Using Fermi choppers to shape the neutron pulse

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Abstract:

This work is part of a series of papers [1, 2] about benchmarking studies related to Fermi choppers (FC) used for pulse shaping of neutron scattering instruments. Here we discuss the comparison of simulated and analytical results to experimental data of the pulse shape observed immediately after the FC in the High Energy Transfer (HET) instrument at ISIS. From the simulation side, there is a combination of a better moderator description, new absorbing B_4C apertures and a new geometrical description of the FC that enhanced the original results [1]. Besides, the analytical formalism, recently derived in [2], is applied to the FC module of the Monte Carlo (MC) software package VITESS used in versions 2.5 and 2.5.1. The overall agreement is now very good.

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1. Introduction

The use of a Fermi chopper (FC), either at a pulsed source or in combination with a second chopper, allows for a monochromatic incident neutron beam and the development of high versatility instruments suited for a large variety of applications [3]. Considering that various effects influence the exact shape of the neutron pulse, it is important to benchmark experimental results with simulated and analytical approaches to assist in the calculation of FC instruments with different characteristics. In the particular case of FC instruments the important parameters that have to be taken into account are the following: the frequency of rotation of the chopper (Hz), the phase angle between the rotating FC and the neutron beam, the diameter of the rotor and the length, width and height of the slits through which the neutrons will pass. One also needs to know if the slit package is straight or curved. For curved FC one should determine (i) the radius of curvature that corresponds to the wavelength transmitted with highest probability, and (ii) the wavelength band available in the experiment. An accurate description of the neutron source is also an essential parameter.

In this paper we present a comparison between simulated and analytical results and experimental data measured at the monitor located just after the FC in the HET instrument at ISIS. In the next section the analytical approach is outlined, and the limiting approximations are discussed. The simulations were performed using the Monte Carlo (MC) software package VITESS [4] versions 2.5 and 2.5.1. In order to perform this work the module FC with two options, straight and curved slits, has been developed [1, 5]. The main principle of this module is briefly described in section 3. Finally in section 4, we compare the simulation and analytical results to the data obtained with HET.

2. The analytical approach to calculate the transmission probability

In order to optimize the design of the new instrument EXED (Extreme Environment Diffractometer) actually under construction at the Hahn-Meitner-Institut (HMI) in Berlin, an extension of the analytical calculation of Marseguerra & Pauli [6] has been derived [2] for a straight or curved revolving slit. EXED is a time-of-flight (TOF) high-resolution powder diffractometer that will operate under extreme external sample conditions. To produce the neutron pulse a FC and a counter rotating double disk chopper will be used. While existing FC have mostly a cylindrical form with a diameter of about 10 cm, the slit packages used on EXED are relatively thin: 1 cm for the straight package and 2.5 cm for the curved one, with a radius of curvature R = 214.4 mm [7]. This design was chosen so that higher transmitted intensities could be achieved with short pulses. In this particular case, the slits have a constant length, and only those neutrons which are sufficiently close to the centre at t = 0 and fast enough will be transmitted (see for example figure 1, option "circular").

For the HET FC configuration, the calculation of the transmission probability had to be further adapted. For instance, one has to sum over all slits and over the absorption layers in between, where no transmission is possible. Then the rotation axis has to be considered to be at the center of the most central slit. Other effects, such as the divergence of the neutron beam and the phase angle of the FC with respect to the incoming neutron beam, were also taken into account.

In the approach presented in [2], the calculation of the neutron transmission probability through one revolving slit is based on the consideration whether the neutron can or cannot pass through the chopper without hitting the walls and being absorbed. To achieve this a comparison is made between the y-coordinate (horizontal direction, as defined in VITESS) of the neutron path and the y-coordinate of the left and right plane of the slit for one and the same

x-coordinate (cf. figure 1). The neutron velocity (v) and the angular velocity (ω) of the chopper are kept constant.

If the slit is far from the chopper centre, the situation is slightly different. For the neutrons arriving on the left side of the chopper on a package that is moving in opposite direction to the incident neutron beam, the neutron becomes faster relative to the chopper. However, on the right side of the chopper, both velocities point into the same direction and the neutron becomes slower with respect to the chopper. As a result, in the former case, the velocities have to be subtracted, while in the latter case they have to be added.

Another remark is in order here: Marseguerra and Pauli suggested in [6] a parabolic slit to follow ideally the path of a neutron having a given velocity v_0 and passing through the centre of the slit at t = 0. The corresponding neutron trajectory is then described by the following equations:

$$\begin{aligned} x &= v_0 t \cos \omega t \\ y &= -v_0 t \sin \omega t \end{aligned} . \tag{1}$$

As we are using the same approximations as the authors mentioned above:

$$\sin \omega t \approx tg\omega t \approx \omega t \quad \text{and} \quad \cos \omega t \approx 1, \tag{2}$$

which have been proved to be justified for slits with a small ratio of height over length, we obtain the following equation for the trajectory

$$y \approx -\frac{\omega}{v_0} x^2 . \tag{3}$$

Let us consider that in practice, the curved slits of the FC are circular, and that for a circle with the minimum at the origin the equation of the trajectory is given by:

$$y = R \pm \sqrt{R^2 - x^2} , \tag{4}$$

where R is the radius of curvature. If y/R « 1, the expansion of expression (4) gives:

$$y \approx -\frac{x^2}{2R} - \frac{x^4}{8R^3} + \ldots . \tag{5}$$

This shows that in the leading order, both approximations are in agreement. If we identify now the two coefficients in front of x^2 in eq. (3) and eq. (5), we get for the radius of curvature R:

$$R \approx \frac{v_0}{2\omega}. \qquad (6)$$

Starting from eq. (5) and using ref. [8], a higher order calculation of R gives:

$$R = \frac{(1 + y'^2(x))^{3/2}}{y''(x)} = \frac{v_0}{2\omega}(1 + (\frac{2\omega x}{v_0})^2)^{3/2}. \qquad (7)$$

3. The simulation of Fermi choppers with VITESS

The FC module in VITESS works with two options: straight and curved. The algorithm of the two FC modules does not include analytic transmission approximations and takes into account the particular shape and position of each individual channel. The mathematical formulation, which is not straightforward, is based on rotating coordinate systems and will be described elsewhere [5].

The geometry of a straight chopper consists of a rectangular shape ‘package’ representing a set of vertical channels. This package is inserted into a cylindrical frame so that the neutrons that fly through without passing the channels are not transmitted. The main input parameters are the length, width and height of the FC, as well as the number of the channels and the thickness of their walls. In this option the channels of the FC are straight, i.e. the very fast neutrons are practically transmitted with only time modulation while the lower speed neutrons are modulated both in time of flight and wavelength.

On the other hand, the curved chopper consists of a set of vertical channels placed in a cylinder. In this option the FC has curved channels, i.e. the neutrons are transmitted with a time and wavelength modulation. In the VITESS 2.5 only the channel option “ideal” was available [and used in ref. 1 and 2]. In this case, as seen from the coordinate system, the walls of the channels have the shape of ideal trajectories for $\lambda_{optimal}$ for which the highest transmission should be obtained, for a given frequency (*f*). At the entrance all channels are defined as having the same width, while at the exit the width slightly depends on the horizontal position of the channel, on *f* and on *R*. Thus with infinitely thin channels all neutrons having zero divergence and $\lambda_{optimal}$ will be transmitted, while the neutrons reflected on the channel walls will be absorbed. For a finite-width channel, other trajectories close to the ideal one will be transmitted, as well as neutrons with wavelengths slightly different from the $\lambda_{optimal}$.

Given the radius of curvature (*R*) is known, one can obtain $\lambda_{optimal}$ as follows:

$$\lambda_{optimal} = \frac{3956}{4\pi f R} \qquad (8),$$

where the wavelength ($\lambda_{optimal}$) is given in Å, the frequency (*f*) in Hz and the radius of curvature (*R*) in meters. It is worth noting that although the shape of the channel walls is not exactly circular, the radius of curvature is *R* in the centre and only slightly differs at the circumference.

Figure 1

The option “circular” was included in the latest version of VITESS 2.5.1. In this approach *R* is constant for all channels, and the channels have a fixed length. In case of option “ideal”, the channel lengths are determined by the envelope radius and any value given explicitly is ignored. The curvature of the channels is then closed to a parabolic shape (cf. fig. 1).

Figure 2 illustrates a comparison of pulse shapes calculated with the two options, ideal and circular, for λ = 1.2 Å. Figure 2(a) shows the result of a simulation for the HET FC slit package S (see below in Table 1 the definitions of these modules) rotating at 200 Hz, where the ratio *y/R* = 0.00175, and Figure 2(b) shows the curved slit package, which will be used for the EXED instrument at the HMI [7] rotating with 600 Hz and which has also a small ratio *y/R* = 0.0011.

Figure 2

In both cases, the peak width is comparable for the two options. As the HET FC has a large diameter of 10 cm, the effect due to different channel lengths is minor, but for the EXED FC with a small diameter of 2.5 cm and thus a broad channel length distribution an asymmetry of the peak shape becomes visible, which is due to the effect described in section 2. Thus for small slit packages it seems much more advantageous to use a constant channel length as realised for the EXED FC.

4. Comparison with real data obtained at HET at ISIS

The HET spectrometer at ISIS is optimized to measure high-energy magnetic excitations (>50 meV) with energy resolution of 2 to 6% depending on the choice of the FC package [9]. In order to further improve the results recently obtained using VITESS in the first benchmarking simulation of HET [1], the following steps were undertaken:

(1) the ISIS water moderator function was carefully calculated using the MCNPX simulation package [10], and the new description was entered as an input parameter in the simulations;

(2) through a geometrical description, where the sample was considered the focus point, the entrance and exit of the series of absorbing B_4C apertures was re-calculated;

(3) the size of each FC package (see Table 1) used in the simulation was carefully re-measured and the new values were used as input parameters in the FC module.

Table 1

The description of the various FC packages used in the MC simulations is given in Table 1. The most requested slit package is the S, and the slit package B is used in about 5 % of the experiments. Both slit packages B and S are generally run at frequencies *f* between 50 and 600

Hz and with the selected incident energy E_{in} ranging from ~10meV − ~1 eV. Their diameter is 10 cm and the thickness of the absorbing material between the slits is 0.055 cm. The comparison of experimental, simulated and analytical results, shown at the monitor straight after the FC, are given in Figure 3. The area under the curves has been normalized to unity and some curves are slightly shifted in time so they can be correctly superposed. This procedure was chosen because the efficiency of the monitor is not analytical. This criterion is much stronger than a simple normalization of the peak maximum to unity, as done in [1]. Nevertheless, the achieved overall agreement is very good and improved with respect to the results obtained in [1].

Figure 3

From Figure 3 it is important to notice that changes in frequency are not only related to changes of resolution but also to changes in intensity. This feature allows for best matching of the resolution/intensity to experimental requirements. Furthermore the comparison of absolute flux is of high interest. A complete HET instrument simulation was performed for a standard Vanadium Sample at room temperature. Data were simulated for the ^{3}He detectors 2.5 m from the sample [9]. The real data in this case *can* be corrected for the efficiency of the detectors at different wavelengths. A variety of different incident energies were simulated with different frequencies of rotation appropriate to those used on the beamline (see Fig. 4). In both cases the data were box integrated over the whole of the recorded signal. To be compared with the experimental data the simulated data need to be multiplied by an arbitrary scale factor. Over all the simulated runs this scale factor was $1.66 \times 10^{15} \pm 0.2 \times 10^{15}$. This shows a good and consistent spread of values. The main discrepancies in the data are most likely due to that fact that VITESS does not simulate phonons in the Vanadium sample [11,12] and only the elastic signal is generated. On the other hand the HET experimental data contains such phonon contribution, which is very difficult to separate. In order to overcome these difficulties and to reduce the phonon contributions the VITESS simulation results should be compared to Vanadium data at 10 K.

Figure 4

This is a test not only for the quality of the modules used in the simulation but also for the moderator description.

5. Final remarks

The ultimate aim of this work is to provide a Virtual Neutron Source (VNS) for a neutron scattering instrument. The idea of using a VNS is that a user can do a virtual experiment, testing suitability and configuration of neutron instruments that best match his/her experiment. However to achieve this final vision, where the VNS is not only a tool for the neutron instrumentation designer, it is necessary to understand each step of a simulation and how well existing instruments can be described. In this way the comparison of the simulated results to analytical calculations and experimental results to benchmark existing instruments is extremely important [1,2,13].

From this work we can conclude that the curved FC module developed by the VITESS group reproduces very well the first component of the resolution function of HET, i.e. the time-energy distribution of a typical neutron pulse. Thus the next natural step is to describe the sample-dependent component of the resolution function, for that the development of various modules describing model scattering functions is required. Furthermore we would like to point out that an accurate description of the source spectrum is extremely important, and the only way to obtain accurate flux.

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Figures and Tables

Figure 1: Geometries of the FC slit packages with the two options “ideal” and “circular” of version 2.5.1. In the first case, the maximum channel length is about 2.78 cm with a broad length distribution, in the second case, the channel length is constant and equal to 2.5 cm and can be much smaller than the FC diameter.

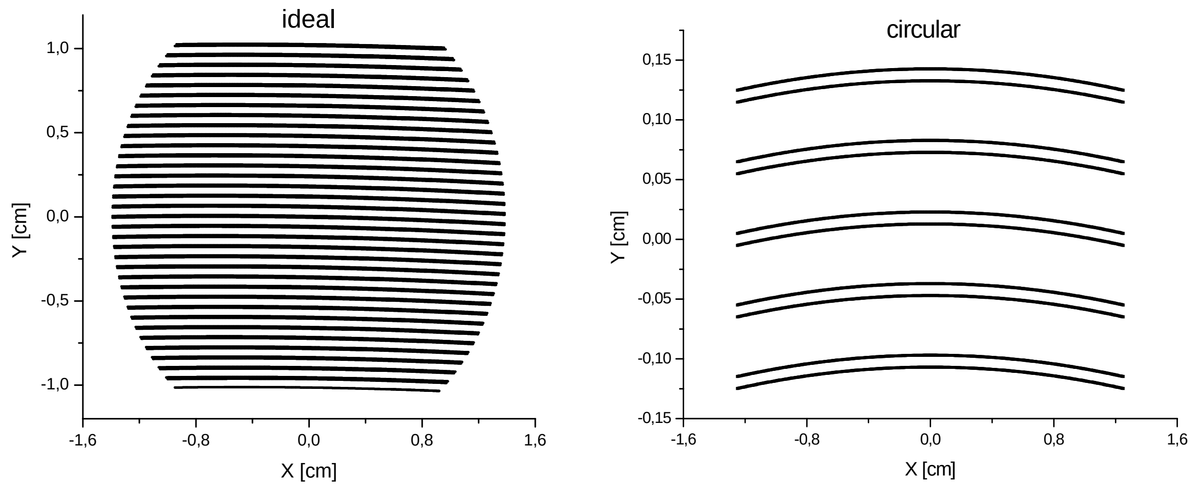

Figure 2: FC peak shape simulated with the two options “ideal” and “circular” of the curved FC module of version 2.5.1. The wavelength is λ = 1.2 Å and a continuous source with constant flux has been used.

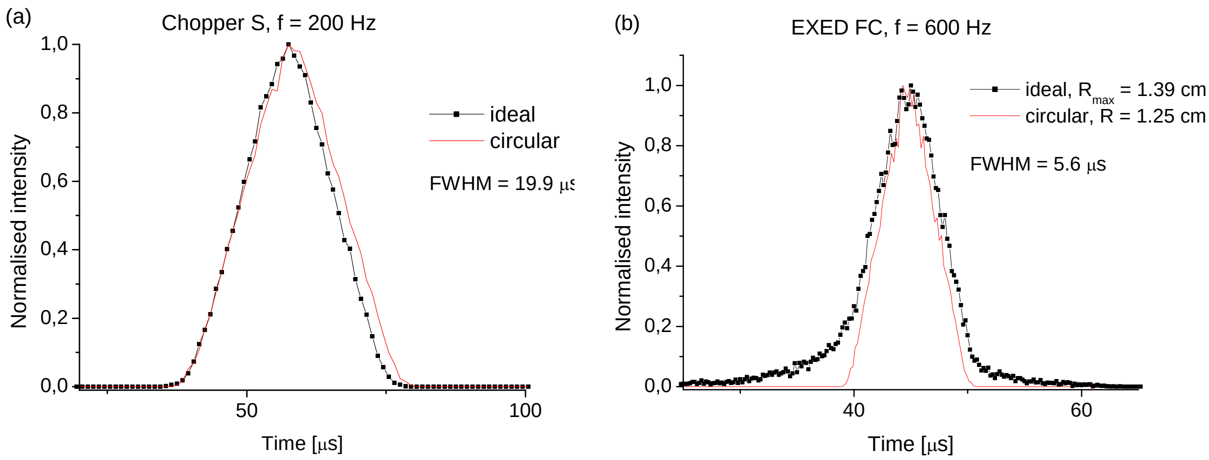

Figure 3: Simulation, analytical results and experimental data showing the time spread immediately after the FC considering the packages B (a) and S (b - d) of HET at ISIS, as described on Table 1. The FWHM's of the curves are: 12.7 μs (a), 27.8 μs (b), 14.6 μs (c) and 7.2 μs (d), depending on the chopper frequency and the incident energy. The corresponding energy resolutions are given in the figures.

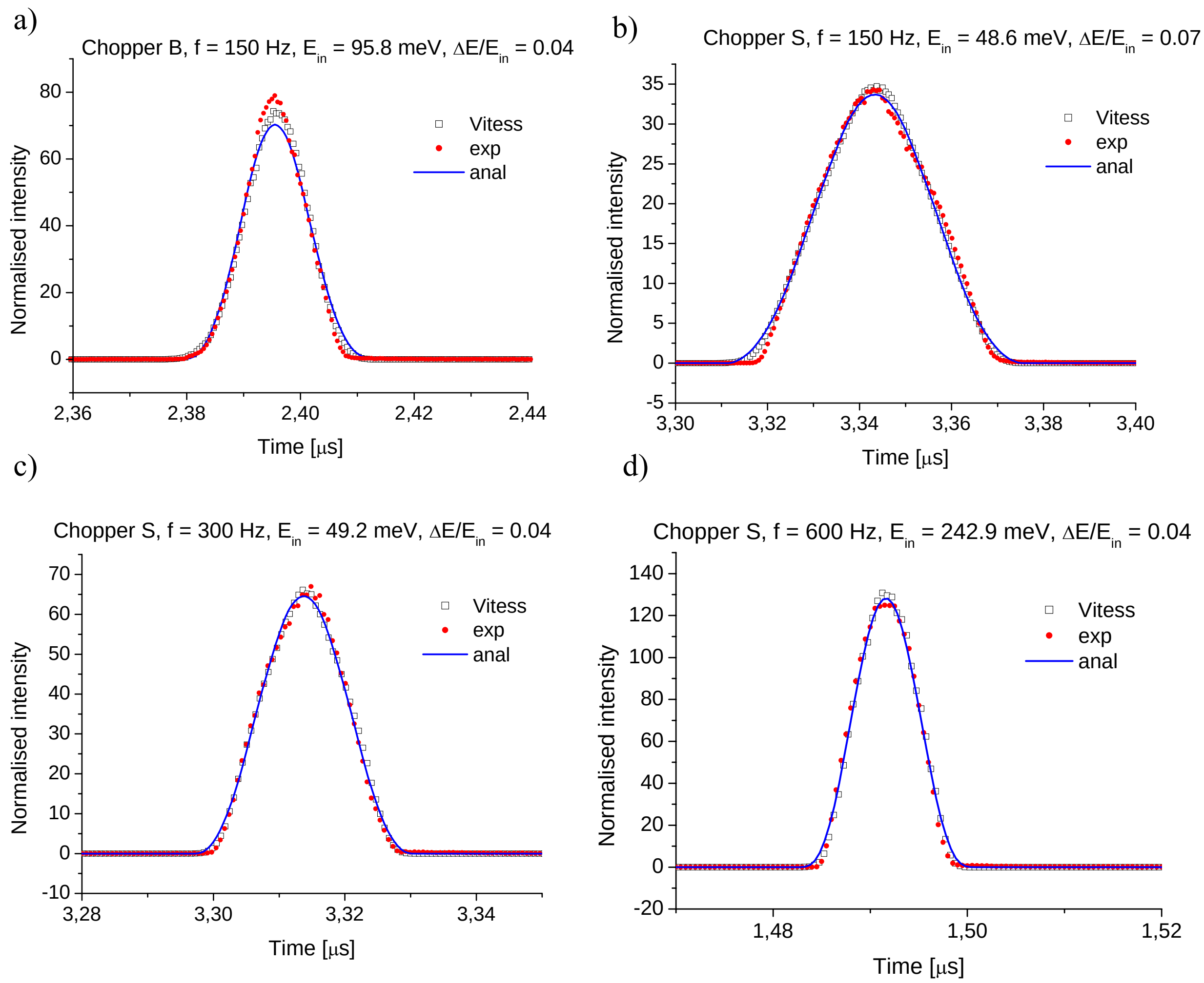

Figure 4: Comparison between experimental (full symbols) and simulated (open symbols) data for the integral intensity in a bank of detectors 2.5 m from the sample position, for an HET instrument using the S chopper package. In this figure the simulated data are scaled by a constant factor of 1.66×10^{15}.

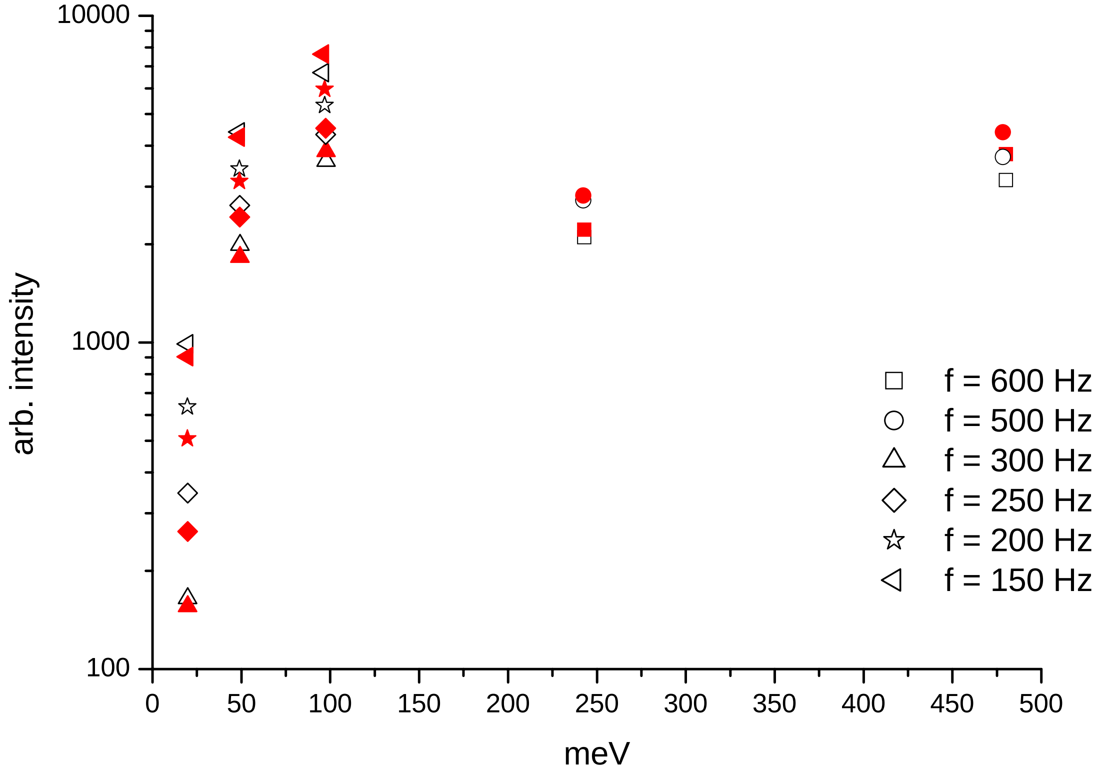

Table 1: Geometrical description of the FC packages B and S corresponding to the VITESS input

Slit package	Height (mm)	Width (mm)	Number of channels	Radius of curvature (mm)
B	52	44.71	24	920
S	64	45.83	16	1300