# Study of liquids with polarized neutrons on D3

A – Instrument and measurements

A-1: First ("old") setup: polarizing Heusler monochromator

In this setup, the polarization of the neutron beam impinging on the sample is constant throughout the experiment. However, there is always some uncertainty on its value, since one can only measure the product of the polarizer and analyzer efficiencies.
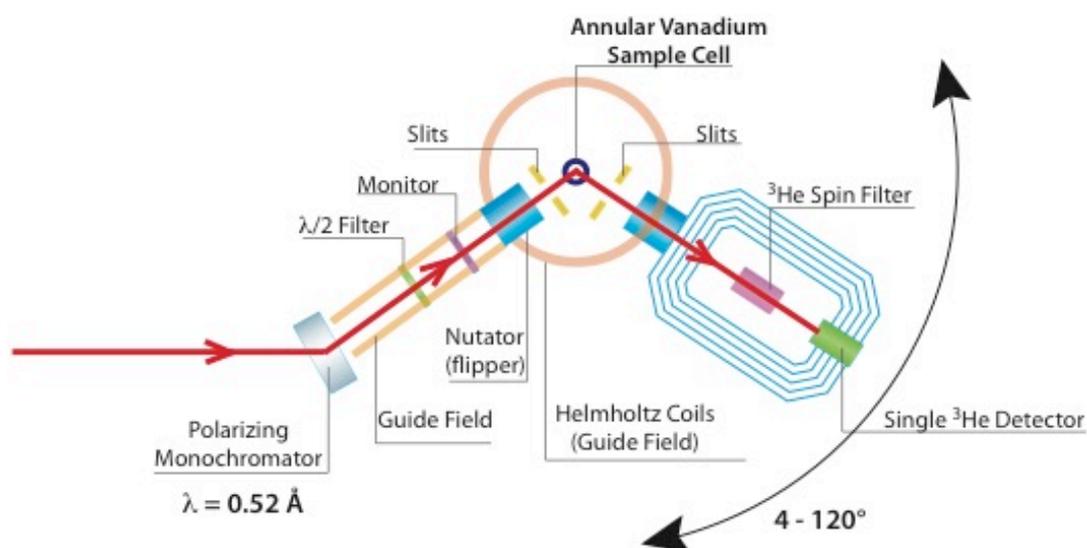

The main limitation of this setup is however the extremely poor Q-resolution resulting from the very small scattering angle of the Heusler (1 1 1) Bragg reflection ($\theta_{Bragg} = 4.26°$ at $\lambda = 0.5$ Å) and the fact that the monochromator is used in transmission geometry.

A-2: Second ("new") setup: Cu monochromator + spin filter

In this setup, the (0 0 2) Bragg reflection from a Cu monochromator produces an unpolarized beam ($\theta_{Bragg} = 7.95°$ at $\lambda = 0.5$ Å). The beam is polarized by a ^{3}He spin filter. The polarizer efficiency is extracted directly from the filter transmission (see below).
The resolution, while still lower than on D4, is much improved, as shown in the figure.
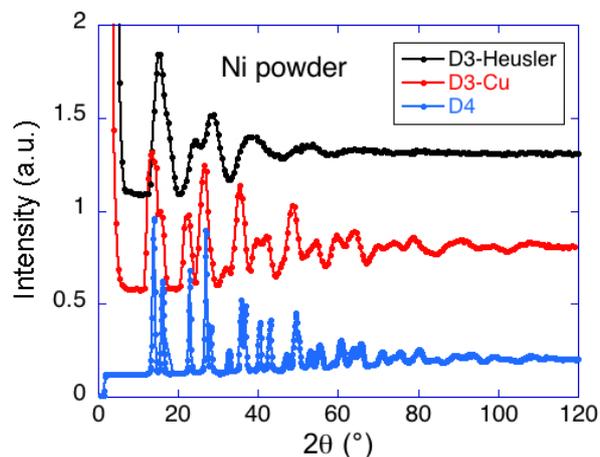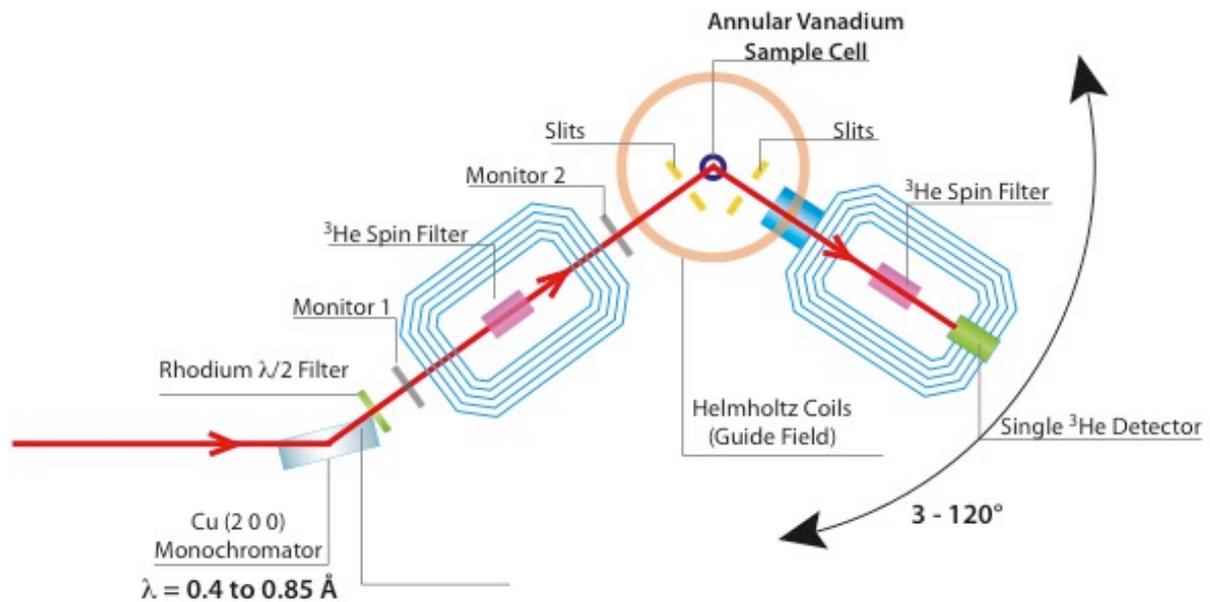
A-3: Beam size and sample container

Upstream window: 13 (horizontal) x 21 (vertical) mm^2.
Downstream window: 13 (horizontal) x 25 (vertical) mm^2.
Annular vanadium cell:
Dimensions of the sample space: $\emptyset_{in}$ = 0.312"=7.93 mm, $\emptyset_{out}$ = 0.426" = 10.82 mm.
Considering the illuminated sample height, the sample volume is about 0.9 cm^3.
The inner and outer walls of the vanadium can have a thickness of 0.006"= 0.15 mm.
A single crystal is mounted on top of the sample container to monitor the efficiency of the analyzer spin filter.

A-4: Measurements

The measurements consist in recording horizontal angular scans of the single detector in both polarization channels: I^+ and I^-.
The step size is usually 1° at high angle (>25°) and 0.5° at low angle (≤25°).
Considering the lifetime of the spin filters, of the order of 70-100 hours, the decay of the polarization is sufficiently slow to integrate each measurement over up to 4 minutes.

Every 2-3 hours, the single crystal on top of the sample container is (automatically) driven into the beam, to record the polarization, product of the efficiencies of the polarizer and the analyzer.

A typical sequence of measurements is:

```
ptz 19.28                    (moves the sample into the beam)
fls ga fr -25 -2.5 .5 240s (scan the detector (25° to 2.5°, in 0.5° steps, 240 seconds/pt)
xbu polar                    (measure the polarization using the "polar.xbu" script
ptz 19.28
fls ga fr -60 -26 1 240s
xbu polar
ptz 19.28
fls ga fr -90 -61 1 240s
xbu polar
ptz 19.28
fls ga fr -120 -91 1 240s
xbu polar
```

```
polar.xbu:
------------------------
par cet = = = 10000 2000 (reset the counting times)
par sps 30s
ptz -23.7                (drives the crystal into the beam)
hkl1 1 1 1        (rotate the detector and sample into predetermined (111) Bragg conditions)
pga -9.00
pom -28.41
spi 1            (set the polarization channels to + +)
spo 1
cen om .7 11     (small rocking curve to center the)
bpb              (background-peak-background, "bpb" scan, to measure the polarization)
```

The heights are the following:
For 3 cells: tz = -13 and   Wafer: fz = 0
                              Top can: fz = 58
                              Middle can: fz = 120
                              Bottom can: fz = 182

For 2 cells: tz = -13 and   Wafer: fz = 62
                              Top can: fz = 120
                              Bottom can: fz = 182

For 1 cell: tz = -13 and   Wafer: fz = 124
                              Can: fz =182

The transmission of the spin filters highly depends on the (decaying) ^{3}He polarization. For example, at $\lambda = 0.5$ Å, the chosen ^{3}He pressure is usually 3.2 bars. With an initial ^{3}He polarization of $\approx 80\%$ and a lifetime of 70-100 hours, the (unpolarised) transmission varies from $\approx 36\%$ to $\approx 24\%$ in the first 24 hours. For that reason, the spin filters are usually replaced every day.
When replacing a filter, it is important to:
- Measure the polarization obtained with the old filter (mandatory) ("bpb" on Bragg peak),
- Measure the transmissions of the depolarized filters (optional, but helps to cross-check the characteristics of the filter, as provided by the ^{3}He lab),
- Declare the new filter in MAD or NOMAD ("par nsf" and "par nsf2",
- Measure the polarization obtained with the new filters ("bpb"),
A detailed procedure is available on the instrument, and given in the appendix.

B – Theory

Neutron beam intensity: $I = I^+ + I^-$

Transmission of unpolarized beam (here ignoring the windows transmission, or empty spin filter transmission) :

$$I^{\pm} = T^{\pm} \frac{I_{in}}{2}$$

$$I = I^+ + I^- = (T^+ + T^-) \frac{I_{in}}{2} = T\, I_{in}$$

$$T = \frac{T^+ + T^-}{2}$$

Neutron polarization

$$P_n = \frac{I^+ - I^-}{I^+ + I^-} = \frac{T^+ - T^-}{T^+ + T^-}$$

$$I^+ = I\, \frac{1 + P_n}{2}$$

$$I^- = I\, \frac{1 - P_n}{2}$$

Spin filter transmission

$$T^{\pm} = e^{-O(\lambda)} e^{\pm O(\lambda) P_{He}}$$

$$P_{He} = P_{He}^0\, e^{-\frac{t}{T_1}}$$

$$O(\lambda) = 7.32 * 10^{-2} * p[\text{bar}] * L[\text{cm}] * \lambda[\text{A}]$$

P_{He} is the ³He polarization, T_1 the relaxation time, $O(\lambda)$ the opacity

Spin filter transmission of unpolarized beam

$$T = \frac{T^+ + T^-}{2} = e^{-O(\lambda)} \cosh[O(\lambda) P_{He}]$$

Transmission of unpolarized beam through depolarized spin filter:

$$P_{He} = 0$$

$$T_0^+ = T_0^- = e^{-O(\lambda)}$$

$$T_0 = \frac{T_0^+ + T_0^-}{2} = e^{-O(\lambda)}$$

Transmitted polarization:

$$P_n = \tanh[O(\lambda) P_{He}]$$

note:

$$\frac{T}{T_0} = \cosh[O(\lambda)P_{He}]$$

since $\cosh^2 x - \sinh^2 x = 1$

$$P_n = \sqrt{1 - \left(\frac{T_0}{T}\right)^2} \qquad (1)$$

This is what we use to determine the polarization of the beam impinging on the sample, from the Monitor2 measurements

Decay:

The relaxation time T_1 is obtained by fitting:

$$P_n = \tanh\left[O(\lambda)\ P_{He}^0\ e^{-\frac{t}{T_1}}\right] \qquad (2)$$

For a polarized primary beam, with polarization P_{in} one has to use:

$$P_n = P_{in}\tanh\left[O(\lambda)\ P_{He}^0\ e^{-\frac{t}{T_1}}\right] \qquad (2')$$

Beam path:
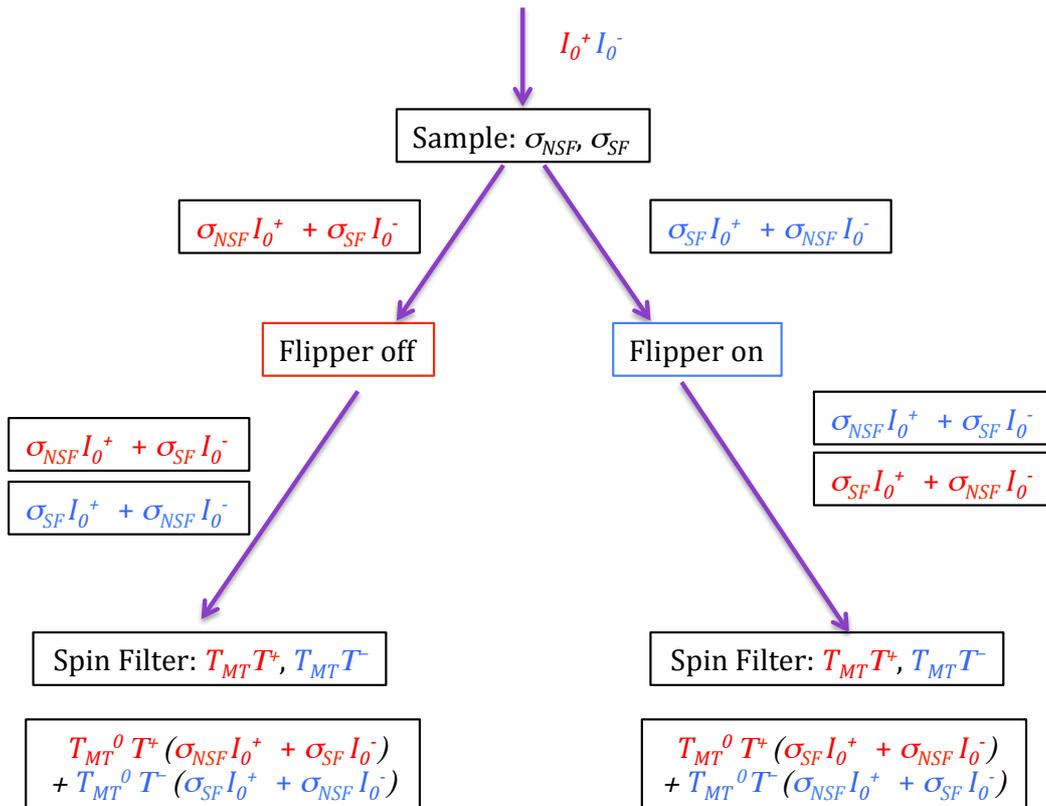
We use $I_0^\pm = T_{MT}^0\ I_{in}^\pm$, where T_{MT}^0 is the magic box empty filter transmission.
$T_{MT}^0 = 1$ if there is no magic box (polarization from Heusler monochromator).

Measured intensities:

Flipper off: $I_m^+ = T_{MT} [T^+(\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-) + T^-(\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-)]$

Flipper on: $I_m^- = T_{MT} [T^+(\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-) + T^-(\sigma_{SNF} I_0^+ + \sigma_{SF} I_0^-)]$

$$\frac{I_m^+}{T_{MT}} = \sigma_{NSF} (T^+ I_0^+ + T^- I_0^-) + \sigma_{SF} (T^+ I_0^- + T^- I_0^+)$$

$$\frac{I_m^-}{T_{MT}} = \sigma_{NSF} (T^+ I_0^- + T^- I_0^+) + \sigma_{SF} (T^+ I_0^+ + T^- I_0^-)$$

$$\sigma_{NSF} = \frac{(T^+ I_0^+ + T^- I_0^-)\frac{I_m^+}{T_{MT}} - (T^+ I_0^- + T^- I_0^+)\frac{I_m^-}{T_{MT}}}{(T^+ I_0^+ + T^- I_0^-)^2 - (T^+ I_0^- + T^- I_0^+)^2}$$

$$= \frac{(T^+ I_0^+ + T^- I_0^-)\frac{I_m^+}{T_{MT}} - (T^+ I_0^- + T^- I_0^+)\frac{I_m^-}{T_{MT}}}{(I_0^{+2} - I_0^{-2})(T^{+2} - T^{-2})}$$

$$\sigma_{SF} = \frac{(T^+ I_0^+ + T^- I_0^-)\frac{I_m^-}{T_{MT}} - (T^+ I_0^- + T^- I_0^+)\frac{I_m^+}{T_{MT}}}{(T^+ I_0^+ + T^- I_0^-)^2 - (T^+ I_0^- + T^- I_0^+)^2}$$

$$= \frac{(T^+ I_0^+ + T^- I_0^-)\frac{I_m^-}{T_{MT}} - (T^+ I_0^- + T^- I_0^+)\frac{I_m^+}{T_{MT}}}{(I_0^{+2} - I_0^{-2})(T^{+2} - T^{-2})}$$

We want to re-write the equations as functions of the incoming polarization and the spin filter parameters
We note P_{in} the incoming neutron polarization

$$P_{in} = \frac{I_0^+ - I_0^-}{I_0^+ + I_0^-} = \frac{I_0^{+2} - I_0^{-2}}{(I_0^+ + I_0^-)^2} = \frac{I_0^{+2} - I_0^{-2}}{I_0^2}$$

resulting in: $I_0^{+2} - I_0^{-2} = P_{in} I_0^2$

$$I_0^+ = I_0 \frac{1 + P_{in}}{2} \quad \text{and} \quad I_0^- = I_0 \frac{1 - P_{in}}{2}$$

To simplify, we will write: $T^\pm = \alpha e^{\pm\beta}$, $\alpha = e^{-O(\lambda)}$, $\beta = O(\lambda) P_{He}^0 e^{-\frac{t}{T_1}}$. Then:

$$T^+ I_0^+ + T^- I_0^- = I_0 \alpha \left[e^\beta \frac{1 + P_{in}}{2} + e^{-\beta} \frac{1 - P_{in}}{2} \right]$$

$$T^+ I_0^- + T^- I_0^+ = I_0 \alpha \left[e^\beta \frac{1 - P_{in}}{2} + e^{-\beta} \frac{1 + P_{in}}{2} \right]$$

$$T^+ I_0^+ + T^- I_0^- = I_0 \alpha \left[\cosh\beta + P_{in} \sinh\beta \right]$$

$$T^+ I_0^- + T^- I_0^+ = I_0 \alpha \left[\cosh\beta - P_{in} \sinh\beta \right]$$

$$T^{+2} - T^{-2} = \alpha^2 e^{2\beta} - \alpha^2 e^{-2\beta} = 2 \alpha^2 \sinh(2\beta)$$

$$T^{+2} - T^{-2} = 4 \alpha^2 \sinh\beta \cosh\beta$$

$$\sigma_{NSF} = \frac{I_0 \alpha \left[\cosh\beta + P_{in} \sinh\beta \right] \frac{I_m^+}{T_{MT}} - I_0 \alpha \left[\cosh\beta - P_{in} \sinh\beta \right] \frac{I_m^-}{T_{MT}}}{P_{in} I_0^2 \, 4 \, \alpha^2 \sinh\beta \cosh\beta}$$

$$\sigma_{NSF} = \frac{\left[1 + P_{in} \tanh\beta \right] I_m^+ - \left[1 - P_{in} \tanh\beta \right] I_m^-}{4 \, P_{in} \, I_0 \alpha \sinh\beta \, T_{MT}} \qquad (3)$$

similarly:

$$\sigma_{SF} = \frac{-\left[1 - P_{in} \tanh\beta \right] I_m^+ + \left[1 + P_{in} \tanh\beta \right] I_m^-}{4 \, P_{in} \, I_0 \alpha \sinh\beta \, T_{MT}} \qquad (4)$$

As shown in equation (2'), $P_{in} \tanh\beta$ is actually the neutron polarization measured on a nuclear coherent Bragg peak, P_{meas}:

$$\sigma_{NSF} = \frac{\left[1 + P_{meas} \right] I_m^+ - \left[1 - P_{meas} \right] I_m^-}{4 \, P_{in} \, I_0 \alpha \sinh\beta \, T_{MT}} \qquad (3')$$

similarly:

$$\sigma_{SF} = \frac{-\left[1 - P_{meas} \right] I_m^+ + \left[1 + P_{meas} \right] I_m^-}{4 \, P_{in} \, I_0 \alpha \sinh\beta \, T_{MT}} \qquad (4')$$

Due to the fact that the P_{meas} measurements (Si single crystal measurements) do not perfectly sample the beam properties (wavelength distribution as well polarization and intensity profile), it is actually safer to use $P_{in} \tanh\beta$ rather than the fit to P_{meas} in the calculations.

If the primary beam polarization is obtained with a spin filter (magic box setup), P_{in} is obtained by fitting the time evolution of the transmission ("Monitor2" measurements) using equations (1) and (2). If the beam polarization is produced by the Heusler polarizing monochromator, one should calibrate it separately, *i.e.* using a Si wafer or rather a large, mosaic, single crystal.

The characteristics of the analyzer spin filter are obtained by fitting the Si polarization measurements to equation (2'). Equation (2') actually involves 3 parameters: P_{in}, T_1, and $O(\lambda) P_{He}^0$. They are rather highly correlated and one can choose to fit either P_{in} and T_1, or $O(\lambda) P_{He}^0$ and T_1, depending on how accurately $O(\lambda) P_{He}^0$ or P_{in} are known.

Once this is done, one calculates the actual non-spin-flip and spin-flip intensities using equations (3) and (4) or (3') and (4').

Considerations about the flipper efficiency

We assume that the first flipper ("Flipper in") before the sample is perfect, *i.e.* has an efficiency = 1 (magic box). If the second flipper has an efficiency $e < 1$, the above cartoon maust be modified:

General case
Flipper out: e < 1

$I_0^+ I_0^-$

Sample: $\sigma_{NSF}, \sigma_{SF}$

$\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-, \sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-$

Flipper off

Flipper on, e < 1

$\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-$

$\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-$

$e (\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-) + (1-e) (\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-)$
$= (\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-) + e (\sigma_{NSF} - \sigma_{SF}) (I_0^+ - I_0^-)$

$e (\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-) + (1-e) (\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-)$
$= (\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-) - e (\sigma_{NSF} - \sigma_{SF}) (I_0^+ - I_0^-)$

Spin Filter: $T_{MT} T^+, T_{MT} T^-$

Spin Filter: $T_{MT} T^+, T_{MT} T^-$

$T_{MT} T^+ (\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-)$
$+ T_{MT} T^- (\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-)$

$T_{MT} T^+ [(\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-) - e (\sigma_{NSF} - \sigma_{SF}) (I_0^+ - I_0^-)]$
$+ T_{MT} T^- [(\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-) + e (\sigma_{NSF} - \sigma_{SF}) (I_0^+ - I_0^-)]$
$= T_{MT} [T^+ (\sigma_{NSF} I_0^+ + \sigma_{SF} I_0^-) + T^- (\sigma_{SF} I_0^+ + \sigma_{NSF} I_0^-)$
$- e (\sigma_{NSF} - \sigma_{SF}) (I_0^+ - I_0^-) (T^+ - T^-)]$

For a nuclear Bragg peak ($\sigma_{NSF} = \sigma$ and $\sigma_{SF} = 0$) the measured intensities reduce to:

Flipper off: $I_m^+ = T_{MT} (T^+ \sigma I_0^+ + T^- \sigma I_0^-)$

Flipper on: $I_m^- = T_{MT} [(T^+ \sigma I_0^+ + T^- \sigma I_0^-) - e \sigma (I_0^+ - I_0^-)(T^+ - T^-)]$

And the measured polarization is:

$$P_{meas} = \frac{e (I_0^+ - I_0^-)(T^+ - T^-)}{2(T^+ I_0^+ + T^- I_0^-) - e (I_0^+ - I_0^-)(T^+ - T^-)}$$

which can be transformed into:

$$\frac{1}{P_{meas}} = \frac{2(T^+ I_0^+ + T^- I_0^-) - e\,(I_0^+ - I_0^-)(T^+ - T^-)}{e\,(I_0^+ - I_0^-)(T^+ - T^-)}$$

$$\frac{1}{P_{meas}} = \frac{(I_0^+ + I_0^-)(T^+ + T^-) + (I_0^+ - I_0^-)(T^+ - T^-)}{e\,(I_0^+ - I_0^-)(T^+ - T^-)} - 1$$

$$\frac{1}{P_{meas}} = \frac{1}{e\,P_{in}P_{out}} + \frac{1}{e} - 1 = \frac{1 + P_{in}P_{out} - e\,P_{in}P_{out}}{e\,P_{in}P_{out}}$$

$$e\,P_{in}P_{out} = P_{meas}(1 + P_{in}P_{out} - e\,P_{in}P_{out})$$

$$P_{out}(e\,P_{in} - P_{in}P_{meas} + eP_{in}P_{meas}) = P_{meas}$$

$$P_{out}P_{in}(e - P_{meas} + eP_{meas}) = P_{meas}$$

$$P_{out} = \frac{P_{meas}}{P_{in}\big(e - P_{meas}(1 - e)\big)}$$

From the sample, we measure :

$$I_m^+ = T_{MT}\big[\sigma_{NSF}(T^+ I_0^+ + T^- I_0^-) + \sigma_{SF}(T^+ I_0^- + T^- I_0^+)\big]$$

$$I_m^- = T_{MT}\big[\sigma_{NSF}(T^+ I_0^+ + T^- I_0^-) + \sigma_{SF}(T^+ I_0^- + T^- I_0^+) - e\,(\sigma_{NSF} - \sigma_{SF})(I_0^+ - I_0^-)(T^+ - T^-)\big]$$

We note that: $\qquad I_m^- = I_m^+ - T_{MT}\big[e\,(\sigma_{NSF} - \sigma_{SF})(I_0^+ - I_0^-)(T^+ - T^-)\big]$

We obtain the system of linear equations:

$$\begin{cases} \sigma_{NSF} - \sigma_{SF} = \dfrac{I_m^+ - I_m^-}{T_{MT}\,e\,(I_0^+ - I_0^-)(T^+ - T^-)} \\[4mm] \sigma_{NSF}(T^+ I_0^+ + T^- I_0^-) + \sigma_{SF}(T^+ I_0^- + T^- I_0^+) = \dfrac{I_m^+}{T_{MT}} \end{cases}$$

Using the previously defined α and β parameters, this system is re-written:

$$\begin{cases} \sigma_{NSF} - \sigma_{SF} = \dfrac{I_m^+ - I_m^-}{T_{MT}\,e\,P_{in}\,2\,I_0\,\alpha\,\sinh\beta} \\[4mm] \sigma_{NSF}I_0\alpha\,[\cosh\beta + P_{in}\sinh\beta] + \sigma_{SF}\,I_0\alpha\,[\cosh\beta - P_{in}\sinh\beta] = \dfrac{I_m^+}{T_{MT}} \end{cases}$$

$$\begin{cases} \sigma_{SF} = \sigma_{NSF} - \dfrac{I_m^+ - I_m^-}{T_{MT}\ e\ 2\ P_{in}I_0\ \alpha\ \sinh\beta} \\[4ex] \sigma_{NSF}2\ \cosh\beta\ I_0\alpha - \dfrac{(I_m^+ - I_m^-)(\cosh\beta\ -\ P_{in}\ \sinh\beta)}{T_{MT}\ e\ P_{in}\ 2\ \sinh\beta} = \dfrac{I_m^+}{T_{MT}} \end{cases}$$

$$\begin{cases} \sigma_{NSF} = \dfrac{(I_m^+ - I_m^-)(1\ -\ P_{in}\ \tanh\beta) + I_m^+(2eP_{in}\ \tanh\beta)}{T_{MT}\ e\ 4P_{in}\ I_0\alpha\ \sinh\beta} \\[4ex] \sigma_{SF} = \dfrac{(I_m^+ - I_m^-)(-1\ -\ P_{in}\ \tanh\beta) + I_m^+(2eP_{in}\ \tanh\beta)}{T_{MT}\ e\ 4P_{in}\ I_0\alpha\ \sinh\beta} \end{cases}$$

Errors and propagation

The error on a measured intensity I is taken as $\sqrt{I}$ (Poisson).

$$d\left(\frac{I_m}{I_0}\right) = \frac{I_m}{I_0}\sqrt{\frac{1}{I_m} + \frac{1}{I_0}}$$

$I_m = I_m^+$ or I_m^- and I_0 = monitor or, if using the magic box, Monitor2.

The uncertainty on the opacity can be estimated:

$$\frac{d[O(\lambda)]}{O(\lambda)} = \sqrt{\left(\frac{dp}{p}\right)^2 + \left(\frac{dL}{L}\right)^2 + \left(\frac{d\lambda}{\lambda}\right)^2}$$

$\dfrac{dp}{p} \approx 0.003,\ \dfrac{dL}{L} \approx 0.007,\ \dfrac{d\lambda}{\lambda} \approx 0.005$ resulting in $\dfrac{d[O(\lambda)]}{O(\lambda)} \approx 0.0085.$

When using the magic box setup, the polarization P_{in} is obtained from the fit of the Monitor2 measurements to equation (1). With this method, we can estimate that the accuracy dP_{in} of P_{in} is better than 0.005. The scripts use dP_{in} = 0.005.
In the "old" setup (Heusler monochromator and no magic box), the actual value of the polarization is quite tricky, since there is no direct measurement, and so is the accuracy. At the moment, the data reduction scripts include a fixed error dP_{in} = 0.002.

Similarly, the product $\beta = O(\lambda)\ P_{He}^0$ (value of the order of 1.2 to 1.5 at $\lambda = 0.5$) may be either the result of the fit of the polarization decay to (2'), or simply calculated from the theoretical values of the spin filter cell characteristics. For calculated β, The calculations use a fixed, reasonable value, including also the uncertainty on the relaxation time T_1:

$$d\beta = d\left(O(\lambda)\ P_{He}^0 e^{-\frac{t}{T_1}}\right) \approx 0.01.$$

The transmissions of the empty spin filter cells, T_{MT}, are of the order of 0.85 to 0.9 (exact value depending on the cell and the wavelength). They have been measured directly, with accuracies $d(T_{MT}) \approx 0.002\ to\ 0.005$.

$$d(1 \pm P_{in}\tanh\beta) = dP_{in}\tanh\beta + \frac{P_{in}\,d\beta}{(\cosh\beta)^2}$$

$$d(1 \pm P_{in}\tanh\beta) = d(P_{in}\tanh\beta) = P_{in}\tanh\beta\sqrt{\left(\frac{dP_{in}}{P_{in}}\right)^2 + \left(\frac{d\beta}{(\cosh\beta\sinh\beta)}\right)^2}$$

$$d\left[(1 \pm P_{in}\tanh\beta)\frac{I_m^+}{I_0}\right] = \sqrt{\left[d\left(\frac{I_m^+}{I_0}\right)\right]^2 + \left(P_{in}\tanh\beta\frac{I_m^+}{I_0}\right)^2\left[\left(\frac{d(P_{in}\tanh\beta)}{P_{in}\tanh\beta}\right)^2 + \left(\frac{d(\frac{I_m^+}{I_0})}{\frac{I_m^+}{I_0}}\right)^2\right]}$$

$$= \sqrt{\left[d\left(\frac{I_m^+}{I_0}\right)\right]^2 + \left(P_{in}\tanh\beta\frac{I_m^+}{I_0}\right)^2\left[\left(\frac{dP_{in}}{P_{in}}\right)^2 + \left(\frac{d\beta}{(\cosh\beta\sinh\beta)}\right)^2 + \left(\frac{d(\frac{I_m^+}{I_0})}{\frac{I_m^+}{I_0}}\right)^2\right]}$$

$$d(P_{in}\,\alpha\,\sinh\beta\,T_{MT}) = P_{in}\,\alpha\,\sinh\beta\,T_{MT}\sqrt{\left(\frac{dP_{in}}{P_{in}}\right)^2 + \left(\frac{d\alpha}{\alpha}\right)^2 + \left(\frac{d(\sinh\beta)}{\sinh\beta}\right)^2 + \left(\frac{dT_{MT}}{T_{MT}}\right)^2}$$

$$= P_{in}\,\alpha\,\sinh\beta\,T_{MT}\sqrt{\left(\frac{dP_{in}}{P_{in}}\right)^2 + \left(d(O(\lambda))\right)^2 + \left(\frac{d\beta}{\tanh\beta}\right)^2 + \left(\frac{dT_{MT}}{T_{MT}}\right)^2}$$

$$\frac{d(\sigma_{NSF})}{\sigma_{NSF}} = \sqrt{\left(\frac{d(P_{in}\,\alpha\,\sinh\beta\,T_{MT})}{P_{in}\,\alpha\,\sinh\beta\,T_{MT}}\right)^2 + \frac{\left(d\left((1 \pm P_{in}\tanh\beta)\frac{I_m^+}{I_0}\right)\right)^2 + \left(d\left((1 \pm P_{in}\tanh\beta)\frac{I_m^-}{I_0}\right)\right)^2}{\left((1 + P_{in}\tanh\beta)\frac{I_m^+}{I_0} - (1 \pm P_{in}\tanh\beta)\frac{I_m^-}{I_0}\right)^2}}$$

Average of corrected data

Once the data have been corrected, we can merge the scans. At each angle, the average $\bar{\sigma}$ of the set $\{\sigma_i\}_{i=1,N}$ measured quantities, with errors $\{\delta_i\}$ is:

$$\bar{\sigma} = \frac{\sum \frac{1}{\delta_i^2} \sigma_i}{\sum \frac{1}{\delta_i^2}}$$

Two errors can be calculated:

- the statistical error

$$d\bar{\sigma}_{stat} = \sqrt{\frac{1}{\sum \frac{1}{\delta_i^2}}}$$

- the standard deviation, reflecting the (weighted) distribution of the data points:

$$d\bar{\sigma}_{dist} = \sqrt{\frac{\sum \frac{1}{\delta_i^2} (\sigma_i - \bar{\sigma})^2}{(N-1) \sum \frac{1}{\delta_i^2}}}$$

If the experimental errors have been properly estimated, and the measurements are reproducible, both errors should be equal.
To account for a possible spread of the data, the final error is taken as the highest of both values:

$$d\bar{\sigma} = \max(d\bar{\sigma}_{stat}, d\bar{\sigma}_{dist})$$

C Analysis, "new" setup (magic box)

The data reduction has been divided into separate steps, to allow easy critical analysis at each step. Similarly, each step produces a number of ouput files, most of them useful only for tests, or used as input in the subsequent steps. In the following, the files to be preferably checked at each step will be <mark>highlighted</mark>.

C-1 Edit an ascii file containing all the useful information.

The file (here named "Userfile") must follow the example below:
Most of the file will be prepared by the local contact.
The user should only act on the data/time informations, scan names and scan numbers.
No keyword should be modified.
The sample descriptions and scan numbers must come last in the file, following the keyword "Numors"
There is no limitation to the number of samples on can add to the file
The sample name cannot contain any space

Userfile

```
Cycle: 163
Exp: TEST-2708
Local(1)/Remote(0): 0
Polarisation_file: polar.fli
Nominal_Lambda  0.5
Lambda  0.5
Gamma_Offset: 0
Small_Beam_Pol:  0.89
Full_Beam_Pol:  0.73
Ratio_full_Small:  0.85
Begin: 10-Nov-2016 @ 16:00
End: 20-Nov-2016 @ 12:00
FirstScan: 570524
LastScan: 570993
Numors
MTCan       0.500   570524:570548
Sample-1    0.500   570566:570599 570609:570642 570654:570681
MTI         0.500   570696:570697
Vana        0.500   570734:570735
Sample-2    0.500   570804:570902
Sample-3    0.500   570916:570993
(end with an empty line)
```

C-2 In MATLAB, launch the gui:

Start MATLAB
"cd" to your own directory

magic3('Userfile')

The GUI is subdivided into 6 panels. From top to bottom:

- Information about the experiment. This corresponds to the first part of the user file, prepared by the local contact.
In "Local" mode, the logfiles and polarisations file must first be copied into a subdirectory named "logfiles".
In "Remote" mode, the data will be fetched directly from the server, using the provided information on cycle number and experiment number. In that case, the computer must first be connected to the data server (local contact action)

- Extract the data and analyze the decays of the polarizations in the spin filters. This part is performed for all data within the given date/time range in the blue boxes. Dates and times may be edited but the format should not be modified. See § C-3 for the details of

the operations performed in that panel. All times in the data analysis will use the given starting date and time as reference ("time 0"). In the files and plots, times are given in minutes from "time 0".

- Normalize and correct the data within the range of scan numbers given in the blue boxes. The scan numbers may be edited. See § C-4 for the details of the operations performed in that panel.

- Data treatment for all samples. See § C-5 for details.

- Visualization of results. This panel allows background subtraction and comparison of results. See § C-6 for details

- Test panel (mostly for local contact: check monitors and polarisatopns)

C-3 Extract data and analyze spin filters

First choose the output format using the top left popup menu. Recommended during the experiment is the html format, which will create .html files in the subdirectory "html". The "pdf" option will create .pdf files in the subdirectory "pdf". It is however much slower, and only recommended for exporting results: pdf files are standalone, while in html format, all graphics are saved into separate files.

C-3-1 Extract data:

Click on the Read Log Files button. This will extract all the scans from the logfiles.

Input: logfiles

Output:
- html/pdf output listing the logfiles, the scan numbers, the "bpb" numbers, and the magic box spin filters
- individual scans (whether of "fls" or "bpb" type), saved under their scan numbers into the subdirectory "scans"

```
   scans / 570530
   ----------------------------------------------------------------------------------------
   gammaCount_P  Count_MTime_P   Time_M   Monit_P   Monit_M   Date   Time       pol      dpol     moni2
   -90.00  620.   892.   90.0000   90.0000  27261451.  27255330. 10/11/16 22:02:05 -0.17989  0.08392   641124
   -89.00  649.   893.   90.0000   90.0000  27264880.  27262243. 10/11/16 22:05:10 -0.15824  0.08323   640153
   -88.00  569.   884.   90.0000   90.0000  27262460.  27271780. 10/11/16 22:08:15 -0.21679  0.08531   639168
   -87.01  621.   941.   90.0000   90.0000  27255341.  27248790. 10/11/16 22:11:19 -0.20487  0.08335   637523
   -86.01  624.   892.   90.0000   90.0000  27245310.  27241150. 10/11/16 22:14:25 -0.17678  0.08383   637996
   -85.01  646.   880.   90.0000   90.0000  27253723.  27245414. 10/11/16 22:17:29 -0.15334  0.08346   638696
   .....
     2θ     I+    I-    time(+)    time(-)  monitor(+)  monitor(-)   date     time     Pol   dPol  monitor2
```

- "monitor2" file, which includes the information about changes of magic box spin filters as well the measurements with time, monitor and monitor2 informations (*i.e.*, all fls" and "bpb" scans)

```
   monitor2
------------------------------------------------------------------------------------------
 Magic Box Filter: ge18008 3.19 0.75  10/11/2016  @  13:00
 -120.79     69.     54.    9.0000    9.0000    2748320.   2746449. 10/11/16 16:41:28  0.12195  0.28015    69343
 -117.79  69385. 51685.   72.0000   72.0000  21973912. 21969660. 10/11/16 16:43:57  0.14620  0.01159   555092
 -114.79     62.     44.    9.0000    9.0000    2747013.   2743895. 10/11/16 16:44:17  0.16981  0.29209    69027
 -120.79      8.     21.    1.1200    2.8800     342158.    882683. 10/11/16 16:44:27 -0.01031  0.65063    15923
 .....
     2θ      I+     I-    time(+)    time(-)  monitor(+)  monitor(-)   date       time       Pol      dPol    monitor2
```

- "scan_list" file: a list of all the extracted "fls" scan numbers

```
 scan_list
 --------
 570524
 570527
 570530
 570533
 570536
 570539
 ...
```

- "bpb_list" file: a list of all the extracted "bpb" scan numbers

```
 bpb_list
 --------
 570524
 570527
 570530
 570533
 570536
 570539
```

This step also updates the first and last scan numbers given in the next panel.

The extracted scans are corrected for deadtime (0.43 μs, applied to both monitor count rates)

C-3-2 Fit of the magic box spin filter transmission, equations *(1)* and *(2).*

$$P_n = \sqrt{1 - \left(\frac{T_0}{T}\right)^2} \qquad\qquad (1)$$

$$P_n = \tanh\left[O(\lambda)\ P_{He}^0\ e^{-\frac{t}{T_1}}\right] \qquad\qquad (2)$$

Click on the Magic Box Filters: Fit button.
P_n is calculated using the transmission measurements (monitor2) and the fitted parameters are the product $O(\lambda)P_{He}^0$ and the relaxation time T_1.
We can compare the fitted values of $O(\lambda)P_{He}^0$ with the values calculated using the given helium pressure and initial polarization. They are usually consistent within better than 0.5%.
The results will serve to calculate the polarization P_{in} in steps C-3-3 and C-4, using equation *(2)*.

Input:
"monitor2" file

Output:

- individual files "polariser-*lam-cell*", where lam is the wavelength, as entered in the top panel, and num is the cell order number (starting at 1). This is the fit input.

```
1.6765      11420    0.1870    (opacity O(λ), starting time of the cell (mn), depolarized  cell transmission e^{-O(λ)}
Magic Box Filter: ge18011 3.17 0.75  18/11/2016 @  14:20     (information from logfile)
   9.0000    9.0000   2758013.    2759840. 18/11/16 16:22:00     70317 0.339890 0.001290 0.835001 0.002332
  72.0000  72.0000 22094664. 22105150. 18/11/16 16:24:28    562136 0.339211 0.000455 0.834274 0.002107
   9.0000    9.0000   2759504.    2758031. 18/11/16 16:24:49     70242 0.339547 0.001289 0.834635 0.002336
   0.4000    3.6000    123200.    1107126. 18/11/16 16:24:58     15501 0.336038 0.002716 0.830810 0.003146
  39.1000 130.9000 12003251. 40179103. 18/11/16 16:27:54    663865 0.339316 0.000419 0.834387 0.002101
   0.4000    3.6000    122538.    1102667. 18/11/16 16:28:00     15510 0.337638 0.002728 0.832571 0.003124

.....
   (time(+)    time(-)  monitor(+)  monitor(-)    date       time     monitor2  transm.  d(transm.)    Pol      dPol
```

- individual files "polariser -*lam-cell*.pol": fit output

```
Time(mn) Polar   dPolar Transm dTransm    fit
   0      0.8332 0.0024  0.3547  0.0013 0.8401
   3      0.8327 0.0022  0.3542  0.0005 0.8399
   3      0.8338 0.0024  0.3553  0.0013 0.8399
   3      0.8341 0.0024  0.3556  0.0013 0.8399
   6      0.8300 0.0024  0.3516  0.0013 0.8396
....
```

- summary file "polariser _parameters-*lam*.txt"

Opacity	Tin	Tout	OPolHe	dOPHe	T1(mn)	dT1	T1(hr)	Chisq	T(P=0)	MT-Trans	dMT	Cell#
1.713	41	2594	1.2846	0.0000	4238	11	70.64	12.77	0.1804	0.900	0.004	8
1.692	2628	4048	1.2693	0.0000	4250	4	70.84	0.35	0.1841	0.900	0.004	11
1.713	4085	5499	1.2846	0.0000	4642	5	77.36	0.52	0.1804	0.900	0.004	8
1.687	5536	6835	1.2653	0.0000	4691	5	78.18	0.49	0.1851	0.900	0.004	11
1.702	7028	8366	1.2765	0.0000	4875	5	81.25	0.31	0.1823	0.900	0.004	8
1.629	8397	9741	1.2217	0.0000	4072	8	67.87	1.46	0.1961	0.900	0.004	11
1.707	9770	11482	1.2806	0.0000	4535	6	75.59	1.07	0.1813	0.900	0.004	8
1.677	11542	12821	1.2574	0.0000	3691	20	61.52	11.85	0.1870	0.900	0.004	11
1.745	12850	14057	1.3090	0.0000	4591	4	76.52	0.25	0.1746	0.900	0.004	11

Notes: the "MT-Trans" parameters are the transmissions of the empty filters, and have been measured separately for each filter. The Cell# is the identity of the filter (from ^{3}He lab)

C-3-3 Fit of the analyzer ("decpol") spin filter transmission, equation *(2')*.

Click on the <mark>Analyser Filters: Fit</mark> button.
The incoming beam polarization P_{in} should be known from step 1 above but, since the polarisatin transport is not perfect along the beam path, we need an extra parameter *PolRatio*. The other parameters are the product $\beta = O(\lambda)P_{He}^0$ and the relaxation time T_1. All three parameters are highly correlated and we can fit either *PolRatio* and T_1, or β and T_1.

β can be calculated from the given spin filter parameters, and past experience has shown that theses values are very reliable.
In the first experiment using this setup, we obtain *PolRatio* = 0.94(1).

Input:

-Polarisation file ("Polar.fli" in our example)
When working in <mark>"Local"</mark> mode, this file must be first copied into the <mark>"logfiles"</mark> directory

- "polariser _parameters-*lam*.txt " file from step C-3-2

Output:

<mark>- *html/pdf "magic_analyser" output showing the fits and giving a summary of all the results*</mark>

- individual files "analyser-*lam*-*cell*", where *lam* is the wavelength, as entered in the top panel, and num is the *cell* order number (starting at 1). This is the fit input.
In the file, two values of the incident polarization are given: Pin(fit) and Pin(T), calculated using the parameters from file "polariser _parameters-*lam*.txt", and using the measured transmission (monitor2), respectively. The measured polarization Pol, has been corrected for Pin, ie, relates directly to the analyser filter alone.

```
 1.7242      1160   0.899   0.003 (opacity, starting time of the cell (mn),  empty cell transmission and error)
New cell info ge18009  pressure/init. polar   3.22   0.75 initial date/time  11 11 16  @  11:20
  570557    1212  0.8089  0.0017  0.7507  0.7455
  570565    1260  0.8088  0.0019  0.7458  0.7403
  570568    1333  0.8006  0.0019  0.7384  0.7346
  570571    1456  0.7945  0.0019  0.7259  0.7245
  570574    1564  0.7899  0.0021  0.7147  0.7157
  570577    1669  0.7813  0.0021  0.7038  0.7045
  .....
   numor    time     Pol     dpol    Pin(fit)  Pin(T)
```

- summary file "analyser _parameters-*lam*.txt"

Opacity	Tin	Tout	OPolHe	dOPHe	T1(mn)	dT1	T1(hr)	Chisq	T(P=0)	MT-Trans	dMT	Cell#
1.713	41	2594	1.2846	0.0000	4238	11	70.64	12.77	0.1804	0.900	0.004	8
1.692	2628	4048	1.2693	0.0000	4250	4	70.84	0.35	0.1841	0.900	0.004	11
1.713	4085	5499	1.2846	0.0000	4642	5	77.36	0.52	0.1804	0.900	0.004	8
1.687	5536	6835	1.2653	0.0000	4691	5	78.18	0.49	0.1851	0.900	0.004	11
1.702	7028	8366	1.2765	0.0000	4875	5	81.25	0.31	0.1823	0.900	0.004	8
1.629	8397	9741	1.2217	0.0000	4072	8	67.87	1.46	0.1961	0.900	0.004	11
1.707	9770	11482	1.2806	0.0000	4535	6	75.59	1.07	0.1813	0.900	0.004	8
1.677	11542	12821	1.2574	0.0000	3691	20	61.52	11.85	0.1870	0.900	0.004	11
1.745	12850	14057	1.3090	0.0000	4591	4	76.52	0.25	0.1746	0.900	0.004	11

Notes:
The "MT-Trans" parameters are the transmissions of the empty filters, and have been measured separately for each filter. They have been included into the code.
The Cell# is the identity of the filter (from [3]He lab)

C-4 Normalize and correct

C-4-1 Normalize data to Monitor2.

Click on the ==Normalise to Monitor== button.

Normalisation to monitor takes possible reactor fluctuations into account. In our case, it is all the more mandatory, since it also corrects for the decay of the polarizer transmission.

The recorded Monitor2 (Mon_2) value is the sum of the intensities measured in both polarization channels, so we need to scale the normalized intensities to the amount of time spent in the relevant polarization state.

$$I^{\pm}_{norm} = \frac{I^{\pm}_{meas} \, (Time^+ + Time^-)}{Scale \, \times Mon_2 \times Time^{\pm}}$$

Scale = 300000 * *M1M2* is a scale factor, chosen to obtain normalized intensities of the same order (in cts/s) as the measured intensities:
300000 is an average Monitor1 intensity (cts/s), to convert to
M1M2 is the ratio of monitors efficiencies :
- *M1M2*= 4.165 10^{-2} for experiments in 2016-2017

- *M1M2*= 0.0322 for experiments in March 2018 onwards

==The normalisation is performed for all scans in the given scan range==

Input:
- individual scans *numor*, where "*numor*" is the scan number, from the sub-directory "scans"

Output:

==*- html/pdf output all the normalized scan numbers*==
- individual normalized scans, saved as "norm_*numor*", where "*numor*" is the scan number, into the subdirectory "normalised_scans"
- monitor values of the individual scans, saved as

C-4-2 Correct data for polarizer and analyzer efficiencies.

Click on the <mark style="background-color: magenta">Correct for Filter Efficiency</mark> button.

This is done using equations (3) and (4). The errors are calculated as described above. Since the neutron polarization is currently not homogenous across the beam, there is the possibility to pick e beam profile from the popup menu
<mark style="background-color: yellow">The correction is performed for all scans in the given scan range</mark>.

Input:
- individual scans *numor*, where "*numor*" is the scan number, from the sub-directory "scans"

Output:

<mark style="background-color: yellow">*- html/pdf output all the corrected scan numbers*</mark>
- individual corrected scans, saved as "corr_*numor*", where "*numor*" is the scan number, into the subdirectory "corrected_scans"

C-5- Group scans measured in the same conditions.

Select the sample to treat from the popup menu
(the scan numbers are set automatically but can also be edited)
Click on the <mark style="background-color: magenta">Group and Average</mark> button.

See "average of corrected data".

C-6 Visualization of results.

The <mark style="background-color: yellow">sample names</mark> are those used in the data reduction above. They refer to the ave_*name* files in the "Averages" sub-directory