An Open-Source Software Package for Data Treatment in a MIEZE Experiment

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Abstract. We present a newly-developed open-source software toolkit for handling and analysing the 4-dimensional datasets generated by modern multi-layer time-of-flight (TOF) position-sensitive detectors (PSD). Two such detectors of the type “Cascade” are in operation at the MIEZE beam line MIRA 2 and at the neutron resonance spin-echo spectrometer RESEDA at FRM II. The software consists of several modules for data analysis and instrument parameter calculations to assist the user during experiments, during simulations and in data evaluation. Specifically for the Cascade detector, it contains modules that correct phase-shifts in the MIEZE signal caused by the detector geometry and layout.

1. Introduction

1.1. The MIEZE Technique

MIEZE (Modulation of Intensity Emerging from Zero Effort) \cite{1,2,3,4} is a spin-echo technique related to NSE (Neutron Spin-Echo) \cite{5,6} and NRSE (Neutron Resonance Spin-Echo) \cite{7,8}. All three spin-echo techniques are based on encoding the energy transfer $\Delta E$ at the sample in a change of the neutron spin phase $\Delta \phi$ that is given by

$$\Delta \phi = \tau_M \cdot \Delta E / \hbar. \quad (1)$$

The proportionality factor $\tau_M$ is called the MIEZE time, or spin-echo time.

The MIEZE setup as shown in fig. 1 consists of two RF $\pi$ flipper coils placed between two spin polarisers. The coils are operated at two different frequencies $\omega_A$ and $\omega_B$.

Such a setup leads to a phase change $\phi$ of a polarised neutron beam after passing the second coil of \cite{8,3}

$$\phi = 2\beta \cdot (\omega_B - \omega_A) \cdot \left( t_b - \frac{L_1 + L_b}{v_1} - \frac{L_2}{v_2} \right) + 2\beta \cdot \omega_B \cdot \frac{L_1}{v_1}, \quad (2)$$

where $v_1$ and $v_2$ denote the neutron velocities before and after scattering at the sample, respectively and $t_b$ is the time the neutrons leave the second coil. The factor $\beta$ is used to distinguish between non-bootstrap and bootstrap \cite{3} coils with $\beta = 1$ for the non-bootstrap and $\beta = 2$ for the bootstrap case.

Inserting equ. 2 into equ. 1 and applying a series expansion to first order \cite{3} leads to

$$\frac{\tau_M}{\hbar} \cdot \left( \frac{\partial E}{\partial v_1} \cdot dv_1 + \frac{\partial E}{\partial v_2} \cdot dv_2 \right) = \frac{\partial \phi}{\partial v_1} dv_1 + \frac{\partial \phi}{\partial v_2} dv_2. \quad (3)$$
Figure 1. The MIEZE setup consists of a polariser, two flipper coils and an analyser. The distance between the coils is $L_1$, the distance from the second coil to the sample $L_b$, the distance from the sample to the detector $L_s$.

The piecewise equalisation of the corresponding terms leads to the general inelastic MIEZE condition which is used in the software to help the user determine the optimal detector position or – by extension – a correction factor to the coil frequencies prior to the experiment:

$$L_s = \left( \frac{\omega_A \cdot L_1}{\omega_B - \omega_A} - L_b \right) \cdot \left( \frac{v_1^2 + 2\Delta E/m_n}{v_1^2} \right)^{3/2}.$$  \hspace{1cm} (4)

The inelastic MIEZE condition, equ. 4, is independent of the bootstrap factor $\beta$. For quasi-elastic scattering equ. 4 simplifies to the common MIEZE condition that relates the separation of the coils $L_1$ and the detector distance $L_2 = L_b + L_s$ to the coil frequencies $\omega_A$ and $\omega_B$:

$$L_2 = \frac{\omega_A \cdot L_1}{\omega_B - \omega_A}.$$  \hspace{1cm} (5)

After the analyser, the different frequencies of the two coils produce a sinusoidally varying intensity signal with a beating frequency $\omega_M = 2\beta \cdot (\omega_B - \omega_A)$. The so-called MIEZE contrast $C$ is the ratio of the amplitude $A$ to the offset $B$ of the measured signal.

It can be shown [3] that the MIEZE contrast is the Fourier-cosine transform of the scattering function $S(q, \omega)$ of the sample and therefore the MIEZE equivalent of the polarisation $P$ in NSE and NRSE:

$$C = \int d\omega S(q, \omega) \cos (\omega \tau_M).$$  \hspace{1cm} (6)

The linewidth $\Gamma$ of an excitation can thus be determined by measuring the normalised MIEZE contrast $C$ at different spin-echo times $\tau_M$ followed by fitting an exponentially decaying function, which is the Fourier-cosine transform of an excitation with a Lorentzian spectral weight function, to the $C$ vs. $\tau_M$ data.

1.2. Path Lengths
The MIEZE setup [4] at MIRA [9, 10] uses a Cascade detector system using six GEM foils [11, 12, 13]. Each of the spatially separated foils detects position-sensitive time-of-flight information of the neutron counts.

With its area of 20 · 20 cm$^2$, the time-of-flight data seen by the foils has to be phase-corrected to prevent a loss of contrast especially at high MIEZE times $\tau_M$. At an offset $\Delta x$ and $\Delta y$ away from the center of the detector, the contrast as given by equ. 6 picks up an additional phase $\Delta \phi$ (fig. 2) given by

$$\Delta \phi = \frac{\omega M}{v_2} \cdot \Delta l = \frac{\omega M}{v_2} \left( \sqrt{L_s^2 + \Delta x^2 + \Delta y^2 - L_s} \right).$$  \hspace{1cm} (7)
giving rise to a reduction of the total contrast if $\phi$ is averaged over the whole detector area.

**Figure 2.** Path length differences on a flat PSD. The additional path length $\Delta l$ away from the detector centre causes a non-uniform phase-distribution on the PSD area. The right panel shows the theoretically calculated phase distribution which is used for correcting the experimental dataset shown in fig. 4.

Knowing the theoretical phase distribution as given by equ. 7, the phase changes due to the different path lengths can be corrected for by using appropriate software as shown in the next section.

2. **Software**

The software allows for loading and analysing time-of-flight detector data. Supported data formats include the native data formats used by the Cascade detector, the NICOS\(^1\) data files and the output produced by various McStas [14, 15] components.

The software is written in C++ [16] and Boost\(^2\) for efficiently handling large PSD-TOF datasets. The Qt\(^3\) based graphical front-end employs a multiple document interface (MDI) approach to allow for a simultaneous treatment of multiple detector datasets (fig. 3). The source code for the MIEZE toolkit is available under ref. [17].

2.1. **Correction of Path Length Differences**

For calculating the total contrast, a correction of the phase-differences encountered on a flat PSD is done using the shift theorem [18] of the Discrete Fourier Transform (DFT):

$$\mathcal{F}\{f(t + \Delta t)\} = \mathcal{F}\{f(t)\} \cdot e^{i\omega \Delta t}.$$

Here, $\mathcal{F}$ denotes the DFT. The theorem links a shift $\Delta t$ in the binning of the dataset in real space to a an additional exponential term in Fourier space. Such a technique is necessary in order to be able to rebin the counts arbitrarily without the constraints imposed by the discrete binning. This operation is done on each pixel of the dataset with the theoretical phase offset as given by equ. 7 used as phase correction factor (see fig. 2, right). For performing the DFT we use the FFTW\(^4\) library.

Additionally, a phase-corrected summation of the signal recorded by each GEM foil of the Cascade detector is performed, yielding a total MIEZE signal. A sine function is fitted to this signal using the Minuit\(^5\) library. In the present step, the phase correction factor for the different paths to the different GEM foils of the Cascade detector, and the MIEZE signal is fitted by using the Minuit library.

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1. [http://trac.frm2.tum.de/projects/NICOS](http://trac.frm2.tum.de/projects/NICOS)
2. [http://www.boost.org](http://www.boost.org)
3. [http://qt.digia.com](http://qt.digia.com)
4. [http://www.fftw.org](http://www.fftw.org)
5. [http://seal.web.cern.ch/seal/MathLibs/Minuit2/html/](http://seal.web.cern.ch/seal/MathLibs/Minuit2/html/)
Figure 3. Screenshot of the graphical user interface showing a typical session. Shown in (a) is an example TOF dataset measured at the instrument MIRA, the corresponding phase (c) and contrast (d) images and a total TOF signal inside a selected region of interest (ROI) (b). The software supports loading and analysing of various detector and simulation data formats.

The contrast of the images can either be determined by an elastic reference measurement or – if statistics are sufficient – by a preliminary fitting step for each foil.

Fig. 4 shows the individual steps of reconstructing the total MIEZE signal, here for an example signal of $\tau_M = 127$ ps ($\omega_M = 200 \cdot 2\pi$ kHz) recorded at MIRA. The left panel shows the raw data for each foil and the corresponding phase distribution on the PSD area. The right panel depicts the area-corrected signal which shows a significantly higher contrast due to the phase-corrected addition of the sinusoidal intensity signals at each pixel of the detector. The total signal using the data of all foils is shown in fig. 5. The higher total counts in each bin of the reconstructed total signal lead to better statistics in the final step of fitting the sinusoidal MIEZE signal.

3. Conclusion

We presented a software system which aids the user in the analysis and correction of measured data in MIEZE experiments. The software is already in use at the MIRA instrument at the FRM II. Measurements show that the implemented contrast correction methods lead to statistically stable results. The advantage of the correction algorithms is their independence of the internal layout of the detector (e.g. the distance of the foils in case of the Cascade detector). Another more elaborate detector-dependent contrast correction technique [19] is currently being adapted and implemented as complement to our general method.
Figure 4. Signal on the individual foils before (left) and after (right) phase correction for an example measurement done with the Cascade detector at MIRA. The phase-corrected signal shows a significantly higher MIEZE contrast $C$. The top panel shows the phase distribution before (left) and after (right) pixel-wise phase correction.

Figure 5. Total MIEZE signal after summation of the data from all six foils (see corrected phase information on the right hand side of fig. 4).
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