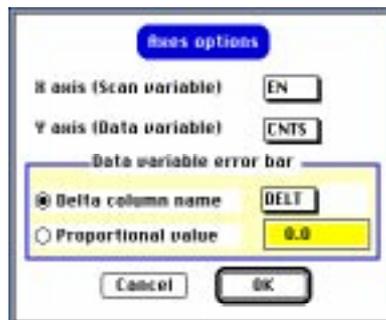


Fig. 12: Axis options dialogue

#### Scan variable:

**PkFit** automatically selects the scan variable (see section 2) but you can override this by selecting the name of another variable. Remember that a scan variable must vary monotonically.

#### Alternate name for CNTS or MES:

**PkFit** takes the counting rate as the default ordinate but you can override this choice by selecting the name of another data column.

#### Calculation mode of errors:

Two modes are available.

- If the current data variable is the counting rate and if DELT (case sensitive) is typed in the field **delta**, the program uses error values read from the data file, if they are present. Otherwise the square root of the neutron number is used.

- If the "proportional error" parameter is set, the experimental error may be taken as a fraction of the ordinate value. E.g., if this parameter is 0.001, the error of the  $i^{\text{th}}$  data point is taken as:

$$\text{error}_i = 0.001 * \text{ordinate value}$$

## 7.4 - Temperature factor

<b>Options</b>	
Energy unit	⌘E
Monitor	⌘M
Axes options	
<b>Temperature</b>	⌘T
kf or ki	⌘K
Absorption	
Current data set header	
General options	
Fit options	
Plot options	
Preferences	
Help	⌘H

The temperature-factor correction can be enabled or disabled at any time. Select **Temperature** from the menu **Options** (keyboard shortcut **command-T**). A dialogue box is shown (Fig. 13) which allows you to set the temperature and to select or deselect the Bose-factor correction.

The default value of the temperature is that of the first point if its value is available in the data file (see section 4).

*Attention: For an energy scan, the Bose factor must be applied if peaks are of the Lorentzian or harmonic oscillator type. To avoid the divergence of the minimization process at zero energy, an  $\omega$  factor is added to the Bose factor.*

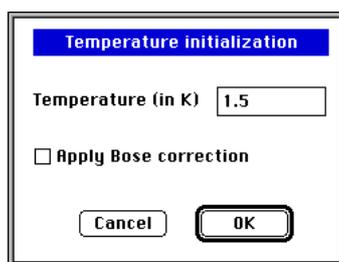


Fig. 13: Setting Bose-factor correction.

## 7.5 - $k_f$ or $k_i$ correction

Options	
Energy unit	⌘E
Monitor	⌘M
Axis options	
Temperature	⌘T
<b><math>k_f</math> or <math>k_i</math></b>	<b>⌘K</b>
Absorption	
Current data set header	
General options	
Fit options	
Plot options	
Preferences	
Help	⌘H

Select  **$k_f$  or  $k_i$**  from the menu **Options** (keyboard shortcut **command-K**). A dialogue box (Fig. 14) allows you to select or deselect the correction. You can choose between a theoretical correction and an experimental correction. The correction can be applied to either the fitted profile or to the data points.



Fig. 14: Dialogue to select/deselect the  $k_f$  or  $k_i$  correction.

### Theoretical correction:

In the case of a fixed  $k_i$  scan the predefined correction is:  $k_f^3 \tan^{-1}(\theta_A)$ . A dialogue (Fig. 15) shows the values of  $k_i$  and  $d_A$  read from the data file. These values, which will be used to calculate  $k_f$  and  $\theta_A$ , can be changed if necessary.



Fig. 15: Dialogue of the theoretical correction in the case of fixed  $k_i$  scan

In the case of a fixed  $k_f$  scan no theoretical correction is presently available; an alert message is thus displayed (Fig. 16).

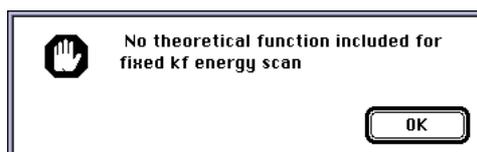
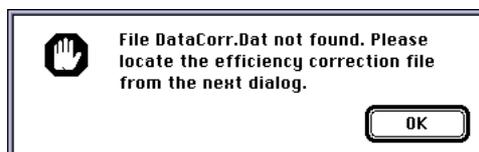


Fig. 16: Alert message when a theoretical correction is selected for a  $k_f$  scan.

*Experimental correction:*

**PkFit** searches for a data correction file with default name 'DataCorr.Dat'. If this file is not found in the working directory an alert message is shown (Fig. 17).



*Fig. 17: Alert message when the data correction file is not found.*

**PkFit** then displays an open file dialogue (Fig. 4) which allows you to select the efficiency correction file to be read. The file format is:

- one comment line, which will be displayed in the output text window
- two columns up to the maximum number of data allowed by the program (see section 3.1). The first column contains the wave vector values in  $\text{\AA}^{-1}$ , the second contains the efficiency correction values. (These are experimental values generally specific to the spectrometer).

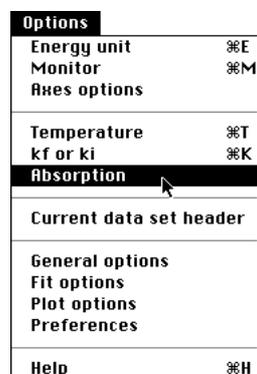
*Data corrected:*

In this mode the correction is applied to the data points. The observed spectrum is thus modified (but the data file content is kept unchanged) as can be seen via the menu item **Draw** (see section 6.1.6).

*Model corrected:*

In this mode the correction is included in the model.

## 7.6 - Absorption



Select **Absorption** from the menu **Options**. A dialogue box (Fig. 18) allows the absorption coefficients to be chosen (see section 3.7 and 11.6).

To add (or remove) the absorption correction to (from) the model, click the check box at the top of the dialogue. Then initialize the absorption coefficients. After clicking button **OK**, the triangle Q-ki-kf is plotted with the absorption parameters and with a cut view of the sample (see section 8.8)

Note that the vector(s) describing the sample orientation must be in the scattering plane, otherwise an alertbox will be shown.

To apply the absorption correction to the background, click the corresponding check box and give the neutron counts BGO of the physical background (from the sample only) at the abscissa value given beside.

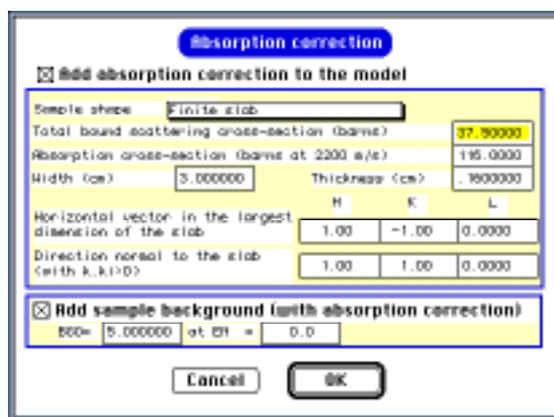


Fig. 18 : Absorption correction dialogue

Here absorption correction is included to the model and to the background.  
 The sample background is 5 counts at an energy of 0 meV.  
 The sample is a finite slab with a width of 3 cm and a thickness of 0.16 mm.

## 7.7 - Data set header

Options	
Energy unit	%E
Monitor	%M
Axes options	
Temperature	%T
Kf or ki	%K
Absorption	
<b>Current data set header</b>	
General options	
Fit options	
Plot options	
Preferences	
Help	%H

Select **Current data set header** from the menu **Options**. A dialogue box (Fig. 19) allows you to edit the contents of the data file header. Changes are kept only if the current data set is saved (see section 5.3) before the graphic window is closed or a new data set is opened.



Fig. 19: Current data set header dialogue

## 7.8 - General options

Options	
Energy unit	⌘E
Monitor	⌘M
Axes options	
Temperature	⌘T
kf or ki	⌘K
Absorption	
Current data set header	
General options	
Fit options	
Plot options	
Preferences	
Help	⌘H

Select **General options** from the menu **Options**. A dialogue box (Fig. 20) allows some miscellaneous program features to be set.

Options are:

### *Peaks plotted separately:*

If enabled, each peak curve is drawn instead of only the calculated spectrum.

### *Extra output during fit:*

If enabled, additional output appears in the text window at each iteration. The normal output is one line with the iteration number, the  $\chi^2$  value and the new parameter values. Extra output are the old, the new values and the uncertainties for each parameter.

### *Enable Draw menu*

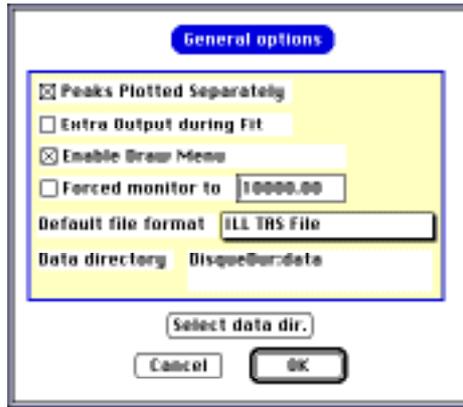
If enabled, the **Draw** item from the menu **Plot** is enabled (See section 8.7).

### *Forced monitor*

If enabled, and if a monitor normalization was selected (see section 7.2), the monitor will be forced to be equal to the corresponding value for the current and subsequent data sets.

### *Default file format*

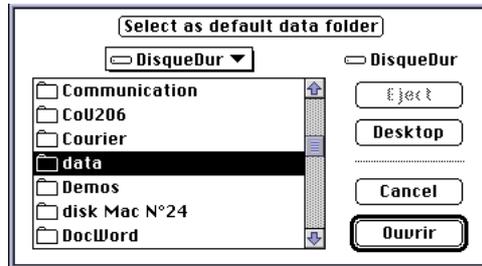
The default file format can be selected through a popup menu. Each time you will open a file this selected file format will be the default, unless you change it in the open file dialogue (see section 5.1)



**Fig. 20:** General *PkFit* setup.

Here individual peak shapes will be plotted; extra output during the fit will be written to the output text window;

When button **Select data dir.** is selected, a dialogue (Fig. 21) allows to choose the default data folder. This folder can be any mounted volume, floppy disk,...



**Fig. 21:** Default data-folder selection dialogue.

## 7.9 - Fit options

Options	Plot	Fit	Rescal
Energy unit			⌘E
Monitor			⌘M
Axis options			
Temperature			⌘T
kf or ki			⌘K
Absorption			
Current data set header			
General options			
Fit options			
Plot options			
Preferences			
Help			⌘H

Select **Fit Options** from the menu **Options**. A dialogue box (Fig. 22) allows for the choice of the resolution deconvolution mode and for the fit mode.

*Integration mode:*

In the case of Lorentzian peak or harmonic oscillator, the convolution with the Gaussian resolution function can be calculated in two ways:

- numerical integration.
- approximate but faster analytic integration. The peak profile (actually a Lorentzian or a harmonic oscillator) is decomposed into a sum of Gaussians.

### *Quick fit mode:*

When the resolution function is included to the model, the fit may take longer to converge if starting values are far from the solution. The "quick fit" mode offers a fit strategy, which is faster when the resolution width is less than the intrinsic width of the peak. The fit is first performed on peak parameters only. At convergence, the convolution of the resolution function and the peak shape is added to the model. This is the default fit mode for the first fit iteration only.

### *Constants defining the fit strategy (for experts only!)*

These parameters are shown at the top of the dialogue window. In general default values are appropriate so change must be performed only in special cases and with extreme care.

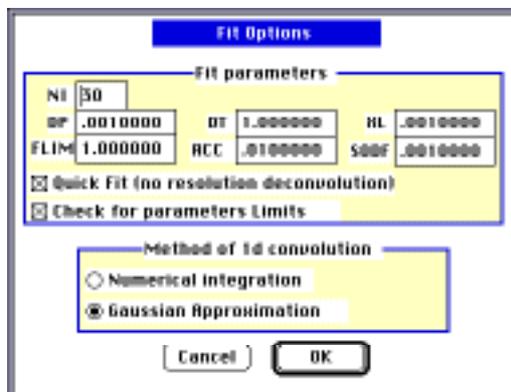
#### List of the fit constants:

- NI        Maximum number of fit iterations (default value = 30). If convergence is not achieved after NI iterations the following message appears in the text window:
- `'JOB TERMINATED: FIT FAILED TO CONVERGE AFTER n ITERATIONS'`
- DP        Starting value of the descent step of the minimization algorithm (default value = 0.001). New parameter values are computed as  $P_{new} = P_{old} + (P_{calc} - P_{old}) * DP$ .
- DT        Increment factor (default value = 1) of the descent step. At each iteration DP, is divided by DT.
- XL        First convergence control parameter (starting value = 0.001). The fit routine calculates the new parameters from the "gauss pivot" of the derived matrix. If the  $\chi^2$  value has increased, XL is multiplied by 10 or divided by 10 otherwise.
- FLIM     Second convergence control parameter. If XL is greater than FLIM then the fit is stopped with the diagnostic "1.Fail". The following message is displayed to the output text window:
- `'CHISQR INCREASED'`  
`'JOB TERMINATED AS AGREEMENT FACTOR DIVERGED'`
- SODF     if the parameter value is less than SODF then the new parameter value takes the value of SODF.
- ACC      Accuracy of the fit (default value = 0.01). The fit is successful if the change in  $\chi^2$  between the last two iterations is less than ACC.

Check for parameter limits:

If this option is enabled (the default) the fit parameters remain in a defined interval.

- The minimum is the start value divided by 10.
- The maximum is the start value multiplied by 10.



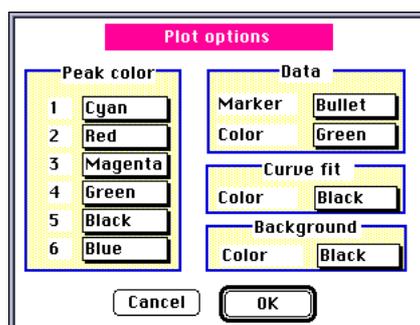
**Fig. 22 :** Options for the resolution-function convolution  
*NI: max. number of fit iterations; DP: starting descent step width; DT: descent step increment; XL,FLIM: fit convergence control parameters; SODF: values for out of range parameters; ACC: requested fit accuracy.*

## 7.10 - Plot options

Options	
Energy unit	%E
Monitor	%M
Axes options	
Temperature	%T
kf or ki	%K
Absorption	
Current data set header	
General options	
Fit options	
<b>Plot options</b>	
Preferences	
Help	%H

Select **Plot options** from the menu **Options**. A dialogue box (Fig. 23) allows plot colors and the shape of data point markers to be changed.

If **PkFit** detects that you are using a black-and-white monitor, the color choice is ignored.



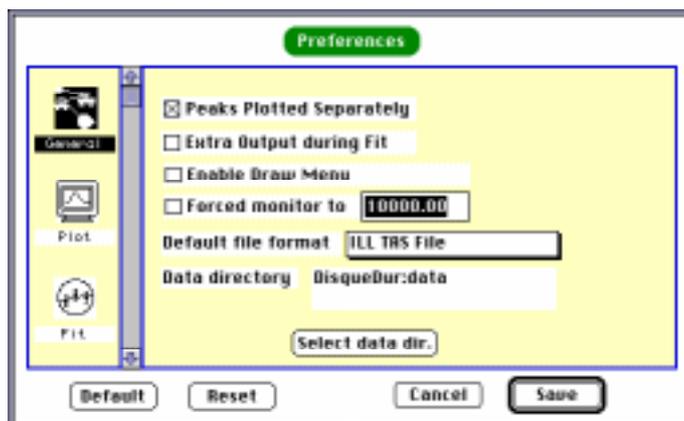
**Fig. 23:** Select the color of each peak curve, of the calculated spectrum and of the data points. Select the symbol of the data points.

## 7.11 - Preferences

Options	
Energy unit	⌘E
Monitor	⌘M
Axis options	
Temperature	⌘T
Kf or ki	⌘K
Absorption	
Current data set header	
General options	
Fit options	
Plot options	
Preferences	
Help	⌘H

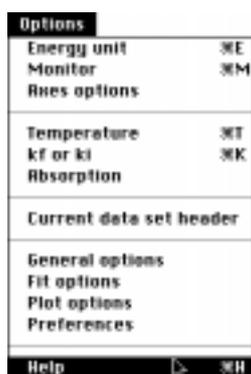
Select **Preferences** from the menu **Options**. A dialogue box (Fig. 24) allows the program configuration to be set and saved in a preference file located in the system folder. This configuration is automatically set next time the program is launched.

The preference-dialogue window exhibits two panes. The left pane shows a set of icons which you can click to select a specific subset of set-up parameters. A vertical scroll bar can be used to move the icons up and down. The right pane shows the dialogue items associated with the selected preference subset.



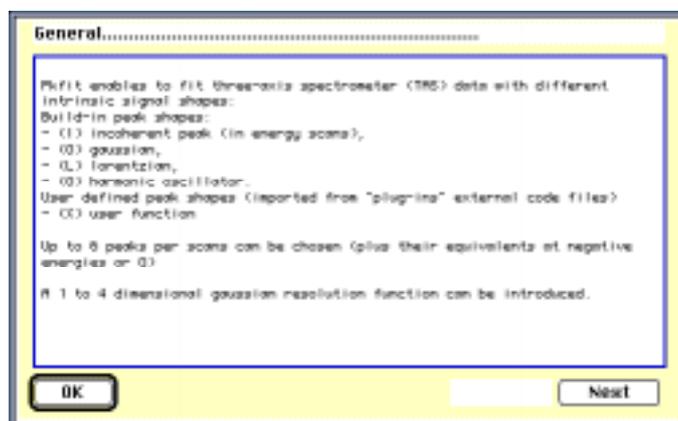
*Fig. 24: The preference dialogue when the subset "General" is selected. Note that button **Select data dir.** can be used to define a default directory (folder) which will be automatically selected when an open-file dialogue will be shown.*

## 7.12 - On-line help



Select **Help** from the menu **Options** (keyboard shortcut **command-H**) to display the help dialogue (Fig. 25). It gives some explanations about the use of **PkFit** and a brief description of its main features.

The help tool looks for a file "Pkf.help" in the application directory. If it is not found the standard open file dialogue is shown. Once the help dialogue is open, click the button **Next** or the button **Previous** to read another help message.



*Fig. 25: The Help dialogue.*

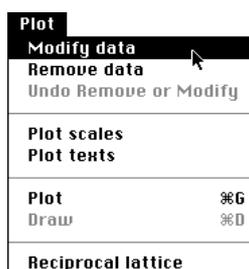
Note that you can easily add your own comments to the help file "Pkf.help" to . Text can be edited with any text editor or word processor (be sure to save the modified file as a plain text file with type 'TEXT'). Figures can be added, replaced and/or positioned in the help message with the help of a resource editor such as ResEdit<sup>TM</sup> 15.

<sup>15</sup> ResEdit is a resource editor developed by Apple Corp.

---

## 8 - Menu Plot

### 8.1 - Modifying data points

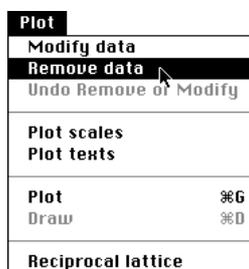


Select **Modify** from the menu **Plot**. Click once on the data point you want to modify. Move the mouse to the new position and click again to set the new intensity.

Press key **E** to exit from the modify option or **Q** to quit without keeping the modification. Note that the message region of the graphic window reminds you how to proceed. The current data set is modified in memory only while the data file is kept unchanged.

*Attention: This option should be used only in very specific and exceptional occasions since modifying data is not the correct way to obtain good results! It is present only to simplify the simulation of scans or to allow for some tests. The authors are not responsible for its misuse.*

### 8.2 - Removing data points



Select **Remove** from the menu **Plot**. Click once on the point you want to remove.

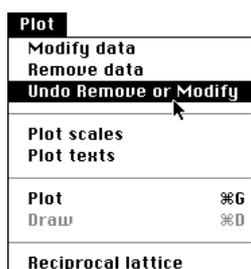
This option may be useful to select only a part of a scan. It can also be used to remove bad points (parasite, interference, ...). However the notion of "bad" point can be very controversial and, as in the previous section, it is rarely advisable to alter the observed data to improve the fit.

The current data set is modified in memory only while the data file is kept unchanged.

A set of keyboard options is proposed in the message region of the graphic window:

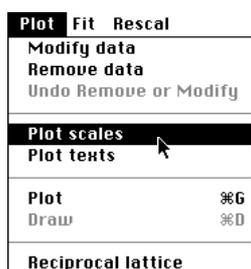
- L** delete all points at the left of the current cursor location
- R** remove all points at the right of the current cursor location
- space** delete the point nearest to the cursor position
- I** delete all points between the current cursor position and that at the previous command (e.g., **I** or **space**)
- E** exit from the current menu option.
- Q** quit without saving modifications.

### 8.3 - Undo Modifying or Removing data points



Select **Undo Remove or Modify** from the menu **Plot**. The last change made with items **Remove data** or **Modify data**.

### 8.4 - Changing the data scale



Select **Plot scales** from the menu **Plot**. A dialogue box (Fig. 26) allows you to change the X and Y data scales.

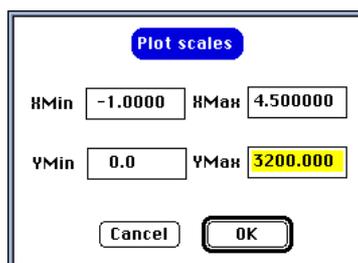
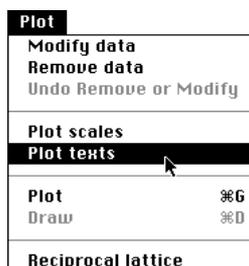


Fig. 26: Changing the scales of the current plot.

## 8.5 - Setting Plot texts



Select **Plot texts** from the menu **Plot**. A dialogue box (Fig. 27) allows you to set plot comments and labels.

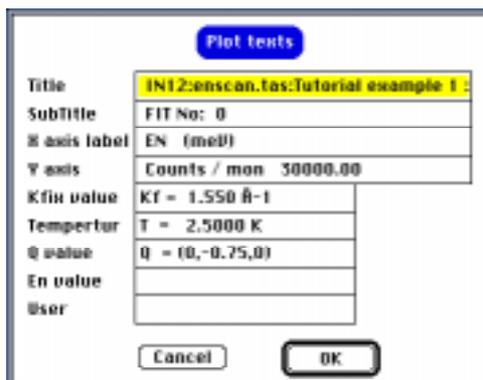
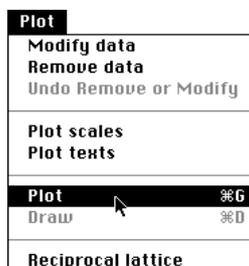


Fig. 27: Changing/adding comments from/to the current plot.

## 8.6 - Plot

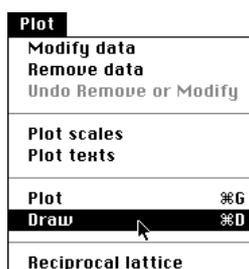


Select **Plot** from the menu **Plot** (keyboard shortcut **command-G**) to update the graphic window.

This option may be useful when some configuration parameters have been changed which do not automatically update the graphic window. This is the case with the following menu items when item **Enable draw menu** is checked in the **General options** dialogue (see section 7.8):

- Set Par** change fit parameters
- Set Peak Par** change peak definitions
- Temperature** change the temperature
- kf or ki** change the correction type

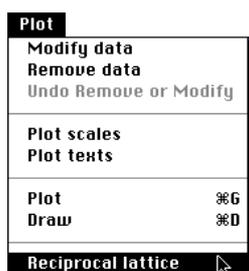
## 8.7 - Draw



Select **Draw** from the menu **Plot** (keyboard shortcut **command-D**). The graphic window is not cleared and new curves are superimposed to the existing ones.

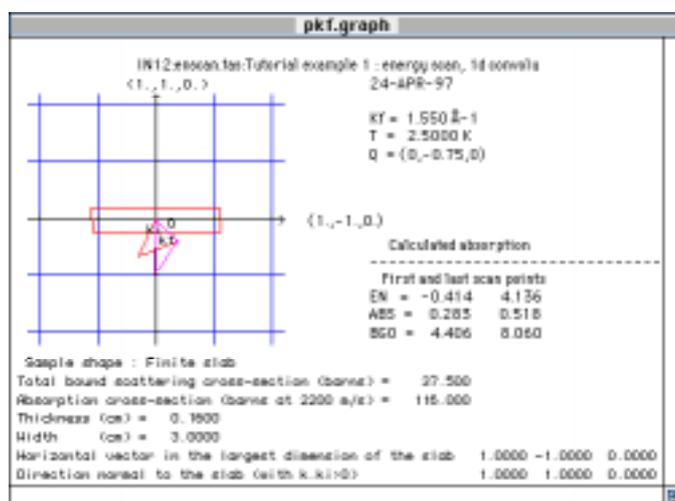
This option may be useful in the same case as the previous one. However instead of clearing the previous plot it allows for a visual comparison of the consequences of the changes. This option is active only if item **Enable draw menu** is checked in the **General options** dialogue (see section 7.8).

## 8.8 - Reciprocal lattice



Select **Reciprocal lattice** from the menu **Plot**. The reciprocal lattice and the triangles  $Q-k_i-k_f$  for the first and the last point of the scan are drawn (Fig. 28) in the graphic window. This window can be printed to the current printer (see section 5.6) or saved in a PICT file (see section 5.3).

The reciprocal lattice in the scattering plan is drawn, with the axis (AX,AY,AZ) in the horizontal direction from left to right, and the second vector (BX,BY,BZ) from bottom to top (in the vertical direction if the vectors are perpendicular). Both vectors are defined in the set of the resolution parameters (see section 10.2).



*Fig. 28: Triangle  $Q-k_i-k_f$  graphic.  
Here absorption parameters are also shown.*

---

## 9 - Menu Fit

The model **PkFit** uses to fit TAS spectra is a linear background plus a series of peak functions. In addition this model may include the Bose factor, a  $k_f$  or  $k_j$  correction, an absorption correction and a convolution of the signal with a one-dimensional or four-dimensional resolution function.

Because PkFit automatically sets:

- the starting background position to a flat background at the position of the lowest point (blue line by default),
- the peak widths by performing a preliminary fit on the widths alone,

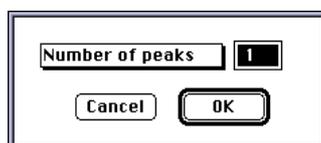
Initializing the model is dead simple:

- set the number of peaks,
- locate the top of each peak,
- set the peak type.

### 9.1 - Initialization of fit parameters



Select **Initialize** from the menu **Fit** (keyboard shortcut **command-I**). A dialogue box (Fig. 29) allows you to set the number of peaks (in the range 0 to 6) in the fit model.

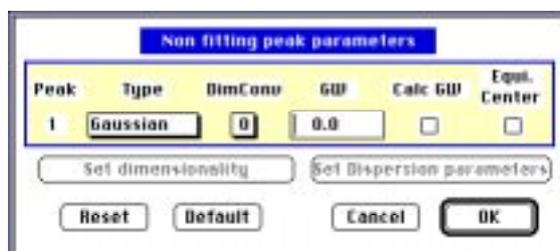


*Fig. 29: Defining the number of peaks in the model.*

Once the number of peaks has been selected, **PkFit** is ready to set the starting peak position(s) and height(s) interactively. When the arrow cursor (  ) is moved to the plot region, it turns to a cross cursor (  ). To initialize the peak parameters, first position the cross cursor at peak maximum and then either click the mouse button for a Gaussian

peak shape or hit one of the following keys. Keys I, G, L, O, B, D or X (case insensitive) respectively stand for an Incoherent, Gaussian, Lorentzian, Harmonic oscillator, Bragg peak, Delta function or a user-defined peak shape.

Then a dialogue is automatically displayed, which allows you to change the peak types and the non-fitting peak-parameters.

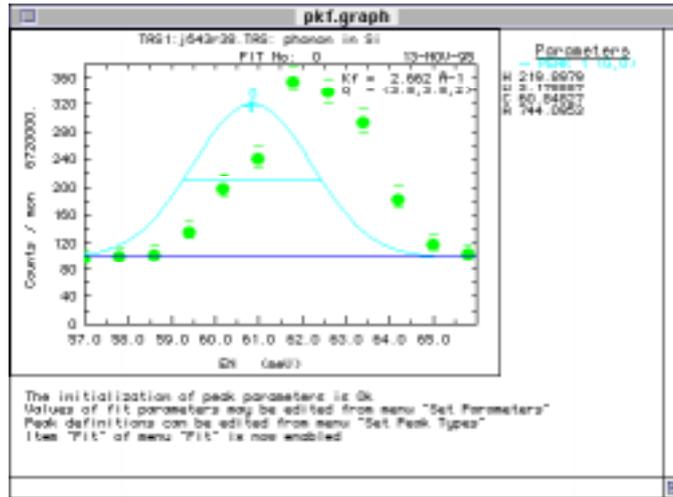


**Fig. 30:** Setting non fitting parameters of peaks (except for "incoherent" ones). Here one Gauss peak has been initialized. The resolution function is not included (DimConv=0) and thus the resolution width ("GW" field) is ignored. The equivalent center option is disabled since the current data set does not come from an energy scan.

You can also open this dialogue box at any time by means of the item **Set peak types** of the menu **Fit** (see section 9.3).

The full widths at half maximum (FWHM) are (arbitrarily) initialized to one third of the plot width divided by the number of peaks. Then a preliminary fit on the widths alone is performed to better estimate the starting peak widths.

Once all fitting parameters have been initialized and non fitting parameters have been set, the different peak(s) are drawn in the graphic window (Fig. 31). **PkFit** displays a cross mark at the selected position and draws a horizontal line which indicates the starting peak width at half maximum (Fig. 31). A message is written in the message region. The item **Fit** of the menu **Fit** is now enabled.



**Fig. 31:** Observed and calculated spectra before the fit. The model parameters (2 background parameters and 3 peak parameters) have been initialized manually. For clarity, the peak has been deliberately initialized here away from its actual position.

## 9.2 - Changing the initial values of the fit parameters

Fit	
Initialize	⌘I
<b>Set parameters</b>	⌘J
Set peak types	⌘U
Oscillator strength	
Fit...	⌘F
Undo fit	
Add a new peak	⌘+
Subtract a peak	⌘-

Select **Set parameters** from the menu **Fit** (keyboard shortcut **command-J**). A dialogue (Fig. 32) allows you to change the starting values of the fit parameters and to apply linear constraints to fit parameters..

The parameter values can be changed. Each parameter can be fixed (excluded from fit) by checking the box at the right of the fit parameter value. By default  $S_0$ , the slope of the background, is fixed. Each peak parameter can be constrained to its analogous parameter of an other peak. In the fit-parameter field, simply replace the parameter value by a formula of the type  $p \cdot X_n + q$  where  $p$  and  $q$  are real numbers,  $X$  is the fit-parameter name (e.g. H,W,C,A, or S) and  $n$  is the peak number. The fit will be performed with the constraint:  $X_m = p \cdot X_n + q$ , e.g.  $C_1 = -C_2$ ,  $A_1 = 0.629 \cdot A_2 - 10$ .

**Fig. 32:** Changing values of fit parameters and setting fit constraints

### 9.3 - Item "Set peak types"

Fit	
Initialize	⌘I
Set parameters	⌘J
Set peak types	⌘U
Oscillator strength	
Fit...	⌘F
Undo fit	
Add a new peak	⌘+
Subtract a peak	⌘-

Select **Set peak types** from the menu **Fit** (keyboard shortcut **command-J**). A dialogue (Fig. 30) allows you to change the peak types and the non fitting peak parameters.

The latter are:

- the peak shape (popup menu)
- the deconvolution dimension (popup menu)
- the resolution width (when the deconvolution dimension is 1)
- the optional computation of the resolution width (see section 6.4)
- the optional computation of the peak at the opposite energy<sup>16</sup> (only for energy scans). This is referred in the following as the "equivalent center option".

#### 9.3.1 - Why a deconvolution ?

The observed peak shapes are generally substantially deformed due to the effect of the instrument resolution. This can be computed as a convolution of the expected profile with the resolution-function of the instrument. In the case of three-axis spectrometers, the latter is a four-dimensional Gaussian, with axes the energy and either the direct or reciprocal space axes.

A 1D deconvolution (convolution in the scan direction only) often suffice, e.g. when the slope of the dispersion curve is small enough (see section 9.3.1 and 11.2.1). Otherwise you should consider using the 4D deconvolution (see section 9.3.2 and 11.2.2).

#### 9.3.2 - Deconvolution at one-dimension

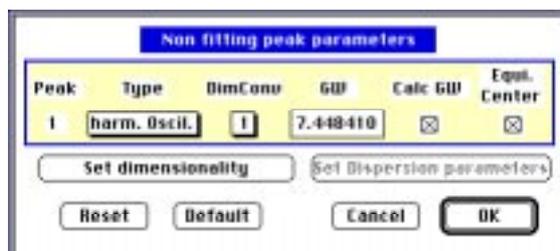
- set the deconvolution dimension **DimConv** to 1 (popup menu)
- set the width **GW** of the resolution function (in the scan direction) to the appropriate value. The latter can be obtained as follows:

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<sup>16</sup> This is referred in the following as the "equivalent center option".

- Edit the value of GW. This value can be estimated, from the width of an adjacent Bragg peak in the case of an angular-scan or of a Q-scan, or estimated from the width of the incoherent peak in the case of an energy scan.
- Check the "Calc GW" box to calculate the resolution width GW.

*Note: the "Calc GW" option is only available for energy scan or Q-scan.*



*Fig. 33: Initialization of the peak types.*

In the example shown in figure 33, the harmonic oscillator is convoluted with a one-dimensional Gauss function (the resolution) with a width of 7.448410 (in the unit of the scan variable). The latter is calculated as the Vanadium width for an energy scan or as the Bragg width for Q-scan (see section 10.6). However, depending on the dimensionality of the model, the convolution can be performed in other directions. The user has the choice among four functions:

three-dimensional: a delta function in three directions. Thus, as for a Bragg peak, the width is directly the corresponding coefficient of the resolution matrix.

Q-independent: a function independent of the Q directions (default case). The resolution function is integrated in these directions. This is the case of the Vanadium width and of an excitation with relatively flat dispersion curves.

two-dimensional: the peak shape function is independent of one of the Q directions (two dimensional compound).

one-dimensional: the peak shape function is independent of two of the Q directions (one dimensional compound).

As an example, let us consider the case of a two-dimensional magnetic compound. The dispersion curve of magnons in the direction normal to the ordered layers is flat. As a consequence, when performing the convolution, we can integrate the resolution function in that direction and this may change the value of the resolution in the scan direction. Since the change occurs not only when the disorder direction is the vertical axis, this is equivalent to a two-dimensional integration.

Click button **Set Dimensionality** to select the dimensionality of the model. A dialogue box appears (Fig. 34). For each peak:

- select the dimensionality via the popup menu in the **Dimensionality** column.
- Define the order direction (one-dimensional crystal) or the normal to the ordered layers (two-dimensional crystal) in the h, k and l columns (in r.l.u).

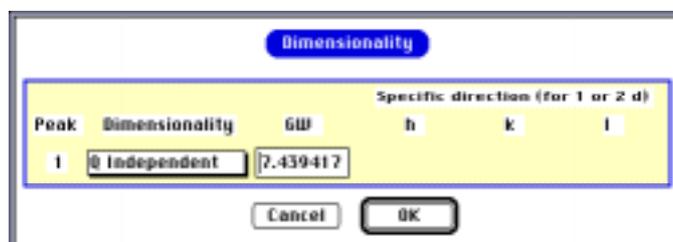


Fig. 34: Initialization of the dimensionality of the model.

### 9.3.3 - Deconvolution at 4 dimensions

The 4 dimensional deconvolution is only available for the following peak shapes:

- Lorentzian
- harmonic Oscillator
- Delta function

Set the deconvolution dimension **DimConv** of the selected peak to 4 (popup menu). A dialogue box (Fig. 35) allows you to initialize the dispersion curve type and the dispersion curve parameters of the selected peak. To select the dispersion curve type, you can either click the popup menu (at the right of the word "Type") or click button **Select**. In this last case, a dialogue box appears (Fig. 36) which displays the predefined dispersion curve expressions and allows you to select one of these. The mathematical expressions of the instrumental resolution function are given in the section 11.2.

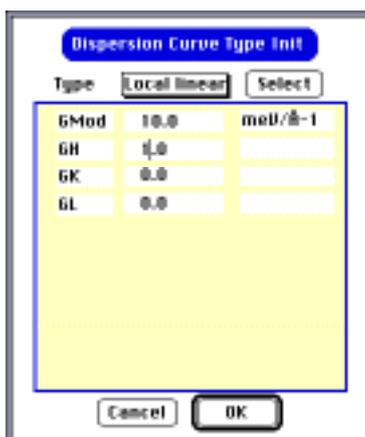


Fig. 35: Initialization of the dispersion curve.

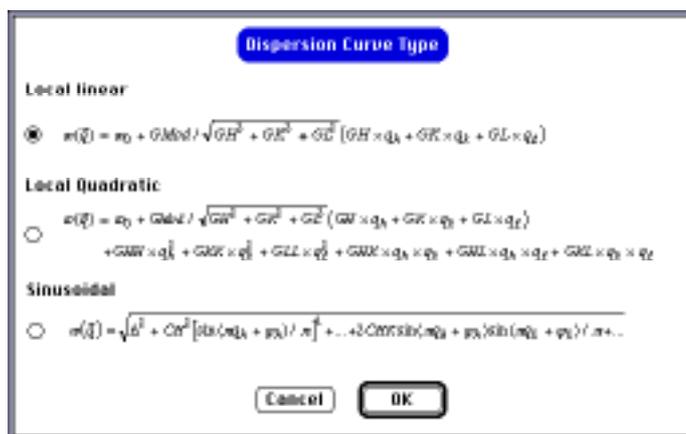


Fig. 36: Selecting the dispersion-curve type.

The button **Set dispersion parameters** of the dialogue **Non fitting peak parameters** (Fig. 33) is now active. It allows you to set the dispersion curves of all the peaks in the same dialogue (Fig. 37). Only two peak parameters can be seen simultaneously. If there is more than two peaks a button **Next** appears which allows you to see the next peak parameters.

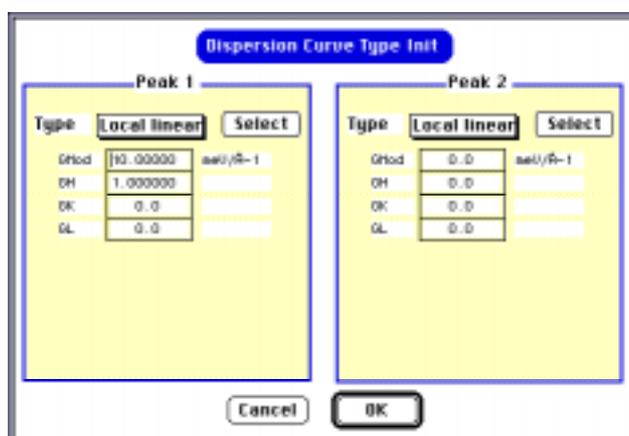


Fig. 37: Initialization of all the dispersion curves. Here two peaks are convoluted with the 4d resolution function.

## 9.4 - "Oscillator strength" constraints



Select **Oscillator strength** from the menu **Fit**. A dialogue box (Fig. 38) allows you to set the constraint.

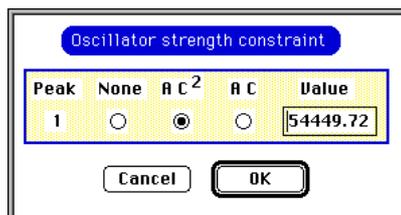


Fig. 38: Oscillator strength constraint dialogue.

In this example, the area and the center of peak 1 are not independent fit parameters. The fit is done with the constraint  $A \cdot C^2 = 54449.72$

## 9.5 - Performing the fit of the model



Select **Fit** from the menu **Fit** (keyboard shortcut **command-F**).

The fit is performed, an error message may appear in the message region of the graphic window, numerical results are written in the text window (Fig. 39) and the observed and calculated plots are redrawn (Fig. 40).

The numerical results are organized in columns:

- # the iteration number
- CHISQR the value of the chi-square statistics
- F0 , S0 background parameters ( $y = F0 + S0 \cdot x$ )
- A1 , W1 , C1 integrated intensity, width and position of peak one.

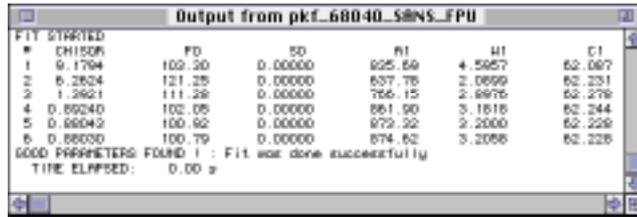


Fig. 39: Example of the numerical results at the end of a fit. Here the model includes one peak only.

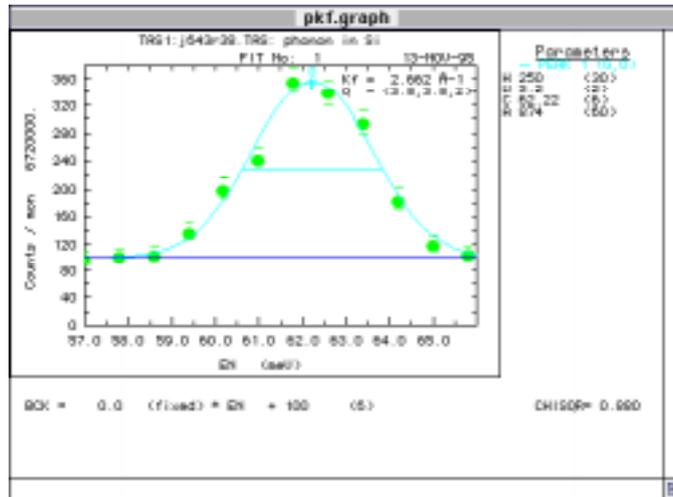


Fig. 40: Example of the graphic window at the end of a fit. The message region contains the background parameters. The parameter region contains the current peak-parameter values.

## 9.6 - Item Undo fit



Select **Undo fit** from the menu **Fit** to restore the fit parameters to those before the fit.

## 9.7 - Item Add a new peak

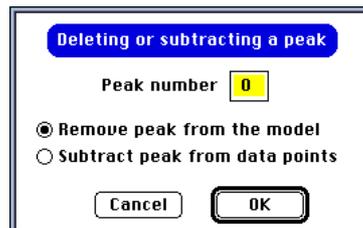


Select **Add a new peak** (shortcut **command-+**) from the menu **Fit** to add a peak to the model. The initialization of an added peak follows the same procedure as that described in section 9.1.

## 9.8 - Item Subtract a peak



Select **Subtract a peak** from the menu **Fit** (shortcut **command--**) to subtract a peak from the model or the data. A dialogue (Fig. 41) allows you to choose between these, and to specify the peak number.

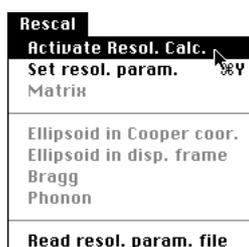


*Fig. 41: Subtracting a peak.*

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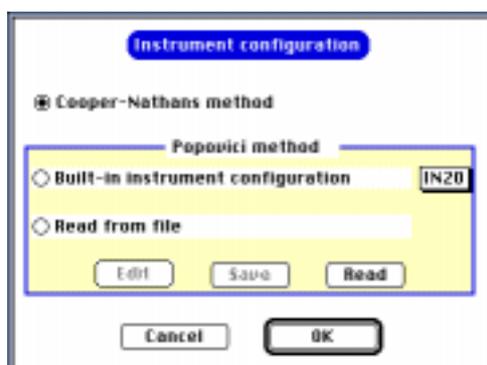
## 10 - ResCal Menu

### 10.1 - Activate the resolution calculation



Select **Activate Resol. Calc.** from the menu **ResCal** (keyboard shortcut **command-Y**). A dialogue box is shown which allows you to select the resolution-calculation method (Fig. 42) and thus to enable the items of the menu **ResCal**.

The resolution function is calculated by means of either the Cooper-Nathans method [1] or the Popovici method [6]. In the latter case, either select the radio button **built-in configuration parameters** and the ILL instrument from the Popup menu or select the radio button **Read from file** and click the button **Read** to read the configuration parameters from a file (see the TAS configuration file format in section 4.3).



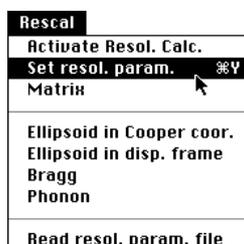
*Fig. 42 : Activate the resolution calculation.*

Both methods use the resolution parameters of the current data set. Be sure that they are realistic (see section 10.2) otherwise the program will give many alerts.

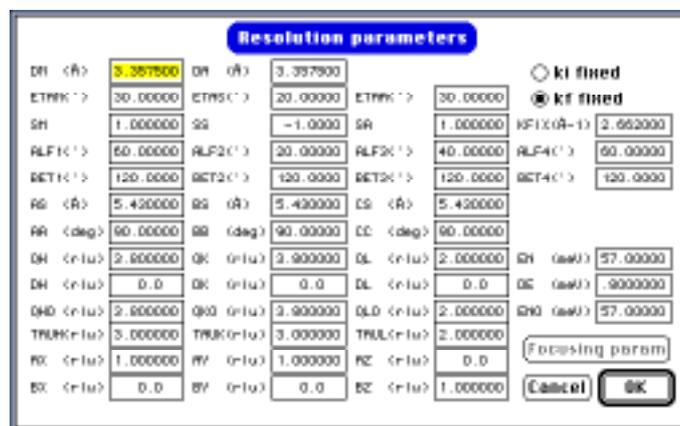
The calculation of the resolution function by means of the Popovici method requires extra parameters describing the instrument, not available in the data files. A built-in table of the parameters of the ILL three-axis spectrometers has been implemented. Thus

a configuration file is no longer necessary, except to define either a non-standard configuration of ILL spectrometers or the configuration of a non-ILL spectrometer.

## 10.2 - Setting the resolution parameters



Select **Set resol. param.** from the menu **Rescal** (keyboard shortcut **command-Y**). A dialogue box (Fig. 43) displays the current values of the resolution parameters.



*Fig. 43 : Set the resolution parameters.*

**PkFit** reads the initial value of the resolution parameters in the file header (see section 4.2). However, if it does not contain all the parameters required the user has to set the correct values for parameters listed below. The program provides default values except for QH, QK, QL, EN which define the point in the ( $\omega, q$ ) plane to be computed:

- QH0, QK0, QL0, EN0 : coordinates of the center of the scan (ILL) or first point of the scan (Saclay).

These values are written at the top right of the graphic window, and are used to calculate the (Q,EN) coordinates along the scan direction. It is essential to initialize these values correctly in the case of a multiple scan variable. In fact, for a QH, QK scan the plot is a projection of the scan on the QH axis and the QK value is always calculated from the equation:  $QK=QK0+(QH-QH0)/DQH*DQK$ .

- TAUH, TAUk, TAUL: coordinates of the nearest zone center.

The default values are the nearest integer of QH, QK, QL (respectively). These parameters are used to calculate the coordinates of the q vector, which are necessary in the dispersion-curve calculations.

When the Popovici method is used, the button **Set focusing parameters** is enabled. If clicked a dialogue is shown (Fig. 44) which allows you to set the monochromator and analyser curvatures and the sample dimensions.

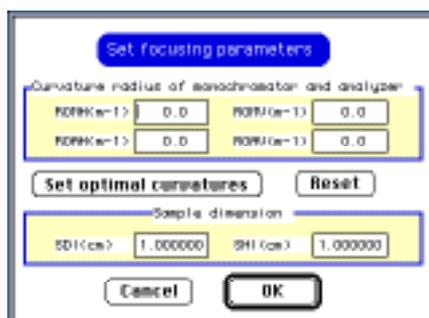
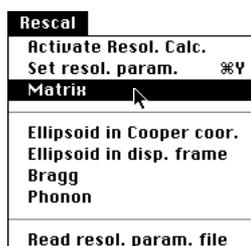


Fig. 44: Set the focalisation parameters.

The button **Set optimal curvatures** helps you to find optimum curvature values of both the monochromator and the analyzer. The monochromator is supposed to focus a parallel beam on the sample, while the analyzer curvatures are set to focus a point at the sample to a point at the detector. Usually these values are not far from the optimum values giving maximum intensities. This option is similar to the command "RO" in Restrax4.1 for Open-VMS/UNIX workstations.

### 10.3 - Resolution matrix



Select **Matrix** from the menu **Rescal**. A dialogue box (Fig. 45) displays the resolution matrix.

This dialogue shows the results of the resolution calculated either by the Cooper-Nathans method [1] or the Popovici method [6]. The results are shown in the form of the following matrices:

Resolution volumes (top line):  $V_i$  and  $V_f$  are volumes of the incident and final wave vectors, giving information on the total measurable "integrated" intensity.

Matrix A (top left pane): the resolution matrix in the coordinate axes reversed with respect to the Cooper-Nathans convention. X is along  $-Q$ , Y is along  $Q_{\perp}$ , Z is the vertical direction and w corresponds to the energy. Elements are in  $\text{\AA}^{-1}$  and in meV or THz, respectively.

Matrix AZ (top right pane): the resolution matrix in the reciprocal lattice coordinates. Elements are in rlu and in meV or THz, respectively.

Matrix ADA (bottom left pane): the diagonalized resolution matrix. Elements are in rlu and in meV or THz, respectively.

Direction cosines matrix (bottom right pane): eigenvectors of the resolution matrix.

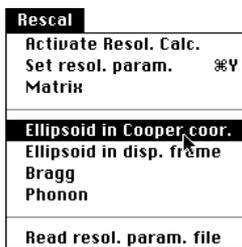
Resolution matrix					RZ in reciprocal lattice coordinates				
A in coordinate axes reversed I.R.T. Cooper-Nathans convention ( $\text{\AA}^{-1}$ and meV)					AZ in reciprocal lattice coordinates (rlu and meV)				
X	Y	Z	w		H	K	L	w	
6081.469	-2837.6	0.0	-274.12		5144.997	4870.078	-870.80	-252.43	
-2837.6	2326.641	0.0	147.9773		4870.078	5144.997	-870.90	-252.43	
0.0	0.0	209.2919	0.0		-870.80	-870.80	1242.993	49.84343	
-274.12	147.9773	0.0	12.98072		w	-252.43	-252.43	49.84343	12.98072

ADA Diagonalized resolution matrix					Direction cosines of axes from RZ to ADA				
X'	Y'	Z'	w'		H	K	L	w	
.0233192	0.0	0.0	0.0		X'	.7000998	-.7071037	.0964934	.0247165
0.0	.1420477	0.0	0.0		Y'	.7000998	.7071068	.0964934	.0247165
0.0	0.0	.0718767	0.0		Z'	-.136295	0.0	.9906451	-.005444
0.0	0.0	0.0	6.714990		w'	-.035370	0.0	.0006237	.9993741

Fig. 45 : The resolution matrix.

## 10.4 - Ellipsoid resolution in Cooper-Nathans coordinates



Select **Ellipsoid in Cooper coor.** from the menu **Rescal**. A dialogue box (Fig. 46) allows for the choice of the visualization plane of the ellipsoid resolution at half the maximum intensity level.

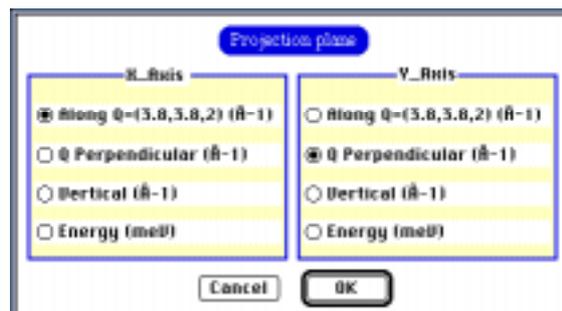


Fig. 46 : Choice of X and Y axes in Cooper-Nathans frame

Both the cut of the resolution ellipsoid by the selected plane, and the projection of the 4 dimensional ellipsoid on the selected plane, are plotted (Fig. 47). The corresponding resolution equations are written at the bottom of the plot.

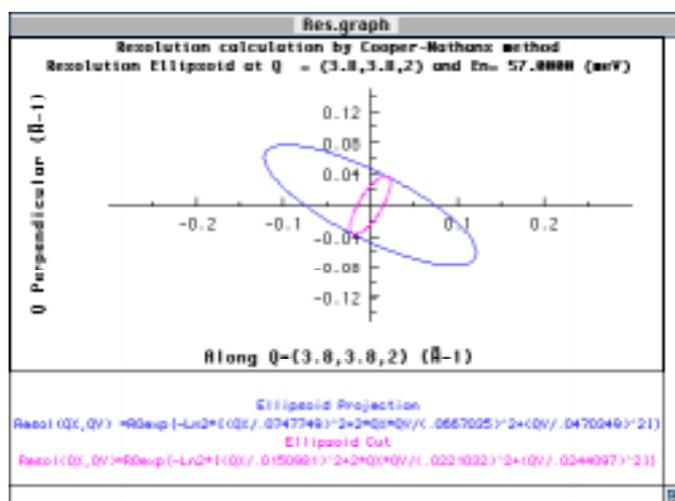
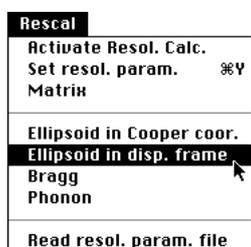


Fig. 47: The resolution ellipsoid in Cooper-Nathans axes.

### 10.5 - Ellipsoid resolution in the q direction



Select **Ellipsoid in disp. frame** from the menu **Rescal**. A dialogue box (Fig. 48) permits a choice of the visualization plane of the ellipsoid resolution in the "dispersion" frame defined by  $q_x$ ,  $q_y$ , the vertical axis and the energy.



Fig. 48: Choice of X and Y axis in dispersion frame

Both the cut of the resolution ellipsoid by the selected plane, and the projection of the 4 dimensional ellipsoid on the selected plane, are plotted (Fig. 49). The corresponding resolution equations are written at the bottom of the plot.

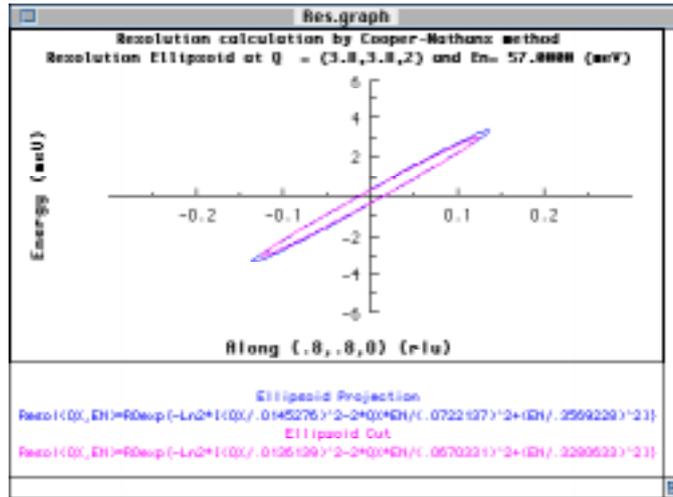
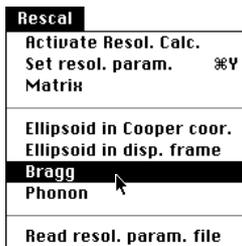


Fig. 49 : The resolution ellipsoid in the dispersion frame.

## 10.6 - Visualization of Bragg widths



Select **Bragg** from the menu **Rescal**. Bragg widths are plotted in the graphic window (Fig. 50).

The four Bragg widths (FWHM)  $W_{Q_h}$ ,  $W_{Q_k}$ ,  $W_{Q_l}$ ,  $W_{E_n}$ , are calculated in reciprocal lattice unit and in meV or THz, respectively. These widths directly correspond to the resolution width, or to the convolution of a delta function in four dimensions with the resolution function.

In the bottom part of the window **PkFit** also plots a convolution of the resolution function with a function which is a delta function in the energy direction and which is independent of  $Q$ .  $\Gamma_{inc}$  is the energy width of that convoluted function. This plot is especially useful to visualize the shape of the incoherent scattering in the  $Q$ ,Energy space.

*Note: For simplicity we use the terms "Bragg Width" and "Vanadium width" even in the case of finite energy.*

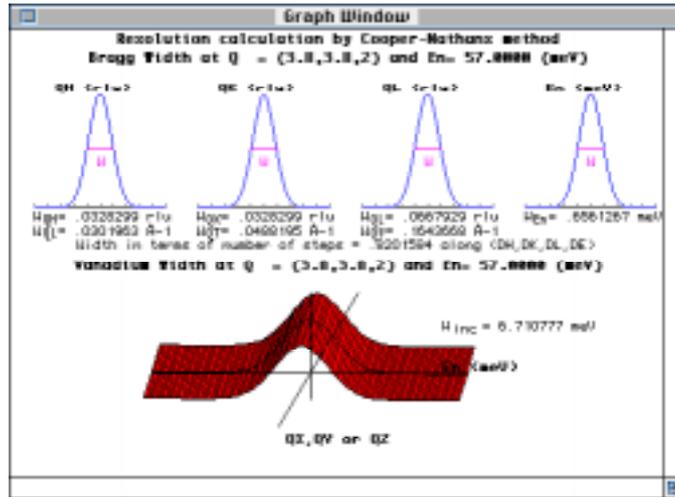
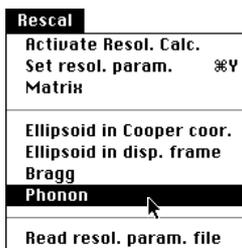


Fig. 50 : Bragg widths

### 10.7 - Visualization of Phonon widths



Select **Phonon** from the menu **Rescal**. A dialogue box (Fig. 51) allows you to select the dispersion-curve type and parameters .

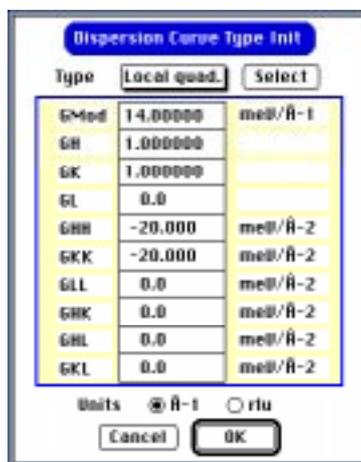


Fig. 51 : The dispersion-curve type and parameters.

The current dispersion-curve type (see section 3.5) is displayed at the top of the dialogue box while the corresponding parameter set is given in the central pane. To select another dispersion-curve type, click on button **Select** to get the corresponding dialogue (Fig. 52), or choose the name of the dispersion-curve type via the popup menu.

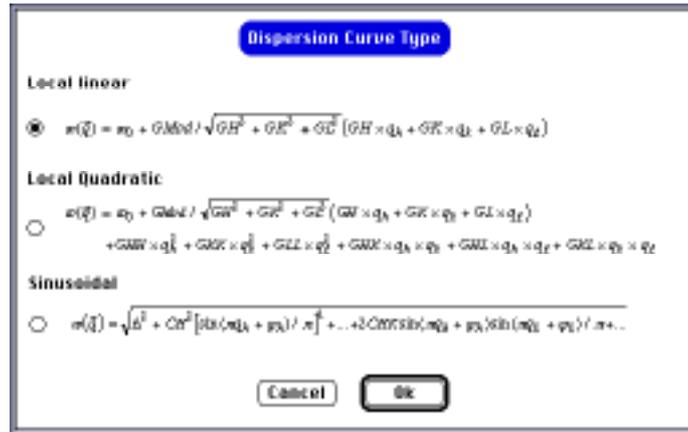


Fig. 52: The dispersion curve type dialogue.

Once both the resolution-curve type and the dispersion-curve parameters have been set (Fig. 51 & 52), the resolution plot in the plane (q,Energy) and the scan simulated by Monte-Carlo integration are drawn (Fig. 53). This is especially useful:

- to simulate an energy scan
- to know whether or not the scan is on the focussing side
- to know if the energy step is well adapted to the phonon width.

The resolution ellipsoid in the plane (q,Energy) is drawn on the left side of the graphic window. The energy is in meV, and q is along the direction [1,1,0]. The plot in figure 53 corresponds to that of the resolution ellipsoid when the user selects the item **Ellipsoid in disp. frame** in the menu **Rescal** and checks item **Along q = (3.8,3.8,2.) (rlu)** for the x axis and **Energy (meV)** for the y axis in the dialogue shown in figure 49. The dispersion curve is drawn in magenta (or light gray) on the same plot and the corresponding equation is written below the two plots.

The dispersion curve is drawn in magenta (or light gray) on the same plot and the corresponding equation is written in the bottom part of the window.

The scan in energy or q, simulated by Monte-Carlo integration (see section 9.3), is drawn on the top right part of the graphic window as a histogram. The width of the histogram is the scan step and the "phonon width"  $\Gamma$  is calculated from the second moment of the point distribution.

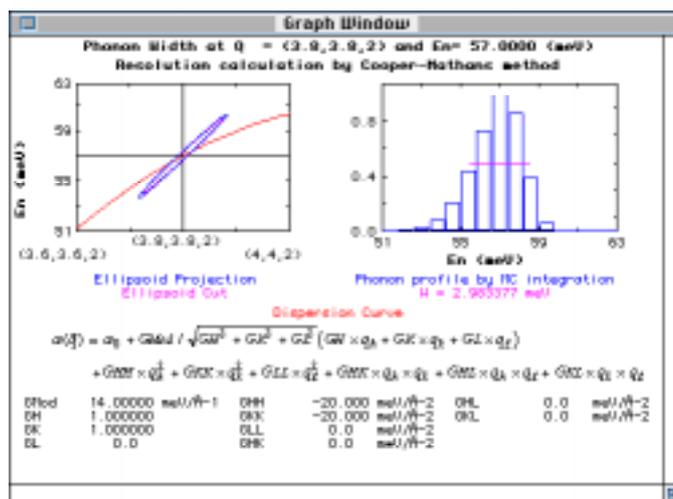
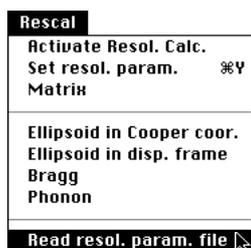


Fig. 53 : Phonon width.

## 10.8 - Read resolution parameters



New resolution parameters (usually read from the data file) are read from a separated file and overwrite the current values. Select **Read resol. param.** from the menu **Options**. A dialogue box (Fig. 54) allows you to select the type of the resolution-parameter file (see section 4).

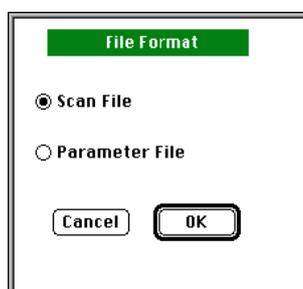


Fig. 54: Selecting the type of the resolution-parameter file.

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## 11 - Mathematical background

The model used by **PkFit** to fit three-axes spectrometer data is:

$$I(X) = F0 + S0 X + I_{Q,\omega}(X)$$

where

X	the scan variable
F0 and S0	linear background parameters
Q	wave vector $\vec{Q} = \vec{k}_f - \vec{k}_i$
$\omega$	transfer energy of the neutron $\hbar\omega = E_i - E_f = \frac{\hbar^2}{2m_n}(k_i^2 - k_f^2)$
$I_{Q,\omega}(X)$	elastic or inelastic scattering intensity
I(X)	detector counts at scan point X

When the one-dimensional Gaussian resolution function is included, the inelastic scattering contribution is given by:

$$I_{Q,\omega}(X) = \int_{-\infty}^{+\infty} S_{Q,\omega}(X - X') R_{Q,\omega}(X') dX'$$

where

$S_{Q,\omega}(X - X')$  is the scattering function

and

$R_{Q,\omega}(X')$  is the resolution function.

When no resolution function is included the above inelastic scattering function is directly the scattering function which depends only on the physical problem. Since a general expression cannot be obtained, **PkFit** relies on several semi-empirical functions which are of common use for this type of calculation [9, 10, 11].

In **PkFit** the built-in scattering functions are the conventional Gauss, Lorentz and damped harmonic-oscillator functions plus extra functions corresponding to specific types of signal (section 11.1). These extra functions, described below, are the incoherent elastic scattering, the Bragg diffraction, or the signal of dispersive excitations (e.g. phonon/magnon). In addition, the user can provide his own functions

in standalone code, i.e. code which is dynamically linked at runtime (see section 13 and [5]).

## 11.1 - Peak functions

Peak functions have three fit parameters:

W the full width at half maximum (FWHM).

C the position.

A the area scaled to the selected monitor value.

A fourth parameter is often useful:

H peak height (in neutron counts).

H can be used to initialize A, but is never directly fitted since it is not independent from the three former parameters:  $H = f(A, W)$ .

### 11.1.1 - Incoherent elastic scattering peaks

The physical definition of the incoherent scattering is:

$$S_{Q,\omega}(X) = A\delta(\omega)$$

In **PkFit**, the incoherent elastic scattering is directly accounted for by the resolution function.

$$I_{Q,\omega}(\omega) = \sqrt{\frac{\ln 2}{\pi}} \frac{A}{W/2} \exp\left[-\ln 2 \left(\frac{\omega - C}{W/2}\right)^2\right]$$

The incoherent peak can only be used in the case of an energy scan. It is then defined as a Gaussian peak located at C and with a width, W, that can be set, or calculated from the resolution matrix, but never fitted. The incoherent-peak location C can be fitted to account for the zero energy shift due, e.g., to a misalignment of the analyser. No temperature correction is applied to this type of peak.

### 11.1.2 - Bragg Peak

The Bragg peak is a one dimensional gaussian with the width equal to the resolution ones calculated by Cooper-Nathans method [1] or the Popovici method [6]. No temperature correction is applied on this type of peaks.

### 11.1.3 - Delta function

The delta function is accounted to describe an excitation of phonon type, i.e., an excitation with a dispersion and with coherence lengths much bigger than the resolution. Thus the physical definition of the delta function is:

$$S_{Q,\omega}(X) = A\delta(\omega - \omega_0(\vec{q}))\delta(\vec{Q} - \vec{Q}_0)$$

It is directly accounted for by the 4 dimensional resolution function. The scattering intensity is given by a Monte-Carlo integration (see section 11.3) and the fit is performed on the scale factor, A, on the peak position,  $C = \omega_0(\vec{q})$ , and on one of the dispersion curve parameter, i.e., the slope (local linear or quadratic curve) or the gap  $\Delta$  (sinusoidal curve).

$$I_{Q,\omega}(X) = \sqrt{\frac{\ln 2}{\pi}} \frac{A}{W/2} \exp\left[-\ln 2 \left(\frac{X-C}{W/2}\right)^2\right]$$

### 11.1.4 - Gaussian peak

This peak shape can be convoluted with the Gaussian resolution function. The other corrections ( $k_f$ ,  $k_i$ , temperature and absorption) can be applied as scale factors.

$$S_{Q,\omega}(X) = \sqrt{\frac{\ln 2}{\pi}} \frac{A}{W/2} \exp\left[-\ln 2 \left(\frac{X-C}{W/2}\right)^2\right]$$

### 11.1.5 - Lorentzian peak

The Lorentzian peak shape can be defined as follows:

$$S_{Q,\omega}(X) = \frac{1}{\pi} \frac{A}{W/2} \frac{1}{1 + \left(\frac{X-C}{W/2}\right)^2}$$

In the case of an energy scan an extra factor must be added to satisfy the sum rule. Thus we have:

$$S_{Q,\omega}(\omega) = \frac{\omega}{1 - \exp(-\omega / T)} \frac{1}{\pi} \frac{A}{W / 2} \frac{1}{1 + \left( \frac{\omega - C}{W / 2} \right)^2}$$

*Attention:* In this case, the peak area  $A$  is not the integral of the scattering function which diverges, but the integral of the dynamic susceptibility:

$$A = \chi(Q) = \int_{-\infty}^{+\infty} \frac{\chi_{Q,\omega}(\omega)}{\omega} d\omega = \int_{-\infty}^{+\infty} [1 - \exp(-\omega / T)] \frac{S_{Q,\omega}(\omega)}{\omega} d\omega$$

### 11.1.6 - Harmonic Oscillator

The harmonic oscillator can be used only in the case of an energy scan and the resolution correction-factor is then included in the fit model. The scattering function has the following expression:

$$S_{Q,\omega}(\omega) = \frac{\omega}{1 - \exp(-\omega / T)} \frac{1}{\pi} \frac{A}{W / 2} \frac{W^2 C^2}{(\omega^2 - C^2)^2 + \omega^2 W^2}$$

An equivalent expression, which uses Lorentzian shape is:

$$S_{Q,\omega}(\omega) = \frac{1}{1 - \exp(-\omega / T)} \frac{1}{\pi} \frac{A}{W / 2} \frac{C_L^2 + (W / 2)^2}{C_L} \left[ \frac{1}{1 + \left( \frac{\omega - C_L}{W / 2} \right)^2} - \frac{1}{1 + \left( \frac{\omega + C_L}{W / 2} \right)^2} \right]$$

with

$$C = \sqrt{C_L^2 + (W / 2)^2}$$

## 11.2 - Resolution function

Generally the vertical and horizontal resolutions are independent, due to the specific geometry of a three-axis spectrometer. This may not be entirely true when a vertically focusing monochromator or analyzer is used. **PkFit** does not take account of these cases.

### 11.2.1 - at one dimension

The resolution function implemented in **PkFit** is of a Gaussian shape. The normalized expression is:

$$R_{Q,\omega}(X) = \sqrt{\frac{\ln 2}{\pi}} \frac{1}{GW/2} \exp\left[-\ln 2 \left(\frac{X}{GW/2}\right)^2\right]$$

where GW is the full width at half maximum (FWHM) of the Gaussian. This parameter depends on the scan position ( $Q, \omega$ ) and is either supplied by the user or calculated by the program (see section 9.3).

### 11.2.2 - at four dimensions

The TAS instrumental resolution function implemented in PkFit is of the normalised Gaussian type:

$$R(\omega, x, y, z) = R_0 \exp\left(-\ln 2 \left[ B_{\omega\omega} \omega^2 + B_{xx} x^2 + B_{yy} y^2 + B_{zz} z^2 + 2 B_{\omega x} \omega x + 2 B_{\omega y} \omega y + 2 B_{xy} xy \right]\right)$$

where

$R_0$  the normalisation factor (the 4D integral of the resolution function is equal to 1):

$$R_0 = \left(\frac{\ln(2)}{\pi}\right)^2 \sqrt{B_{zz} \left( B_{\omega\omega} B_{xx} B_{yy} - B_{\omega\omega} B_{xy}^2 - B_{xx} B_{\omega y}^2 - B_{yy} B_{\omega x}^2 + 2 B_{\omega x} B_{\omega y} B_{xy} \right)}$$

$x$  and  $y$  two directions defining the scattering plane,

$z$  the vertical direction of the spectrometer.

Generally the vertical and horizontal resolutions are independent ( $B_{\omega z}, B_{xz}, B_{yz}=0$ ) due to the specific geometry of the three-axis spectrometers. This may not be entirely true when a vertically-focusing monochromator and/or analyser is used. **PkFit** does

not take account of these cases. The resolution parameters  $B_{ij}$  are those given by the Cooper-Nathans method [1] or the Popovici method [6] for a given set of spectrometer-configuration parameters.

$$M = \begin{pmatrix} B_{\omega\omega} & B_{\omega x} & B_{\omega y} & 0 \\ B_{\omega x} & B_{xx} & B_{xy} & 0 \\ B_{\omega y} & B_{xy} & B_{yy} & 0 \\ 0 & 0 & 0 & B_{zz} \end{pmatrix}$$

In the case of a constant  $k_i$  scan, the resolution volume is accounted for by the  $k_f^3 \operatorname{tg}^{-1}(\theta_A)$  correction. In the case of a constant  $k_f$  scan the resolution volume, when multiplied by the monitor efficiency (in  $1/k_i$ ) and by the term  $k_f/k_i$  of the cross section, is simply a constant. In **PkFit** the monitor efficiency is assumed to account for the multiple order contamination.

The "Bragg width" are directly calculated from the diagonal elements of the resolution matrix,  $W_i = \sqrt{8Ln(2) / B_i}$ , when the "Vanadium width" is given by the following expression, obtained after integrating the resolution function in x and y:

$$W_{inc} = \sqrt{8Ln(2) / \left[ B_{\omega x} - B_{\omega\omega}^2 / B_{xx} - (B_{\omega y} B_{xx} - B_{\omega x} B_{xy})^2 / B_{\omega\omega} / (B_{yy} B_{xx} - B_{xy}^2) \right]}$$

### 11.3 - Monte-Carlo integration

In general, the intensity profile  $I(\omega_s)$  of a phonon peak observed in a TAS scan is given by an overlap integral,

$$I(\omega_s) = I_0 \int S(\vec{Q}, \omega) R(\vec{Q}, \omega - \omega_s) d\omega d\vec{Q} \quad (1)$$

where  $S(\vec{Q}, \omega)$  and  $R(\vec{Q}, \omega)$  are the scattering function and the resolution functions. Within RESCAL only undamped phonons are considered whose scattering function is then a  $\delta$ -function,

$$S(\vec{Q}, \omega) = \delta(\omega(\vec{q}) - \omega) \quad (2)$$

In the case of undamped excitations (the scattering function is a delta function (2)), the calculation of the integral (1) corresponds to the determination of the section of the resolution ellipsoid by the dispersion surface. This can be carried out analytically in case of a planar dispersion (cf. Cooper & Nathans [1]), but this is often quite

complicated and time-consuming. Many of the problems are avoided by using a Monte-Carlo (MC) integration technique based on the following two ideas:

- a set of random points, with a Gaussian probability density, can be directly generated in the  $(\bar{Q}, \omega)$  space to simulate the  $R(\bar{Q}, \omega)$  function.
- integral (1) is approximated by the volume of the slice of the resolution ellipsoid bounded by the dispersion surfaces corresponding to two subsequent scan positions.

By using the Gaussian distribution, mentioned in the first point, instead of a uniform distribution, the “hit-or-miss” Monte-Carlo integration technique, described in the second point, becomes a crude MC integration technique, which is more efficient (see reference [12]). The value of integral (1) is easily obtained as the number of MC events for which the value of  $\omega(\bar{q}) - \omega$  lies within  $\omega_s \pm \Delta\omega_s/2$ , where  $\Delta\omega_s$  is the step-length of the scan. It is also assumed that the TAS resolution function does not change in the peak region. As a consequence during a single summation over a set of the random points, the simulated profile is accumulated by binning the differences  $\omega(\bar{q}) - \omega$  into a histogram with step length  $\Delta\omega_s$ .

The above algorithm is directly applicable to any type of dispersion as long as the dispersion equation is resolved with respect to the energy. For linear dispersion in  $(\bar{Q}, \omega)$  space, it can be generalised to any scan direction. While for curved dispersion surfaces, their expression cannot always be resolved with respect to the scan variable. In the latter case, even if an interpolation is performed the computation time will be long. Therefore, to preserve the interactivity, **PkFit** calculates scan profiles by means of the MC method only for general scan directions and planar dispersion surfaces (equivalent to the Cooper and Nathans method) or for scans at  $\bar{Q} = \text{constant}$ . Since we consider here undamped excitations, whose scattering function is a delta function, the profile calculated as explained before is directly the peak function to be used to fit the data. Therefore the fit parameters are the peak center, the intensity and one of the dispersion curve parameter (e.g., the slope in the case of a linear dispersion curve).

In **PkFit** the case of damped excitations (with a finite lifetime) is treated as an extension of the undamped case. This is done through a numerical convolution of the histogram with a normalised scattering function. Therefore both the undamped and damped dispersive excitations can be treated by means of the 4D convolution method above. In other words, convoluting the resolution function with the signal is simple since it requires only that one of the built-in scattering functions (delta, Lorentzian or damped harmonic oscillator) and the type of the dispersion curve be selected (see section 11.4).

## 11.4 - Dispersion curves and structure factors

The equation of the dispersion curves available in **PkFit** are:

- a local linear dispersion curve

$$\omega(\vec{q}) = \omega_0 + G_{Mod} / \sqrt{GH^2 + GK^2 + GL^2} [GH \times q_h + GK \times q_k + GL \times q_\ell]$$

- a local quadratic dispersion curve

$$\omega(\vec{q}) = \omega_0 + G_{Mod} / \sqrt{GH^2 + GK^2 + GL^2} [GH \times q_h + GK \times q_k + GL \times q_\ell] \\ + G_{HH} \times q_h^2 + G_{KK} \times q_k^2 + G_{LL} \times q_\ell^2 + G_{HK} \times q_h q_k + G_{HL} \times q_h q_\ell + G_{KL} \times q_k q_\ell$$

- a sinusoidal dispersion curve

$$\omega(\vec{q}) = \sqrt{\Delta^2 + CH^2 [\sin(\pi q_h + \varphi_h) / \pi]^2 + \dots + 2CHK \sin(\pi q_h + \varphi_h) \sin(\pi q_k + \varphi_k) / \pi + \dots}$$

Future versions will enable the user to implement his own dispersion curves in external code resources.

## 11.5 - Gauss-Newton method

This algorithm calculates changes in parameters at each step,  $\Delta x$ , from the normal equation:

$$M[1 + \lambda \text{diag}(M)] \Delta x = N$$

with

$$M_{jk} = \sum_i \frac{1}{\sigma_i^2} \frac{\partial F_{calc}}{\partial p_j}(x_i) \frac{\partial F_{calc}}{\partial p_k}(x_i) \\ N_j = \sum_i \frac{1}{\sigma_i^2} [F_{obs}(x_i) - F_{calc}(x_i)] \frac{\partial F_{calc}}{\partial p_j}(x_i)$$

and

$p_j$	the parameter j,
$x_i$	the abscissa of point i,
$F_{obs}$	the observed intensity array,
$F_{calc}$	the calculated function,
$\sigma_i$	the experimental error.

In **PkFit**, the Choleski decomposition of the symmetric, positive definite matrix, M, and back solution for the consistent system of linear equations are performed. In cases where M is non positive definite, an error message is written on the text window.

A new set of x,x' is readily obtained by,

$$x' = x + \Delta x(\lambda)$$

The initial value of the damping factor,  $\lambda$  (XL in section 8.2), is set at 0.001. If  $\chi^2$ , defined below, does not decrease with x',  $\lambda$  is multiplied by 10, and x' is calculated again. Otherwise,  $\lambda$  is divided by 10, and the step to calculate the derived matrix (DP) is divided by DT (see section 8.2), before performing another iteration.

$$\chi^2 = \sum_i \left[ \frac{F_{obs}(x_i) - F_{calc}(x_i)}{\sigma_i} \right]^2$$

When  $\lambda$  (or XL) is greater than FLIM (default value is 1.), the fit is stopped with the diagnostic "1.Fail".

The fit procedure is considered successful when the difference between two successive calculations of  $\chi^2$  is smaller than ACC (default value is 0.01). The standard deviations of parameters are calculated from diagonal elements in the inverse of the coefficient matrix M according to the procedure proposed by Scott (1983).

## 11.6 - Absorption calculation

Neutron absorption depends on the sample shape and nature. It is described by the following triple integral:

$$A(Q, \omega) = \frac{1}{Vol} \iiint_{Vol} e^{-\mu_i T1 - \mu_f T2} dV$$

where

$\mu_i, \mu_f$  are the linear absorption coefficients  $\mu = \sum_{atoms j} \frac{\sigma_j}{v_0}$  for the initial and final

neutron energies respectively,

$v_0$  is the cell volume.

T1 is the path-length of the neutron inside the sample before the scattering process.

T2 is the path-length of the neutron inside the sample after the scattering process. (fig. 55)

$\sigma_j$  is the total cross section of atom j

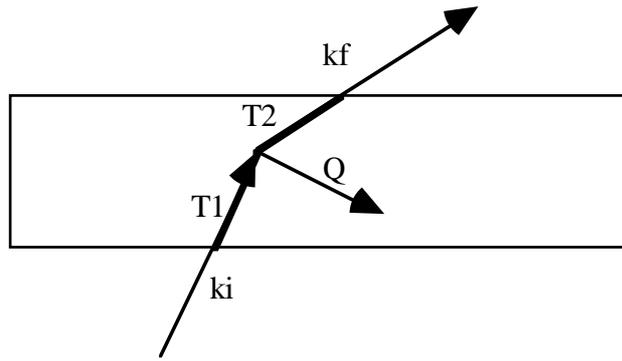


Fig. 55: Scattering geometry for absorption calculations: Slab sample

$\sigma_j$  is the sum of the scattering cross section,  $\sigma_j^d$ , and of the absorption cross section,  $\sigma_j^a$ . Except for those nucleides that have a resonance at thermal-neutron energies,  $\sigma_j^d$  is constant and  $\sigma_j^a$  is inversely proportional to  $k_0$  and, hence, to the velocity,  $v$ , of the incident neutron. The expression uses in **PkFit** is:

$$\sigma_j = \sigma_j^d + \sigma_j^a \sqrt{\frac{25.29}{E_n}} = \sigma_j^d + \sigma_j^a \frac{3.4942}{k_n}$$

where  $\sigma_j^a$  is the absorption cross section conventionally tabulated for  $v=2200$  m/s which corresponds to  $k_0=3.4942 \text{ \AA}^{-1}$  and  $E_n, k_n$  respectively the energy and the wave vector of the neutron.

### 11.6.1 - Infinite slab of thickness $e$

The approach below assumes thick enough samples and a neutron beam with an infinite section. Thus the sample volume in the neutron beam is a constant and the integral over the volume becomes a simple integral over the thickness.

In the transmission case we have:

$$A = \frac{1}{e} \int_0^e \exp\left(-\mu_i \frac{x}{\cos(\theta)} - \mu_f \frac{e-x}{\cos(\theta')}\right) dx$$

and:

$$A = \begin{cases} \exp(-\mu_i e / \cos(\theta)) & \text{if } \mu_i e / \cos(\theta) = \mu_f e / \cos(\theta') \\ \frac{\exp(-\mu_f e / \cos(\theta')) - \exp(-\mu_i e / \cos(\theta))}{\mu_i e / \cos(\theta) - \mu_f e / \cos(\theta')} & \text{otherwise} \end{cases}$$

In the reflection case we have:

$$A = \frac{1}{e} \int_0^e \exp\left(-\mu_i \frac{x}{\cos(\theta)} - \mu_f \frac{x}{\cos(\theta')}\right) dx$$

and:

$$A = \frac{1 - \exp(-\mu_f e / \cos(\theta') - \mu_i e / \cos(\theta))}{\mu_i e / \cos(\theta) + \mu_f e / \cos(\theta')}$$

### 11.6.2 - Finite slab of thickness e and width L

In this case the absorption calculation is fastidious and will not be described here. However it has been done analytically, so that the cost of CPU is negligible even in a computer without floating point unit (coprocessor). The basic integral expression is:

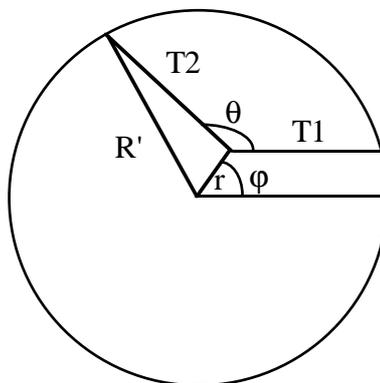
$$A = \frac{1}{L e} \int_0^e dx \int_0^L dy \exp(-\mu_i T1 - \mu_f T2)$$

### 11.6.3 - Cylinder of thickness e and radius R with axis in the scattering planes

Here an integration along the vertical axis, z, has to be performed. This is done numerically by replacing L by :  $2 \sqrt{R^2 - z^2}$ , and by integrating z from -R to R.

### 11.6.4 - Sphere of radius R

In this case, the integration is made numerically in the three directions of space. This is time-consuming and it is thus advisable to use a computer equipped with a floating point unit.



*Fig. 56: Scattering geometry for absorption calculation: Spherical sample*

The integral is written:

$$A(\theta) = \frac{1}{4/3 \pi R^3} 4 \int_0^R dz \int_0^{\sqrt{R^2 - z^2}} r dr \int_0^{\pi} \sin(\varphi) d\varphi e^{-\mu_i T1 - \mu_f T2}$$

with

$$T1 = \sqrt{R^2 - z^2 - r^2 \sin^2(\varphi)}$$

and

$$T2 = \sqrt{(x - r \cos(\varphi))^2 - (y - r \sin(\varphi))^2}$$

where

$$x = \frac{A \tan(\theta) + \sqrt{(R^2 - z^2)(1 + \tan^2(\theta)) - A^2}}{1 + \tan^2(\theta)}$$

and

$$y = \frac{A(1 + \tan^2(\theta)) + \sqrt{(R^2 - z^2)(1 + \tan^2(\theta)) - A^2}}{1 + \tan^2(\theta)}$$

with

$$A = r \sin(\varphi) - r \cos(\varphi) \tan(\theta)$$

### 11.6.5 - Cylinder of radius R with vertical axis

The calculations are the same as in the preceding case but without the integration over z and with z=0.

## **11.7 - Gaussian approximation**

In the general case the numerical convolution of the resolution function with the scattering function takes a lot of CPU time especially in the 4D case. However, since the resolution function is of the Gaussian type, a much faster analytic convolution is possible when the scattering function is also of Gaussian type. Therefore, whenever possible, non-Gaussian scattering functions are approximated by a sum of Gaussians. E.g. for a Lorentzian at the power p, the following expression is used:

### 11.7.1 - Approximation of a Lorentzian by a sum of Gaussians.

We used the following expression:

$$\frac{1}{1 + X^2} = \sum_{n=1}^{N_{\max}+1} b_n \exp(-\ln(2) a_n^2 X^2)$$

with

$$b_1 = \frac{1 - \beta}{1 - \beta^{N_{\max}+1}} \gamma \quad \text{and} \quad b_n = b_{n-1} * \beta \quad \text{for } n=1, N_{\max}$$

$$a_1 = \delta \quad \text{and} \quad a_n = a_{n-1} * \alpha \quad \text{for} \quad n=1, N_{\max}$$

$$b_{N_{\max}+1} = 1 - \gamma$$

$$a_{N_{\max}+1} = 1/\epsilon$$

For a better approximation at high X, and to limit the numbers of fit parameters to five ( $\alpha, \beta, \gamma, \delta$  and  $\epsilon$ ) whatever the Gaussian number may be, a dependency is introduced between the parameters of the different Gaussians [13]. The best fit in the range  $-35 < X < 35$  (or  $1/(1+X^2) > 10^{-3}$ ) is obtained for the following parameter values:

Function	$N_{\max} + 1$	$\alpha$	$\beta$	$\delta$	$\gamma$	$\epsilon$
Lorentzian (p=1)	17	0.605483	0.378768	0.759196	0.539198	0.645745
Square Lorentzian (p=2)	9	0.681772	0.244425	1.10383	0.413822	0.507653

The relative error takes a maximum of 0.046 at X equal 5.43 and its mean-square value is 0.0007.

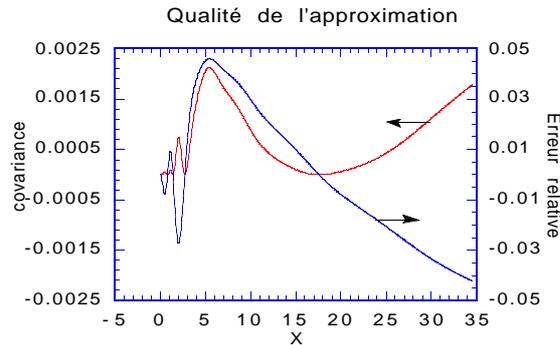


Fig. 57: Gaussian approximation quality

This approximation can also be used for a multidimensional Lorentzian by simply replacing  $X^2$  by  $X_1^2 + 2X_1X_2 + X_2^2 + \dots$  and thus the analytic integration is still easy. In the 4D case the expressions are too cumbersome to be written here, and thus only the 1D equations are given in section 11.7.2.

### 11.7.2 - One-dimensional convolution.

We calculated the convolution product of a sum of Gaussians with the resolution function which is also of the Gaussian type:

$$R_0 \int_{-\infty}^{+\infty} \sum_{n=1}^{N_{\max}+1} b_n \exp\left(-4 \ln(2) a_n^2 \frac{(x' - C_x)^2}{W_x^2}\right) \exp(-\ln(2) B_{xx} (x - x')^2) dx'$$

$$= \sqrt{\frac{\pi}{\ln(2)}} R_0 \sum_{n=1}^{N_{\max}+1} \frac{b_n}{A_x} \exp\left(-4 \ln(2) \frac{(x - C_x)^2}{W_n^2}\right)$$

with

$$A_x = \sqrt{\frac{4 a_n^2}{W_x^2} + B_{xx}} \quad \text{and} \quad W_n = \sqrt{\frac{W_x^2}{4 a_n^2} + \frac{1}{B_{xx}}}$$

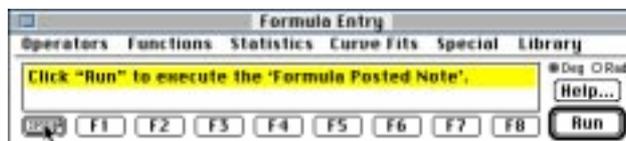
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## 12 - Reading Log Files with Kaleidagraph

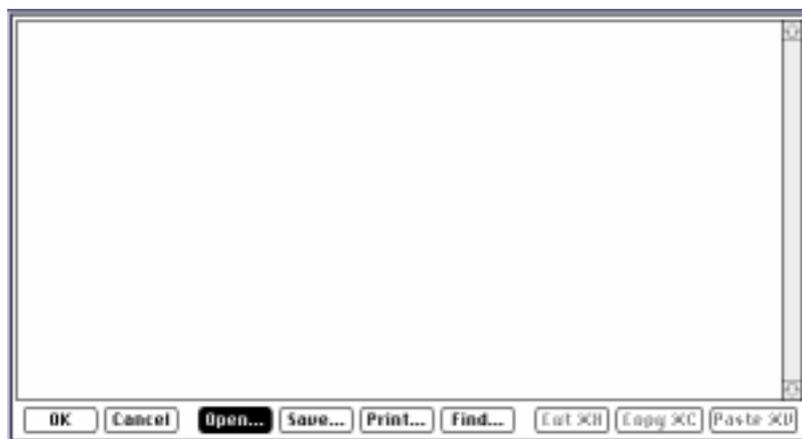
Each time PkFit creates a log file (see section 4.4), it also creates a file with extension `.KGSscript` which contains a Kaleidagraph script. Running these scripts with Kaleidagraph 3.0 or higher, automatically plots the data and the fitted curves and thus helps you producing documents with publishing quality. See an example below.

*Attention!!! Be sure that files `PkfitPlotScript.plot` and `PkfitPlotScript`, given in the TAS software package, are present in your PkFit folder otherwise the program will not be able to run the scripts.*

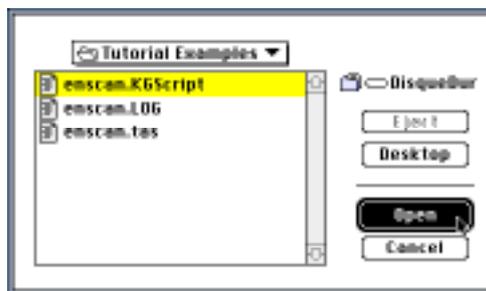
- 1 Launch Kaleidagraph.
- 2 Select the item "Formula Entry" from the menu "Windows".
- 3 Click the button "Formula Posted Note" (Bottom-left button of the window "Formula Entry").



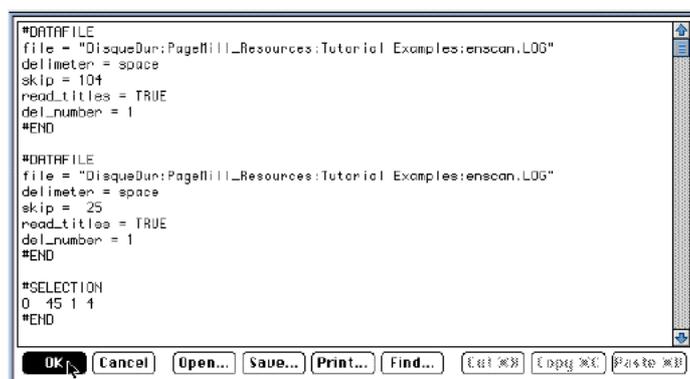
- 4 Click the button "Open" in the dialogue "Formula Posted Note". A standard open-file dialogue is shown.



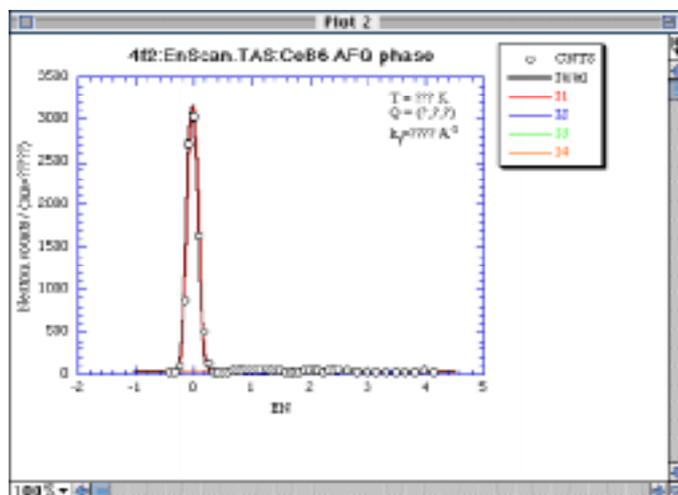
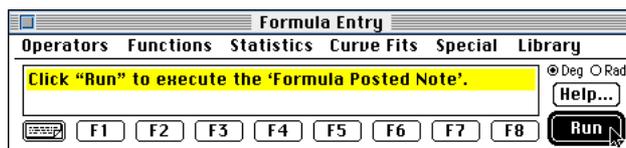
- 5 Select the file `enscan.KGScript` and click the button "Open". Then the contents of the script file is displayed in the window "Formula Posted Note".



- 6 Click the button "OK" in the dialog "Formula Posted Note".



- 7 Click the button "Run" in the window "Formula Entry". The log file `enscan.log`, saved in PkFit, is opened and copied to two data-windows. Both the observed and fitted spectrum are displayed.



Note that in the texts, the numerical values of the parameters are replaced by "?" characters. Thus the correct values must be set by hand by the user.



---

## 13 - Standalone code

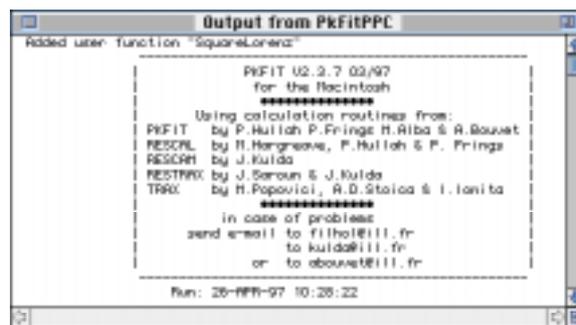
In **PkFit**, you can add your own peak-shape to the built-in list, by means of "standalone code", i.e. plug-ins files. The latter is the code of a subroutine which can be dynamically linked at runtime. Of course the arguments of the subroutine must strictly conform to what is expected by the program. The "standalone code" must be compiled with the same options and linked with the same libraries than the main program. **PkFit** also assumes that the file containing the "standalone code" is placed in the subdirectory "Plug-ins" of the application folder.

In the case of a 68K Macintosh, the standalone code must be placed in resources with type C68K which are stored in the resource fork of the plug-ins file. In the case of a PowerPC Macintosh, the standalone code is more likely stored in a PPC fragment which is placed in the data fork of the plug-ins file. The PPC version of **PkFit** can import both 68K resources and/or PPC fragments.

*Note that before using a subroutine in the form of a "standalone code" it is advisable to execute it in the usual manner from within a small test program since there is no easy way to debug a "standalone code".*

### 13.1 - Using plug-ins peak shapes

At launch time **PkFit** writes a message to the text window indicating whether or not user defined functions were found (Fig. 58).



*Fig. 58: User defined function message.*

The full name of each user defined function is appended to the popup menu in the dialogue **Non-fitting peak parameters** (Fig. 59).



*Fig. 59: User function name selection.  
Here a function named "SquareLorenz" has been added to the function list*

## 13.2 - Syntax

A user-defined peak function for PkFit:

- must take only one argument: a structure "MyStruct" declared as below.
- must have its name typed in UPPER CASE (at least for 68k resources C68K).

The FORTRAN structure containing the function parameters must be declared as follows:

```

Structure /TypeMyStruct/
  Character UserFuncName*12
  Integer   NUSE, IN(N_Max_Data)
  real      YTMP(N_Max_Data), XIN(N_Max_Data), A_BoseCorr(N_Max_Data)
  real      Hight, CENT, WID, AREA
End Structure

```

where the following are input parameters:

MyStruct.NUSE	Number of points used
MyStruct.IN	Index array of points used
MyStruct.XIN	A vector of N_Max_Data abscissa values.
MaStruct.Cent	The peak position.
MaStruct.Width	FWHM of the peak.
MaStruct.Area	Peak area.
MyStruct.A_BoseCorr	A vector of N_Max_Data Bose-factor correction with the $\omega$ -factor (see section 3.7).

where the following are output parameters:

MyStruct.UserFuncName	Name (up to 12 characters) of the user function.
MyStruct.Height	Peak height
MyStruct.YTMP	A vector of N_Max_Data values of the user function at the abscissa XIN.

PkFit uses the `MyStruct.UserFuncName` in two distinct ways:

- The full name is appended to the popup menu in the dialogue **Non-fitting peak parameters** (Fig. 59).
- The first character is used as a marker of the top of the calculated peak in the graphic window. It is thus advisable to choose a name whose first character is not yet used (i.e., avoid using the following letters: I[ncoherent], G[aussian], L[orentzian], O[scillator], B[ragg], D[elta function].).

`MyStruct.Height` must be a constant multiplied by the ratio `MyStruct.Area/MyStruct.Width`. If not, **PkFit** will compute wrong peak heights.

### 13.3 - Compiling and linking with MPW

The TAS-prog software package provides the code of a sample user-function and the make file to create the standalone code. These files are in the folder `makePlug-ins`:

- `UserFunc.f`: the FORTRAN code of a sample user function which computes a "square Lorentz" peak function.
- `PkFitUserFunc68k.make`: a make file to compile and link it as a "68k code resource" with MPW.
- `PkFitUserFuncPPC.make`: a make file to compile and link it as a "PPC code fragment" with MPW.

The standalone code of a Square-lorentzian peak shape is in the folder `Plug-ins`:

- `PkFitUserFunc68k`: a file which contains a resource C68K with ID 1001.
- `PkFitUserFuncPPC`: a file which contains a "PPC code fragment".

To create your own 68k code resource with MPW:

- 1 modify the FORTRAN code of the subroutine `USERFUNC` in the file `UserFunc.f`.
- 2 increment the ID of the resource (for example `ResID=1002`) in the make file `PkFitUserFunc68k.make`.
- 3 select the item **Set Directory...** from the menu **Directory** and select the folder `makePlug-ins` as the current directory.

- 4 select the item **Build...** from the menu **Build** (keyboard shortcut command-B) and type `PkFitUserFunc68k` in the edit text "Program name?".
- 5 The new code resource will be added to the file `PkFitUserFunc68k` in the directory `Plug-ins`.

To create your own PPC code fragment in MPW:

- 1 duplicate the FORTRAN code of the subroutine `USERFUNC` in the file `UserFunc.f`.
- 2 rename the subroutine, i.e. `USERFUNC2` and modify its contents.
- 3 duplicate the line `-export USERFUNC` in the link options of the make file `PkFitUserFuncPPC.make` and replace `USERFUNC` by the name of your subroutine (e.g. `USERFUNC2`).
- 4 select the item **Set Directory...** from the menu **Directory** and select the folder `makePlug-ins` as the current directory.
- 5 select the item **Build...** from the menu **Build** (keyboard shortcut command-B) and type `PkFitUserFuncPPC` in the edit text "Program name?".
- 6 The new PPC code fragment will be added to the file `PkFitUserFuncPPC` in the directory `Plug-ins`.

### 13.4 - Sample FORTRAN code

We give below:

- the FORTRAN code of a sample user function which computes a "square Lorentz" peak function.
- a make file to compile and link it as a code resource with MPW. If left unchanged:
  - It assumes that the FORTRAN file is in the same folder as the make file.
  - It will create in the file `::Plug-ins:PkFitUserFunc68K` a resource `C68K` with an ID of 1001, compiled for a Macintosh with a 68020 processor but with no floating point unit.
- a make file to compile and link it as a PPC fragment with MPW. If left unchanged:
  - It assumes that the FORTRAN file is in the same folder as the make file.
  - It will create in the file `::Plug-ins:PkFitUserFuncPPC` a PPC fragment with entry point `USERFUNC`.

In the make files you can redefine the MPW variables `ResID`, `FCompileOptions`, `FLinkOptions` so they match your needs.

ResID                   ID of the new code resource C68K.  
*Pkfit assumes that the ID is in the range 1001 to 1010.*

FCompileOptions   the compiler options e.g.:  
                   -mc68020 -opt=3  
                   -mc68040 -fpu -opt=3

FLinkOptions       the link options

Contents of file UserFunc.f (identical for the 68K and PPC cases).

```

Subroutine USERFUNC(MaStruct)
C-----6-----2-----0
C----- Note that the name of the subroutine MUST be given CAPITALIZED
C----- and exactly as in the options of the linker:
C-----   -m           when creating a 68k code resource
C-----   or -main and -export when creating a PPC fragment
C-----6-----2-----0
C      Implicit None
C
C      integer I,K,N_Max_Data
C      Parameter (N_Max_Data=500)
C      Real Pi
C      Parameter (Pi=3.141593)
C
C      Structure /MonTypeStruct/
C      Character UserFuncName*12
C      Integer   NUSE,IN(N_Max_Data)
C      real      YTMP(N_Max_Data),XIN(N_Max_Data),A_BoseCorr(N_Max_Data)
C      real      Hight,CENT,WID,AREA
C      End Structure
C      Record   /MonTypeStruct/ MaStruct
C
C      MaStruct.UserFuncName='SquareLorenz'
C      If (MaStruct.WID.le.0.) RETURN
C      MaStruct.Hight=MaStruct.Area/PI/MaStruct.WID*.5
C      Do I=1,MaStruct.NUse
C          K=MaStruct.IN(I)
C          MaStruct.YTMP(K)=MaStruct.A_BoseCorr(K)*MaStruct.Hight
1          / (1.+((MaStruct.XIN(K)-MaStruct.CENT)/MaStruct.WID)**2)**2
C      End Do
C
C      Return
C      END

```

Make file to create a 68K resource with type C68K.

Note that if you want to add several peak shapes to PkFit, you must create as many resources C68K as necessary but with different ID numbers. All these resources must be placed in the same plug-ins file PkFitUserFunc68k .

```
#----- Make file of the code resource -----
# File:      PkFitUserFunc68k.make
# Target:    PkFitUserFunc68k
# Sources:   PkFitUserFunc.f
# Created:   Friday, January 31, 1997 5:36:33 PM
#
#===== Part which could be modified =====
ResID      =    1001
#=====

#----- Tool names -----
Fortran     = FORTRAN
Link        = Link

#----- Plug-ins folder -----
PI          = "::Plug-ins:"
OB          = ":object:"

#----- Options de compilation et de Link -----
FCompileOptions = -mc68020 -opt=3
FLinkOptions    = -w -t '????' -c 'PkFt' -mf
Program         = PkFitUserFunc68k

#
#----- Dependances pour la compilation -----
{Program} ff {Program}.make PkFitUserFunc.f {OB}PkFitUserFunc.f.o
  {Fortran} {FCompileOptions} PkFitUserFunc.f -o {OB}
  {Link} ∅
    -sg {Program} -f -srt -ad 4 {FLinkOptions} ∅
    -rt C68K={ResID} ∅
    -m USERFUNC ∅
    {OB}PkFitUserFunc.f.o ∅
    "{Libraries}"RunTime.o ∅
    "{Libraries}"Interface.o ∅
    "{FLibraries}"FORTRANlib.o ∅
    "{FLibraries}"IntrinsicLib.o ∅
    "{FLibraries}"FSANELib.o ∅
    -o {PI}{Program}
```

Make file to create a standalone PPC fragment.

```
#----- Make file of the PPC fragment -----  
  
# File:      PkFitUserFuncPPC.make  
# Target:    PkFitUserFuncPPC  
# Sources:   PkFitUserFunc.f  
# Created:   Friday, January 31, 1997 5:36:33 PM  
  
#----- Tool names -----  
Fortran      = FORTRAN.PPC  
Link         = PPCLink  
  
#----- Plug-ins folder -----  
PI           = "::Plug-ins:"  
OB           = "::object:"  
  
#----- Options de compilation et de Link -----  
FCompileOptions = -opt=3  
FLinkOptions    = -w -t '????' -c 'PkFt' -mf  
Program         = PkFitUserFuncPPC  
  
#  
#----- Compilation and link -----  
{OB}PkFitUserFunc.f.o f {Program}.make PkFitUserFunc.f  
    {Fortran} {FCompileOptions} PkFitUserFunc.f -o {OB}  
  
{Program} ff {Program}.make {OB}PkFitUserFunc.f.o  
    {Link}  ̈  
        {FLinkOptions} ̈  
        {OB}PkFitUserFunc.f.o ̈  
        "{PPCLibraries}"PPCCRuntime.o ̈  
        "{PPCLibraries}"StdCRuntime.o ̈  
        "{SharedLibraries}"StdCLib ̈  
        "{SharedLibraries}"MathLib ̈  
        "{SharedLibraries}"InterfaceLib ̈  
        "{PPCFLibraries}"FortranLibPPC.o ̈  
        -main USERFUNC ̈  
        -export USERFUNC ̈  
        -o {PI}{Program}
```



---

## 14 - References

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12. J.M. Hammersley and D.C Handscomb, Monte Carlo methods (John Wiley & Sons, London, 1964) p 50.
13. A similar approximation has been made (see reference below) without constraints. The validity domain is narrower. It is only  $-10 < X < 10$  in the case of a Lorentzian approximated by a set of 9 independent Gaussians. W.Schmidt, D.Sieger, H.Tietze-Jaensch, R.Geick (1992) Nuclear Instr. and Methods in Phys. Res. A316, 364.
14. F.Rieutord, program INX, ILL Grenoble (France).



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## Appendix-A : Unified TAS ILL format

This is the default ILL file format since January 1995. Its main features are:

- for compatibility with "ILL Standard Formatted Data" [4], each file starts with a header which will be ignored. The first header line is a line of 80 characters "R" and the last one is a line of 80 "V".
- only lines starting with a known five character identifiers are interpreted by the program, others are ignored. A list of identifiers is given below.
- lines can be in any order but the header lines and the data lines must be contiguous and must immediately follow the data format line.
- depending on its identifier, a line contains either a character string or one or more numerical parameters. The later are generally in the following form:

*<KeyWord=><numerical value> ,*

with however some exceptions.

Note that there is no space between the keyword and the equal sign. The coma is compulsory except for the last parameter in the line.

### Line identifiers:

#### *Instrument line:*

**INSTR :** A6

#### *Experiment Number line:*

**EXPNO :** A72

#### *User Name line:*

**USER\_ :** A72

#### *Local Contact Name line:*

**LOCAL :** A72

#### *File Name line:*

**FILE\_ :** A30

*Experiment date line:*

**DATE\_:** A9 , 1X , A8

*Title line:*

**TITLE:** A72

*Scan Command line:*

**COMND:** A72 (Command = copy of keyboard input on the TAS instrument)

*Comment line:*

**COMM\_:** A72 (comment - any stuff)

*Polarization Analysis line: (only in PA mode)*

**POLAN:** A72 (concatenated version of the .PAL file)

*Q vector, Energy Value and Energy Unit line:*

**POSQE:** QH=F8.4, QK=F8.4, QL=F8.4, EN=F8.3, UN=THz

*Scan Step line:*

**STEPS:** DQH=F8.4, DQK=F8.4, DQL=F8.4, DEN=F7.3,

*Parameter lines:*

**PARAM:** <parameters from the list further in this section>

*Fixed spectrometer variable line:*

**VARIA:** <parameters from the list further in this section>

*Spectrometer Variable Zero line:*

**ZEROS:** <same order as for variables ((F7.2, ', '))>

*Data FORTRAN Format line:*

**FORMAT:** A126

*DATA line:*

**DATA\_:**

The DATA line must be followed by the *variable name line* (without an identifier) which is then followed by a set of *data value lines*.

*variable name line*

A list of 4 character long (including spaces) key words defining each variable to be read from the subsequent data-value lines. Each key word is taken as the label of the corresponding data column and is compared to the predefined table "SPEC" given below. Unknown data names are automatically added to that table.

Predefined data names for the ILL TAS format as listed in table "SPEC":

'EN'	'	energy transfer	(in meV or THz)
'QH'	','QK'	q value	(in r.l.u.)
'KI'	'	initial wave vector	(in Å <sup>-1</sup> )
'CNTS'	'DELTA'	neutron counts and errors	
'TIME'	'	counting time	(in sec.)
'M1'	','M2'	counts of monitors 1 and 2	
'F1'	','F2'	status of flipper 1 and 2	(on/off)
'TT'	'	sample temperature	(in K)

'A1	','A2	'	monochromator angles ( $\omega_M, \theta_M$ )	(in degree)
'A3	','A4	'	sample angles ( $\omega, \theta$ )	(in degree)
'A5	','A6	'	analyzer angles ( $\omega_A, \theta_A$ )	(in degree)

*data value lines*

- They contain numerical values only (except perhaps for the "OFF"/"ON" keywords associated to the flipper states).
- The values are read in the format specified in the *data format line*. If an error occurs during the read process, the line is read again but using a standard free format statement READ(LIN, \*).
- For each line the program assumes that data values are in the same number and order than key words in the *variable name line*.

PARAM keywords: (see section 3.3 and figures 2 & 3)

DM, DA,	( $d_M, d_A$ ) monochromator and analyzer d-spacing	(in $\text{\AA}^{-1}$ )
ETAM, ETAA, ETAS,	( $\eta_M, \eta_A, \eta_S$ ) monochromator, analyzer and sample mosaic	(in minutes)
SM, SA, SS,	( $S_M, S_A, S_S$ ) monochromator, analyzer and sample scattering-sense coefficients	(1 or -1)
KFIX,	value of fixed k vector	(in $\text{\AA}^{-1}$ )
FX,	1=fixed $k_i$ scan, any other value = fixed $k_f$ scan	
ALF1, ALF2, ALF3, ALF4,	( $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ ) horizontal collimations	(in minutes)
BET1, BET2, BET3, BET4,	( $\beta_1, \beta_2, \beta_3, \beta_4$ ) vertical collimations	(in minutes)
AS, BS, CS, AA, BB, CC,	( $a, b, c, \alpha, \beta, \gamma$ ) cell parameters of the sample	(in $\text{\AA}$ and degrees)
AX, AY, AZ,	coordinates of a 1 <sup>st</sup> horizontal wave vector	(in rlu)
BX, BY, BZ,	coordinates of a 2 <sup>nd</sup> horizontal wave vector	(in rlu)

VARIA keywords related to the spectrometer: (see section 3.3 and figure 2)

A1, A2, A3, A4, A5, A6,	spectrometer rotations (degree)
TM, GM, RM,	monochromator translation, goniometer and curvature
GL, GU,	sample goniometers (degree)
TA, GA, RA,	analyzer translation, goniometer and curvature
CH, IM,	magnetic field (T) and intensity (A)
I1 to I8,	Intensities

VARIA keywords related to the sample:

QH, QK, QL,	scattering wave vector (in rlu)
EN	energy transfer (meV or THz)



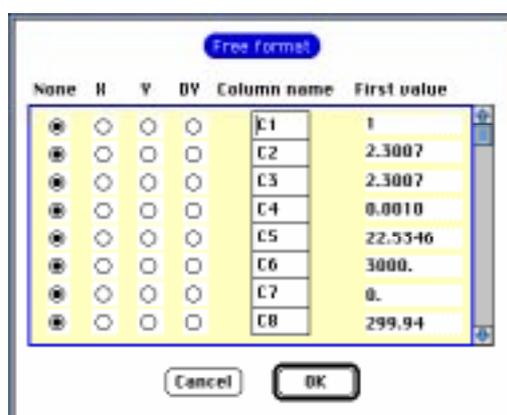
---

## Appendix-B : Free file format

### *Line of the data names*

The program looks for a data name line similar to that described in appendix-A and containing the string "CNTS" (case insensitive).

- If found, the column assignment is performed automatically. The column named "CNTS" is associated with the Y plot-axis and the X plot-axis is associated with the first monotical data-column.
- If no such line is found a dialogue (Fig. 60) is shown which makes it possible:
  - to select manually the columns X, Y (and optionally DY ) columns.
  - to change the column names.



*Fig. 60: Free format dialogue.*

### *Lines of data values*

The program assumes that data values to be read from data lines are in the same number and order than variable names in the variable name line if it exists. Data values are read in free format. The column separators accepted are one or more spaces, a tabulation, a coma, a semicolon, or a slash.

***Attention:** PkFit reads only ASCII Files. E.g. to read **Kaleidagraph** documents, save them as a text document (i.e. select the item **Tab-Delimited Text** from the item **Export** of the menu **File**);*

Example of a free format file with a data name line:

EN	CNTS	DELT	data name line
-0.931000	-0.002000000	.00810000	data lines
-0.827000	0.0040	0.00660000	
-0.620000	0.00200000	0.00890000	
....	etc.		

---

## Appendix-C : CENG file format

### *Comment lines*

Any line starting with a '\*' character is assumed to be a comment line and is ignored.

### *Title line*

The program searches for a line containing the string 'INR', 'SCR' or 'SCA'. The title of the scan is read on the next line.

### *Lines of experiment parameter names*

The program looks for any line - except the title line and the comment line - containing one or more parameter names and compares it to its internal table "HeaderPar\_Name" (case sensitive). This table is not the same as for the ILL file format.

Parameters listed in the internal table "HeaderPar\_Name":  
(See section 3.3 for their definition)

'ICON'	not used
'NPT '	number of data points in the scan <sup>17</sup>
'NLIN'	number of lines in the file
'DM ', 'DA '	( $d_M$ , $d_A$ ) monochromator and analyzer d-spacing (in Å)
'SM ', 'SA ', 'SS '	( $S_M$ , $S_A$ , $S_S$ ) scattering sense coefficients (1 or -1)
'FX '	1 = fixed $k_j$ scan, any value = fixed $k_f$ scan
'KI '	value of fixed $k_j$ vector (in Å <sup>-1</sup> )
'ALF1', 'ALF2', 'ALF3', 'ALF4'	( $\alpha_1$ , $\alpha_2$ , $\alpha_3$ , $\alpha_4$ ) horizontal collimation (in minutes)
'ETAM', 'ETAA', 'ETAE'	( $\eta_M$ , $\eta_A$ , $\eta_S$ ) monochromator, analyzer and sample mosaic (in minutes)
'AE ', 'BE ', 'CE ', 'AA ', 'BA ', 'GA '	(17, a, cell parameters of the sample (in Å and deg.))
'HO ', 'K0 ', 'L0 '	coordinates of a horizontal wave vectors (in r.l.u.)

---

<sup>17</sup> This is the nominal point number. The actual point number may be smaller if the scan has been interrupted.

'U0 ', 'V0 ', 'W0 ' coordinates of a vertical wave vectors (in r.l.u.)  
 'EI ' incident energy (in meV).  
 'MO ', 'AN ' type of monochromator and analyzer  
 G1 for graphite (1,1,1), CU for copper, ...

*Lines of experiment parameter values*

The program assumes that parameter values, to be read from the line following the parameter name line, are in the same number and order as parameter names. The format of the parameter values is predefined in the table "FormB".

Format	Parameters
(F7.3,5X)	DM, DA, KI, EI
(F4.0,5X)	SM, SS, SA, FX ALF1-ALF4, BET1-BET4, ETAM, ETAA, ETAE
(F6.3,6X)	AE, BE, CE HO, KO, LO, UO, VO, WO
(F8.3,5X)	AA, BA, GA
(4A1,8X)	MO, AN

Internal table "FormB": parameters names and formats

*Line of the data names*

The program looks for a line containing the string 'MES' and assumes it is the data name line that will be immediately followed by a line with the unit and by a series of data value lines. If no such line is found, an error message is given.

The data name line describes the contents of the subsequent data value lines. The name of each measured variable is 4 character long (including spaces) and is taken as the label of the corresponding column of values in the subsequent lines. Each data name read from the data name line is compared to a predefined table "SPEC". Unknown data names are automatically added to that table.

Predefined data names for the CENG file format as listed in table "SPEC":

'EN ' energy transfer (in meV or THz)  
 'QH ', 'QK ', 'QL ' q value (in r.l.u.)  
 'EI ', 'EF ' initial and final energies (in meV or THz)  
 'KI ' initial wave vector (in Å<sup>-1</sup>)  
 'MES ', 'DELTA' neutron counts and errors  
 'TS ' counting time (in sec.)  
 'MN ', 'M2 ' counts of monitors 1 and 2  
 'F1 ', 'F2 ' status of flipper 1 and 2 (on/off)  
 'HX ', 'HY ', 'HZ ' Helmholtz magnetic field (T)  
 'TECH', 'TK ' sample temperature (in K)  
 'RM ' sample temperature (in Ω)  
 'OE ', 'TE ' sample angles (ω, θ) (in degree)  
 'OA ', 'TA ' analyzer angles (ω, θ) (in degree)  
 'OM ', 'CMO ', 'TMO ', 'BMO ' monochromator variables

'BAN '	'CAN '	'TAN '	analyzer variables	
'BEB '	'PH '		sample holder rotation	(in degree)
'HE '			helium level	(in mm)
'CH '			magnetic field	(in T)
'IA '			amplifier intensity	(in A)
'VB '	'V1 ' to 'V8 '		voltmeter	(in V)
'MU '			azimutal angle (for spectrometer DN3)	(in degree)
'TREG'			regulation temperature	(in K)
'NP '			scan point number <sup>18</sup>	

### Lines of data values

The program assumes that data values to be read from data lines are in the same number and order as data names in the data name line. The format of the data values is predefined in the table "Form".

Format	Variables
(F7.3,1X)	EN , QH , QK , QL , EI , EF , KI TECH , TK , VB
(F9.0,1X)	MES
(F6.1,2X)	DELT
(F7.2,1X)	TS , HX , HY , HZ OE , TE , OA , TA , OM , TM , PH CMO , TMO , BMO , BEB , BAN , CAN
(1X,F6.0,1X)	HE
(1X,F6.2,1X)	CH , IA , B1 -B8
(F8.4,1X)	V1 -V8
(F8.3,1X)	MN , M2
(A4,4X)	F1 , F2

Internal table "Form": data names and formats

<sup>18</sup> This is the nominal point number. The actual point number may be smaller if the scan has been interrupted.

## Example of file contents

```

****HELIUM010190.RES      4-NOV-91  15:53:50  DNI
$ DIFTES>
**SCR

HE4 T=1.38K SVP

**** Fichier resultat :   HELIUM010190.RES      4-NOV-91  15:53:51

   MO      DM (Ang)      EI (meV)      KI (A-1)      AN      DA (Ang)
   G1      3.355         14.306         2.627         G1      3.355
AE (Ang)  BE (Ang)      CE (Ang)      AA (Deg)      BA (Deg)  GA (Deg)
 18.      6.283         6.283         90.000        90.000   90.000
  H0      K0           L0           U0           V0       W0
 19.      0.000         0.000         0.000         0.000   1.000
ALF1(')  ALF2(')      ALF3(')      ALF4(')      BET1(')  BET2(')
 110.     20.          30.          30.          90.      90.
BET3(')  BET4(')
 111.     90.
ETAM(')  ETAE(')      ETAA(')
 112.     10.          36.

**** variables non mesurees
BMO (Deg) CMO (Deg)  TMO (V)      TM (Deg)      OM (Deg)      OE (Deg)      PH (Deg)      BEB (Deg)      BEH (Deg)      BAN (Deg)
 113.     4.99        9.82        20.88        20.88        5.29         0.00         0.00         1.07         163.50
CAN (Deg) TAN (V)   IA (A)       CH (kOe)
 114.     2.10        0.00        0.00

NP      MES      QH      QK      QL      EN      TE      TA      RM      TK      KF      MN      M2      TS
      (cps)    (rlu)  (rlu)  (rlu)  (meV)  (Deg)  (Deg)  (Ohm)  (K)    (A-1)  (kc)   (kc)   (s)
 115.   6.      1.930  0.000  0.000  -1.000 -21.13  20.16  32581.  1.322  2.718  228.000  0.000  285.85
 116.   5.      1.930  0.000  0.000  -0.900 -21.18  20.22  32546.  1.323  2.709  228.000  0.000  288.37
 117.   5.      1.930  0.000  0.000  -0.800 -21.22  20.29  32496.  1.323  2.700  228.000  0.000  288.76
 118.   7.      1.930  0.000  0.000  -0.700 -21.27  20.37  32413.  1.324  2.691  228.000  0.000  288.60
 119.  10.      1.930  0.000  0.000  -0.600 -21.31  20.43  32510.  1.323  2.682  228.000  0.000  288.57
 120.  13.      1.930  0.000  0.000  -0.500 -21.35  20.51  32494.  1.323  2.673  228.000  0.000  288.46
 121.  35.      1.930  0.000  0.000  -0.400 -21.40  20.58  32356.  1.325  2.664  228.000  0.000  288.94
 122.  66.      1.930  0.000  0.000  -0.300 -21.43  20.65  32317.  1.325  2.655  228.000  0.000  288.79
 123.  93.      1.930  0.000  0.000  -0.200 -21.47  20.72  32398.  1.324  2.646  228.000  0.000  288.28
 124. 151.     1.930  0.000  0.000  -0.100 -21.51  20.81  32337.  1.325  2.636  228.000  0.000  288.74
 125. 148.     1.930  0.000  0.000  0.000  -21.55  20.88  32320.  1.325  2.627  228.000  0.000  288.61
 126. 137.     1.930  0.000  0.000  0.100  -21.58  20.96  32202.  1.327  2.618  228.000  0.000  288.72
 127. 118.     1.930  0.000  0.000  0.200  -21.63  21.03  32280.  1.326  2.609  228.000  0.000  288.89
 128. 150.     1.930  0.000  0.000  0.300  -21.67  21.11  32265.  1.326  2.600  228.000  0.000  288.59
 129. 269.     1.930  0.000  0.000  0.400  -21.71  21.19  32170.  1.327  2.590  228.000  0.000  288.08
 130. 334.     1.930  0.000  0.000  0.500  -21.75  21.27  32173.  1.327  2.581  228.000  0.000  288.60
 131. 546.     1.930  0.000  0.000  0.600  -21.79  21.35  32101.  1.328  2.572  228.000  0.000  288.69
 132. 719.     1.930  0.000  0.000  0.700  -21.83  21.43  32174.  1.327  2.562  228.000  0.000  288.94
 133. 801.     1.930  0.000  0.000  0.800  -21.86  21.52  32072.  1.328  2.553  228.000  0.000  288.40
 134. 816.     1.930  0.000  0.000  0.900  -21.90  21.60  32159.  1.327  2.543  228.000  0.000  288.17

**** ATTENTION : pendant operation sur les echelles
**** ATTENTION : suspension comptage

**** ATTENTION : pendant operation sur les echelles
**** ATTENTION : reprise comptage
 135. 609.     1.930  0.000  0.000  1.000  -21.93  21.69  32088.  1.328  2.534  228.000  0.000  288.59
 136. 636.     1.930  0.000  0.000  1.100  -21.97  21.76  32044.  1.328  2.524  228.000  0.000  288.25
 137. 494.     1.930  0.000  0.000  1.200  -22.01  21.86  32078.  1.328  2.515  228.000  0.000  288.30
 138. 430.     1.930  0.000  0.000  1.300  -22.06  21.95  32075.  1.328  2.505  228.000  0.000  288.62
 139. 336.     1.930  0.000  0.000  1.400  -22.08  22.04  31995.  1.329  2.495  228.000  0.000  288.35
 140. 212.     1.930  0.000  0.000  1.500  -22.12  22.13  31994.  1.329  2.486  228.000  0.000  288.33
 141. 165.     1.930  0.000  0.000  1.600  -22.17  22.21  32054.  1.328  2.476  228.000  0.000  288.50
 142. 122.     1.930  0.000  0.000  1.700  -22.19  22.31  32036.  1.328  2.466  228.000  0.000  288.04
 143.  69.     1.930  0.000  0.000  1.800  -22.23  22.41  31981.  1.329  2.456  228.000  0.000  288.10
 144.  54.     1.930  0.000  0.000  1.900  -22.27  22.50  31869.  1.330  2.447  228.000  0.000  288.24
 145.  83.     1.930  0.000  0.000  2.000  -22.31  22.59  31946.  1.329  2.437  228.000  0.000  288.36

IMAX =      816.000  IN = 0.764E+04

      PAS      QH      QK      QL      EN
WT (largeur) :      7.95  0.000  0.000  0.000  0.795
MAX (maximum) :     19.90  1.930  0.000  0.000  0.890
ECART (a la valeur theorique):  3.90  0.000  0.000  0.000  0.390

```

---

## Appendix-D : Old ILL formats

The three old ILL formats (Spectra, TAS, Filing), while different, follow common rules. The strategy used by **PkFit** to interpret those three kind of files is described below.

### *Comment lines*

Any line starting with a '!' character is assumed to be a comment line and is ignored.

### *Title line*

**PkFit** performs a three step search for the Title line:

- 1 - search for a line beginning with string 'IN' (TAS or Spectra file)
- 2 - search for a line containing the string 'HEADING' (Filing File). If such a line is found, the title of the scan is read on the next line.
- 3 - if steps 1 and 2 fail, the second line of the file is assumed to be the title line.

### *Lines of experiment parameters*

Any line - except the title line - containing one or more '=' characters is taken as a parameter line. Each '=' is assumed to be preceded by a parameter name (4 character long) and followed by the corresponding parameter value (free format over 8 characters). The program reads each parameter name and compares it to its internal table "HeaderPar\_Name" (case sensitive). If the parameter name is found in the list, the program assigns the input value to that parameter, otherwise the given parameter is ignored.

If several parameters are given on a same line, they must be separated from each other by one or more spaces, by a coma, a semicolon, or a slash.

Parameters listed in the internal table "HeaderPar\_Name":  
(See section 3.1 for their definition)

'ICON'	not used
'NPT '	number of data points in the scan <sup>19</sup>
'NLIN'	number of lines in the file
'DM ','DA '	( $d_M, d_A$ ) monochromator and analyzer d-spacing (in Å)
'SM ','SS ','SA '	( $S_M, S_A, S_S$ ) scattering-sense coefficients (1 or -1)
'FX '	1 = fixed $k_i$ scan, any value = fixed $k_f$ scan
'KFIX'	value of fixed k vector (in Å <sup>-1</sup> )
'ALF1','ALF2','ALF3','ALF4'	( $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ ) horizontal collimation (in minutes)
'ETAM','ETAA','ETAS'	( $\eta_M, \eta_A, \eta_S$ ) monochromator, analyzer and sample mosaic (in minutes)
'AS ','BS ','CS ','AA ','BB ','CC '	3.1. cell parameters of the sample (in Å and deg.)
'AX ','AY ','AZ ','BX ','BY ','BZ '	coordinates of 2 horizontal wave vectors (in r.l.u.).

#### Line of the data names

The program looks for a line containing the string 'CNTS' and assumes it is the data name line that is immediately followed by a series of data value lines. If no such line is found, an error message is given.

The data name line describes the contents of the subsequent data value lines. The name of each measured variable is 4 character long (including spaces) and is taken as the label of the corresponding column of values in the subsequent lines.

Each variable name read from the data name line is compared to a predefined table "SPEC". Unknown variables are automatically added to that table.

Predefined variable names listed in table "SPEC":

'EN '	energy Transfer (in meV or THz)
'QH ','QK ','QL '	q value. (in r.l.u.)
'EI ','EF '	initial and final energies (in meV or THz)
'KI '	initial wave vector (in Å <sup>-1</sup> )
'CNTS','DELT'	neutron counts and errors
'TIME'	counting time (in sec.)
'M1 ','M2 '	monitor counts
'F1 ','F2 '	status of flippers 1 and 2 (on/off)
'HX ','HY ','HZ '	Helmholtz magnetic field (T)
'T '	temperature (in K)
'A2 ','A3 ','A4 ','A5 ','A6 '	spectrometer angles (in degrees)

<sup>19</sup> This is the nominal point number. The actual point number may be smaller if the scan has been interrupted.

## Lines of data values

The program assumes that variable values to be read from data lines are in the same number and order as variable names in the data name line. The numerical field width is assumed to be 8 character long.

## Example of a Spectra file (old ILL format):

```

IN8 009531AUFK KAT 11-FEB-88 04:27:51A001200000 line with keyword "IN"
11-FEB-88 04:27:51 AUFK KAT HKLE 1.00 1.00 0.00 0.00 0.015 0.015 0.000 0.200 30.00 title line
ICONT= 0; NPT= 75; NLINE= 75 experiment parameter lines
3.2. 3.35500; DA= 3.35700; SM= 1.; SS=-1.; SA= 1.; FX= 2.; KFIX= 2.66167
ALF1= 40;ALF2= 40;ALF3= 40;ALF4= 40;BET1= 120;BET2= 120;BET3= 120;BET4= 120;ETAM= 35.; ETAA= 35.
AS= 4.05500; BS= 4.05500; CS= 4.05500; AA= 90.00000; BB= 90.00000; CC= 90.00000; ETAS= 10.
AX= 1.000; AY= 1.000; AZ= 0.000; BX= 0.000; BY= 0.000; BZ= 1.000
!POS 20.60 41.18 23.01 -2.00 20.58 41.17 96.49 90.00 -0.54 1.36 -0.01 0.00 4.35 4.70 14.69
comment
!Z** 0.73 -0.01-202.18-179.62 -91.71-181.00 -86.45 -45.51 -4.99 0.00 -5.00 -5.00 0.00 0.00 0.00
MN= 0.20000E+03

PNT EN(MEV) A3 A4 KI T M1 M2 TIME CNTS data name line
3.3. -7.394 23.01 -2.00 1.875 90.44 200 9862 145.39 268 data value lines
3.4. -7.193 23.01 -2.00 1.901 93.37 200 1760 142.83 576
3.5. -6.993 23.01 -2.00 1.926 95.46 200 1728 138.34 196
3.6. -6.798 23.01 -2.00 1.950 96.85 200 1717 136.55 219
3.7. -6.605 23.01 -2.00 1.975 97.75 200 1375 134.28 322
.....
3.8. 6.987 23.01 -2.00 3.234 100.00 200 1433 61.49 198
3.9. 7.188 23.01 -2.00 3.249 100.00 200 1461 61.53 159
3.10. 7.386 23.01 -2.00 3.263 100.00 200 1492 61.16 180

```

## Example of a Filing file (old ILL format):

```

?SV4335.SCN?12-MAR-91 YBACUO x=6.92 40-40-40
created on: 15-MAR-9 at 10:23:09
Scaling by:M1 scan-variable was:EN
SV4335.SCN* 1.000
SV4337.SCN* 1.000
SV4338.SCN* 1.000
SV4336.SCN* 1.000
HEADING OF FIRST FILE: keyword "HEADING"
12-MAR-91 YBACUO x=6.92 40-40-40 title line
3.11. 1.27800; DA= 1.67850; SM= 1.; SS=-1.; SA=-1.; FX= 2.; KFIX= 6.50007
ALF1= 50;ALF2= 40;ALF3= 40;ALF4= 40;BET1= 120;BET2= 120;BET3= 120;BET4= 120;ETAM= 25.; ETAA= 35.
AS= 3.84200; BS= 3.84200; CS= 11.70000; AA= 90.00000; BB= 90.00000; CC= 90.00000; ETAS= 25.
AX= 0.000; AY= 0.000; AZ= -1.000; BX= 1.000; BY= 1.000; BZ= 0.000
!POS 21.71 43.40 -48.68 -12.51 -16.73 -33.47 89.27 269.95 -0.56 1.41 0.15 -0.05 5.60 5.00 91.58
!Z** 1.39 0.02-363.48-179.32-271.71-181.07 -89.86 -45.00 -4.99 -5.43 -5.00 -5.00 0.00 0.00 0.00
MN= 0.10000E+04

EN CNTS DELT M1 QH QK QL KI TIME M2 T A2 A3 A4
3.12. 2091 45.7 3000 0.50075 0.50075 1.59775 6.50200 1534.9 312 2.08750 44.4300 -42.980 -12.7
3.13. 1435 37.9 3000 0.50000 0.50000 1.59800 6.57500 1688.4 325 2.08750 43.9100 -45.850 -12.6
3.14. 222 14.9 1000 0.50000 0.50000 1.59700 6.64800 545.6 90 2.09000 43.4000 -48.690 -12.5
3.15. 262 16.2 3000 0.50175 0.50175 1.59525 6.72350 1636.6 357 2.08750 42.8925 -51.490 -12.4
3.16. 117 10.8 3000 0.50025 0.50025 1.59925 6.79200 1767.4 343 2.08750 42.4400 -54.280 -12.2
3.17. 111 10.5 3000 0.50025 0.50025 1.59825 6.86300 1836.6 344 2.08750 41.9800 -57.050 -12.0
.....
3.18. 303 17.4 4000 0.50050 0.50050 1.59900 7.72300 3766.1 834 2.08375 37.1200 -97.570 -6.2
3.19. 316 17.8 4000 0.50100 0.50100 1.60025 7.78600 4083.8 1052 2.08375 36.8100 -102.15 -5.3
3.20. 381 19.5 4000 0.49900 0.49900 1.59900 7.84300 4426.1 6733 2.08375 36.5300 -107.66 -4.1

```



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## Appendix-E : The resolution parameters

The resolution parameters used in the dialogue **Set resol. param.** (see section 10.2) are described below:

DM, DA,	( $d_M, d_A$ ) monochromator and analyzer d-spacing (in $\text{\AA}^{-1}$ )
ETAM, ETAA, ETAS,	( $\eta_M, \eta_A, \eta_S$ ) monochromator, analyzer and sample mosaic spread (Half Width) (in minutes)
SM, SA, SS,	( $S_M, S_A, S_S$ ) monochromator, analyzer and sample scattering sense coefficients (1 or -1)
KFIX,	value of fixed k vector (in $\text{\AA}^{-1}$ )
FX,	1=fixed $k_i$ scan, any other value = fixed $k_f$ scan
ALF1, ALF2, ALF3, ALF4,	( $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ ) horizontal collimations (in minutes)
BET1, BET2, BET3, BET4,	( $\beta_1, \beta_2, \beta_3, \beta_4$ ) vertical collimations (in minutes)
AS, BS, CS, AA, BB, CC,	( $a, b, c, \alpha, \beta, \gamma$ ) cell parameters of the sample (in $\text{\AA}$ and degrees)
AX, AY, AZ,	coordinates of a 1 <sup>st</sup> horizontal wave vector (in rlu)
BX, BY, BZ,	coordinates of a 2 <sup>nd</sup> horizontal wave vector (in rlu)
QH, QK, QL, EN,	point at which the resolution is calculated (in rlu and meV or THz)
DH, DK, DL, DE,	scan steps (in rlu and meV or THz)
QH0, QK0, QL0, EN0,	a point of the scan (in rlu and meV or THz)
TAUH, TAUk, TAUL	( $\tau_h, \tau_k, \tau_l$ ) position of the nearest zone center (in rlu)

The focusing parameters used in the dialogue **Set focusing param.** (see section 10.2) are described below:

ROMH, ROAH,	monochromator and analyzer horizontal curvatures (in $\text{m}^{-1}$ )
ROMV, ROMA,	monochromator and analyzer vertical curvatures (in $\text{m}^{-1}$ )
SDI,	Sample diameter (in cm)
SHI,	Sample height (in cm)



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