



Technical Report
RAL-TR-96-077

The Correction of Time-of-Flight Neutron Scattering Spectra for Time-Independent Backgrounds

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October 1996

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ISSN 1358-6254

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The Correction of Time-of-Flight Neutron Scattering Spectra for Time-Independent Backgrounds

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Abstract

A description is given of data analysis software for calculating an empirical correction to time-of-flight neutron spectra for time-independent backgrounds. The programs have been written for analysing data from the Liquids and Amorphous Diffractometer LAD using the ATLAS suite, but are easily capable of modification for use with other instruments or other data analysis methods.

1. Introduction

Time-of-flight neutron scattering spectra often suffer from a background component which is independent of time, but cannot be successfully removed by the subtraction of measured background spectra. The purpose of the software described here is to enable such backgrounds to be removed from neutron spectra by means of a semi-empirical fitting method, using the known time-dependence of the flux from a moderator at long times-of-flight.

Time-independent backgrounds, which will be referred to as 'flat' backgrounds throughout this report since they contribute a constant to a time-of-flight spectrum, have several likely origins:

1. *Electronic noise in the detector system.* This effect is expected to be much larger for scintillator detectors than for gas detectors. For the LAD diffractometer [1] there are lithium glass scintillator detectors at scattering angles of 20°, 35°, 60° and 90°, whilst there are gas detectors at angles of 5°, 10° and 145°.

2. *Sensitivity of detectors to gamma rays from the sample.* Experience on LAD suggests that some samples become activated by the incident beam such that they 'shine' with delayed gamma rays. It appears that the half-life of the activity is long compared to the length of a time-of-flight frame (20,000 µseconds), but sufficiently short that

the activity may not be detected by the time the sample is removed from the beam. Thus, on the time-scale of a time-of-flight frame this contribution to the background is approximately flat. The gamma shine appears to be particularly severe for silver-containing samples. There is also expected to be appreciable gamma shine for vanadium and it is particularly important to correct vanadium data for this effect due to its use in normalising experimental data. The sensitivity to gamma radiation is expected to be very much larger for scintillator detectors than for gas detectors.

3. *Delayed neutrons from the neutron-producing target.* This effect only happens when the target is fissile (i.e. uranium), but not when the target is non-fissile (i.e. tantalum). The effect is due to nuclei in the target undergoing fission at some delayed time after the proton beam has struck the neutron-producing target. The delayed neutrons are moderated and then scattered by the sample as are the prompt neutrons. However, since the half-lives for the fissions may be long compared to the length of a time-of-flight frame, this contribution to the neutron signal is flat.

Effects 2 and 3 are both sample-dependent. Hence they are not successfully removed from the spectra measured for the sample by subtracting background spectra measured with the sample removed. This is the reason why a semi-empirical fitting approach has been adopted here for removing flat backgrounds from neutron scattering data.

2. The Principle of the Method

For a pulsed neutron source the flux distribution of a beam at long times-of-flight t (such that neutron energy is significantly less than kT where T is the temperature of the moderator) the Maxwellian distribution may be used to show that the number of neutrons per unit time is proportional to t^{-4} ;

$$y = Bt^{-4} \quad (1)$$

or $\log y = -4 \log t + B'$,

where B and B' are constants. With the flat background contribution included this becomes;

$$y = Bt^{-4} + C, \quad (2)$$

where C is the flat background constant. Figure 1 shows log-log plots of spectra for the incident beam monitor and a scintillator detector at a

scattering angle of 35° on LAD. For the monitor spectrum there does not seem to be a significant flat background contribution, and at long times the log-log plot is linear. However, for the scintillator detector the log-log plot starts to become linear towards longer times-of-flight, but then at the long time end of the spectrum it flattens off to a constant due to the flat background contribution.

It is possible to obtain a flat background constant for each spectrum by using a trial-and-error method where the constant is adjusted to make the log-log plot linear up to the longest time-of-flight. However, this is an extremely laborious process for the large number of spectra involved, and for this reason the automated method discussed here may be preferred. The software described in this report is designed to fit eqn. (2) to time-of-flight spectra in order to yield the flat background constants C which can then be subtracted from the experimental data.

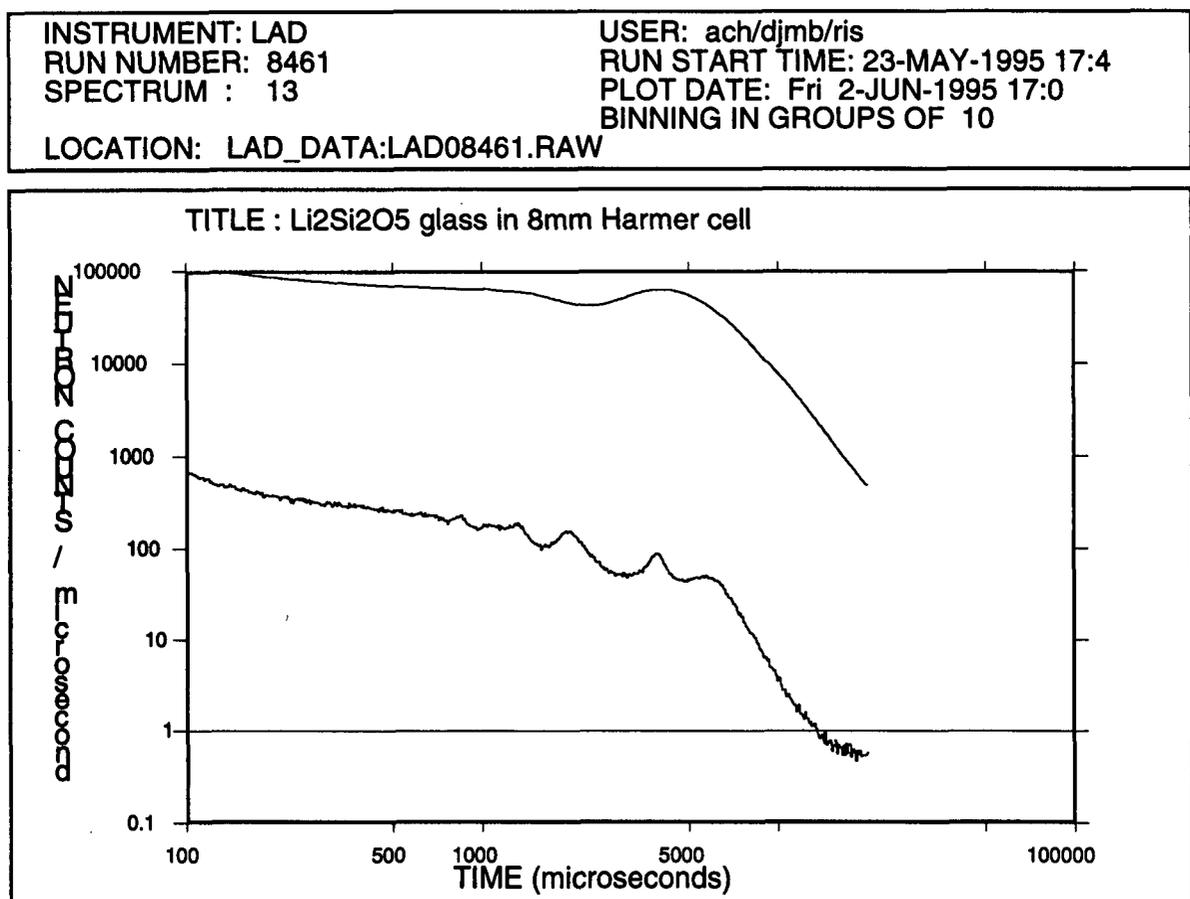


Figure 1. A log-log plot of the LAD time-of-flight spectra for the incident beam monitor (upper curve) and for a scintillator detector at 35° (lower curve) with a lithium disilicate glass sample.

3. How to Use the Software

There are two methods by which it may be judged whether it is necessary to perform a flat background correction of time-of-flight neutron scattering data:

1. either by performing log-log plots like that shown in figure 1 (the GENIE [2] commands TOGGLE LOGX and TOGGLE LOGY should be used) and inspecting whether the spectrum remains linear at long times,

2. or by plotting the data on a Q -scale, as is shown in figure 2, and looking for a turn-up at low Q (such a turn-up is a symptom of a flat background since Q is inversely proportional to time-of-flight).

When analysing experimental data using the ATLAS suite [3,4] there are two stages involved in the subtraction of a flat background:

1. *Produce a .BCK file.* The recommended way to create a .BCK file is to use the ATLAS batch menu (the user should type A_B to run this) and select the flat background option (10). This will run a program which fits eqn. (2) to the spectra for all the LAD detectors, except the monitors. The results are placed in an ASCII file named LAD01234.BCK for example. The first line of the file is used for comments. Otherwise the first entry on each line is the spectrum number, whilst the second and third entries are the flat background constant C for that spectrum and its error σ_C from the fit. The program produces both a preliminary version of the .BCK file and a final version (see below for further details). The fitting can be done in two different ways:

A. The data for each run are fitted entirely separately.

B. The data for several runs may be added together and then fitted. In this case a suitable output .BCK file is still produced for every run number.

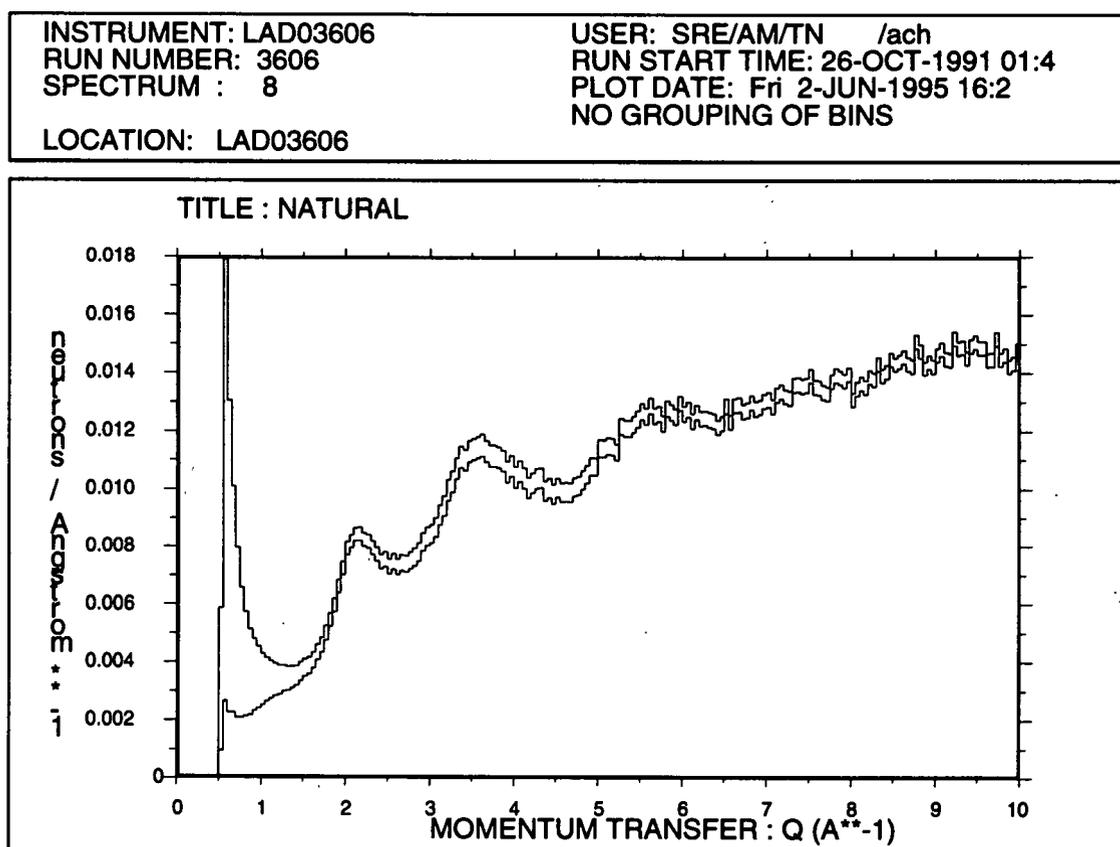


Figure 2. This shows the result of NORM for 35° LAD data for a sample containing natural silver, both with (lower curve) and without (upper curve) a flat background correction.

Method *B* should only be used where all the runs involved are on the same sample and where there is no reason to expect any change in flat background level from one run to another. It has the advantages of being quicker and of having greater statistical accuracy.

2. Use *NORM* to subtract the *.BCK* file from the data. Once the *.BCK* file has been created for a sequence of runs the flat background may be subtracted from the data when running the *NORM* program of the *ATLAS* suite [2,3]. If *NORM* is run from the *ATLAS* batch menu then this is done by selecting the appropriate option. If *NORM* is run interactively then the command *DELAY* (which is not described in the *ATLAS* manual [3]) should be issued before issuing the *RUN* command.

Figure 2 shows an example of the output of the *NORM* program with and without a flat background correction. The small peak at a momentum transfer $\sim 1.15\text{\AA}^{-1}$, which is only apparent for the

spectrum which has been corrected for flat background, is found to be a genuine peak since it can be observed clearly in spectra from lower angle detectors.

4. Further information on the Software

The software for creating a *.BCK* file may be run interactively by use of the command `@g_f:MAKE_BCK` in *GENIE*. It is then possible to select an option where the fitted curve for each spectrum is written to a *GENIE* intermediate file `SYS$SCRATCH:LAD01234.FLAT`. This file can then be used to assess the quality of the fit.

The contents of a *.BCK* file can be loaded into a *GENIE* workspace for graphical display by use of the command `@g_f:BCK_L`. Figure 3 shows the *.BCK* file created for the data shown in figure 2, together with the flat background constants obtained for the same spectra by the trial-and-error method described in section 2.

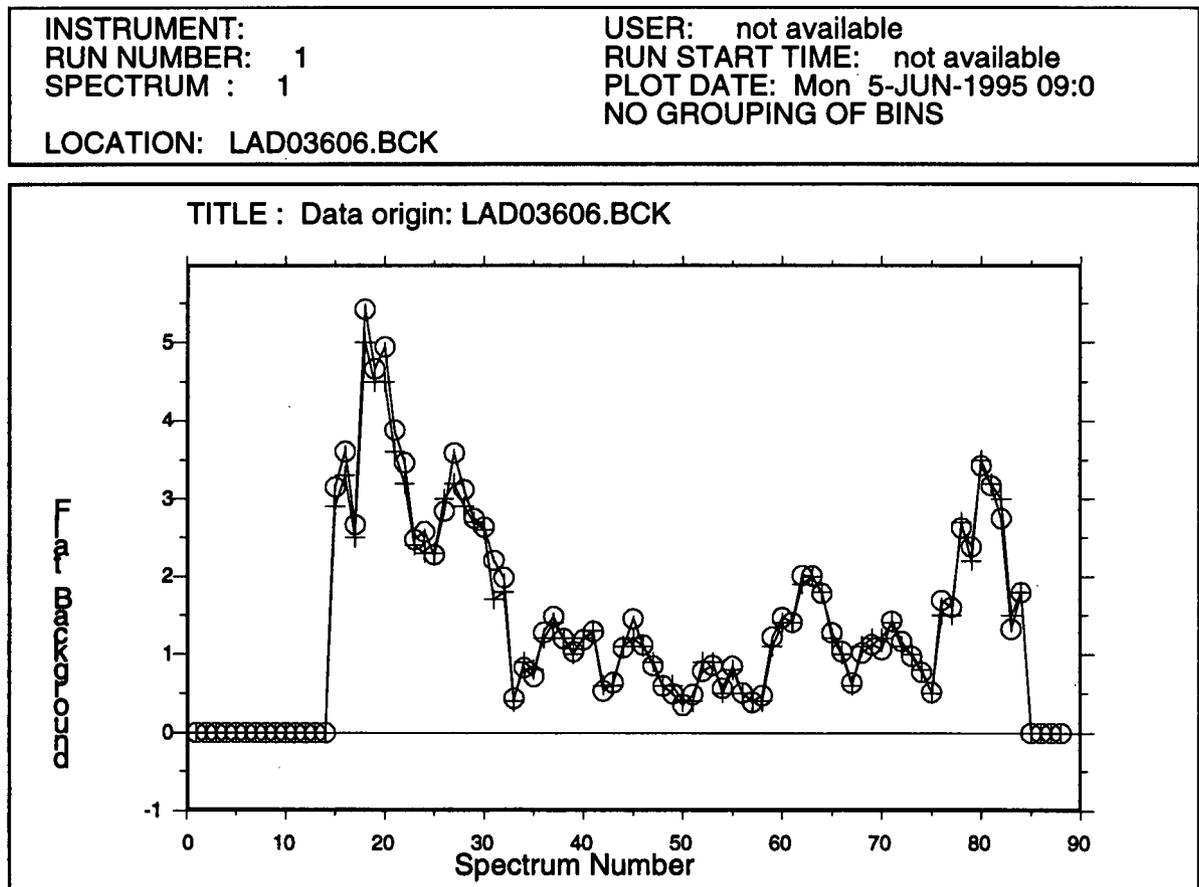


Figure 3. The *.BCK* file created for the data shown in figure 2 (circles), compared with the flat background constants obtained by the trial-and-error method described in section 2 (crosses).

The software produces a preliminary version of the .BCK file, which then undergoes a checking procedure to produce a final version. In the checking procedure any missing spectra (monitors and failed fits) are assigned flat background constants C of zero. Any negative constants from the fit are replaced with a value of zero. Finally constants C which are less than $f\sigma_C$ are replaced by zero. Here σ_C is the standard deviation on the value of C from the fit and f is a tolerance factor which has a default value of 3.0. It is possible to perform the checking procedure with a different value of f by using the program BCK_L to load the preliminary .BCK file into a GENIE workspace Wn, setting the tolerance factor f by typing v19=2.7 say, and then using the command TR Wn g_f:CHECK_BCK Wm.

5. Conclusions

A description has been given of data analysis software for calculating an empirical correction to time-of-flight neutron spectra for time-independent backgrounds. The programs have been written for analysing data from the Liquids and Amorphous Diffractometer LAD using the ATLAS suite, but are easily capable of modification for use with other instruments or other data analysis methods.

References

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