HFBS Data Reduction

§ 1 Introduction

This document describes the data reduction operations for data collected on the HFBS instrument available to users of the DAVE software package. The main interface for the data reduction application is shown in figure 1. This particular screen shot was taken on a WINDOWS PC but it should look similar on the other supported platforms.

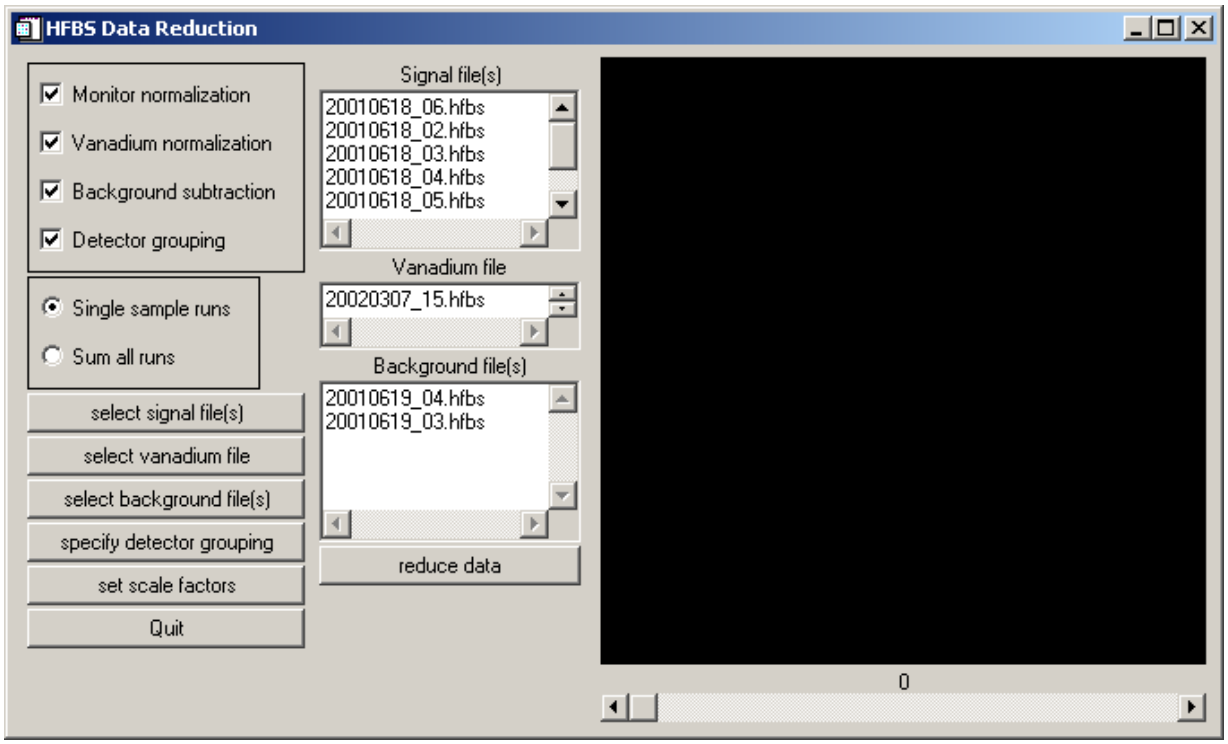

Figure 1 Screen shot from the HFBS data reduction application.

As can be seen in fig. 1, the data reduction interface is a configurable entity allowing one to repeat the same data reduction steps for a large number of data files simultaneously or in sequence.

The data reduction steps are listed below. Those steps always carried out are underlined and all other steps are optional. Those steps requiring further explanation are followed by a section number indicating the section in this document where this procedure is described.

- Read in raw .HFBS file(s)
- Convert from cam bins (channels) to energy channels
- Normalize to p(E) (2)
- Subtract background files (summing them if more than one is present)

- Normalize spectrum to beam monitor (3)
- Normalize spectrum to a vanadium run (4)
- Group detectors
- Write out reduced data to a .DAVE file

§ 2 Normalization to p(E)

The velocity profile of the Doppler monochromator is a function of time. Since the energy transfer to the sample is related to the velocity of the monochromator v_m,

$$E = 2E_o\left(\frac{v_m}{v_o}\right) + E_o\left(\frac{v_m}{v_o}\right)^2,$$

and the velocity of the monochromator varies with time, the amount of time the monochromator spends at each energy varies. In the expression above E_o and v_o are the Bragg energy and velocity respectively. This information is encapsulated in a quantity referred to as p(E), the probability density describing the amount of time the monochromator samples energy transfer E. For a sinusoidal energy profile p(E) is bowl-shaped and is given by the expression,

$$p(E) = \frac{1}{\pi\sqrt{E_o^2 - E_m^2}}.$$

For the last few years the velocity profile of the monochromator is given by a rounded triangle function. This provides a more uniform p(E) than a sinusoid. The spectra observed in each detector are modulated by this function. Therefore this reduction procedure involves simply dividing the data in each detector by this quantity. This quantity is contained in the raw data file and is used in this step.

§ 3 Normalization to beam monitor

After the data have been converted from cam bin to energy and normalized to p(E), the data are normalized to the incident beam monitor, a.k.a. the fission chamber. Since (i) the neutron spectrum from the phase space transformation chopper is not uniform, (ii) there are varying apparent levels of background in each detector, and (iii) there is a significant loss on the neutron energy loss side of the spectrum, this normalization procedure is not straightforward (i.e. simple division of the signal by the monitor is not applicable). The procedure implemented in the HFBS data reduction program is described below.

The monitor spectrum is given by M(E) and the spectra in each detector are given by $I_D(E)$ where D denotes the detector and E is the energy transfer. One main assumption is that there is an energy-independent background B_D in each detector D. Thus the signal in each detector $I_D(E)$ is related to the desired normalized signal $I_{NORM,D}(E)$ through the following relationship:

$$I_{NORM,D}(E) = (I_D(E)-B_D)/M(E).$$

The problem is to find an "appropriate" value of B_D.

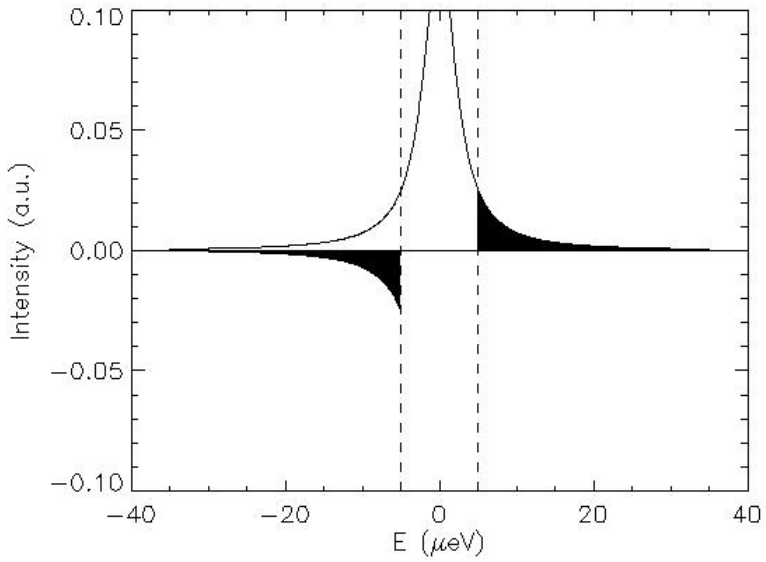

Figure 2 Schematic of the monitor normalization procedure illustrating how the area is calculated for a QENS lineshape as an example. The shaded area must sum to 0.0 for the optimal value of B_D.

The way this is done in the data reduction is through a minimization of the difference in the integrated intensity on both sides of the elastic peak. The primary assumption is that the intrinsic lineshape of the measurement is symmetric about the elastic peak position. This assumption is the condition that gets enforced through the constraint of equivalent integrated intensity on both sides of the elastic peak position. In practice an arbitrary limit of 5 μeV is selected as the region over which the signal is masked off and the integrated intensity is compared between the "left" and "right" sides of the elastic peak. That is the intensity is integrated from (-∞,5) and from (5,∞). Numerically a mask is calculated where the "left" side results in negative area and the "right" side results in positive area as shown in figure 2. The sum of both sides equals 0.0 for the optimal value of B_D. Mathematically the problem is cast as follows:

$$S_D = \int_5^{\infty} dE\, I_{NORM,D}(E) - \int_{-\infty}^{-5} dE\, I_{NORM,D}(E),$$

which can be rewritten as

$$S_D = \int_{-\infty}^{\infty} dE\, w(E) I_{NORM,D}(E),$$

where the weighting or "mask" function introduced into the integral is defined as

$$w(E) = \theta(E-5) - \theta(-5-E),$$

and $\theta(E)$ is the unit step function. The condition we impose on S_D is that it be a minimum absolute value for an optimal value of B_D. This is easier to do and, in fact, can be performed analytically if we choose to minimize S_D^2. This optimality condition is stated as follows:

$$\begin{aligned} 0 &= \left.\frac{\partial S_D^2}{\partial B_D}\right|_{B_D} \\ &= 2S_D \frac{\partial S_D}{\partial B_D} \end{aligned},$$

but $\frac{\partial S_D}{\partial B_D} = -\int_{-\infty}^{\infty} dE \frac{w(E)}{M(E)}$ which we can drop from the optimality condition above since it does not involve a factor of B_D. The first term in the optimality condition above need only be considered.

$$\begin{aligned} 0 &= S_D \\ &= \int_{-\infty}^{\infty} dE\, w(E)\left[\frac{I_D(E) - B_D}{M(E)}\right] \\ &= \int_{-\infty}^{\infty} d\tilde{E}\, w(\tilde{E})\frac{I_D(\tilde{E})}{M(\tilde{E})} - \int_{-\infty}^{\infty} dE\, \frac{w(E)}{M(E)} B_D \end{aligned},$$

which can be solved for B_D,

$$\boxed{B_D = \frac{\int_{-\infty}^{\infty} d\tilde{E}\, w(\tilde{E})\frac{I_D(\tilde{E})}{M(\tilde{E})}}{\int_{-\infty}^{\infty} dE\, \frac{w(E)}{M(E)}}}.$$

This is the result for which we were looking and the integrals are implemented numerically in the data reduction procedure. This can be shown to be a minimum under certain relevant circumstances through explicit calculation of $\frac{\partial^2 S_D^2}{\partial B_D^2}$,

$$\frac{\partial^2 S_D^2}{\partial B_D^2} = 2\left(\frac{\partial S_D}{\partial B_D}\right)^2 + 2S_D \frac{\partial^2 S_D}{\partial B_D^2}$$
$$= 2\left(\frac{\partial S_D}{\partial B_D}\right)^2$$
$$= \left[\int_{-\infty}^{\infty} dE \frac{w(E)}{M(E)}\right]^2 \geq 0$$

Note that the term involving $2S_D \frac{\partial^2 S_D}{\partial B_D^2}$ vanishes since the second partial with respect to B_D is zero. For a flat (i.e. uniform) monitor spectrum the second derivative is zero so really the value of B_D is at an inflection point of the function S_D^2. However on HFBS the monitor spectrum is asymmetric in energy so that the condition for a minimum is satisfied.

§ 4 Normalization to vanadium run

The purpose of normalizing spectra to a vanadium run is that it provides a means to equalize the sample-independent differences in the detectors such as signal levels. Vanadium is to a good approximation an isotropic scatterer. However be aware that vanadium has a significant absorption cross-section and since the beam goes through the sample twice on HFBS this can result in non-negligible angle-dependent attenuation factors. The procedure in the HFBS data reduction does not include calculation nor correction for such attenuation factors.

In this procedure the vanadium spectra are converted to energy transfer, normalized to p(E), and normalized to monitor. A Gaussian function is then fit to the spectra between –5 μeV and +5 μeV in each detector resulting in a 16 element array of integrated intensities, A. If we denote the integrated intensity from the vanadium spectrum in detector D by A_D and the intensity in the same detector of the signal file that we wish to correct as I_D then the "vanadium-normalized" intensity can be expressed as

$$I_{D,V\,NORM} = \frac{I_D}{\left(A_D / \langle A \rangle\right)},$$

where the expression in brackets denotes the average of all of the integrated intensities. In practice only detectors 4 to 16 are included in this average since the first three detectors have such a high count rate in comparison.