



Technical University of Denmark



*McStas*



CAMEA

# Comparison to the Cold Chopper Spectrometer

Author:

J. O. Birk



PAUL SCHERRER INSTITUT



ÉCOLE POLYTECHNIQUE  
FÉDÉRALE DE LAUSANNE

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Kinematic flux calculations</b>	<b>2</b>
<b>3</b>	<b>Flux simulations</b>	<b>3</b>
3.1	Results . . . . .	4
<b>4</b>	<b>Background</b>	<b>4</b>
4.1	Single scattering events. . . . .	4
4.2	Multiple scattering events . . . . .	5
<b>5</b>	<b>Other experimental issues</b>	<b>8</b>
5.1	Coverage . . . . .	8
5.2	High Resolution . . . . .	8
5.3	Time Resolution . . . . .	9
5.4	Thermal Measurements . . . . .	9
5.5	Bragg peaks . . . . .	9
<b>6</b>	<b>Conclusion</b>	<b>9</b>

## 1 Introduction

The cold chopper and CAMEA spectrometers are in many ways equivalent. One uses several incoming energies combined with a continuous outgoing energy band while the other use a continuous incoming band and several outgoing energies, and both have big angular coverage. They do however also have some key differences. CAMEA have a higher flux in each channel while the cold chopper have a bigger angular coverage, bigger resolution flexibility, and more freedom in choosing its energy range. Since CAMEA cannot compete with the cold chopper at very high resolutions it is important to investigate how the CAMEA compares to the cold chopper spectrometer in the primary operational region of CAMEA. For this comparison we have thus concentrated on settings where CAMEA excels (1.4% energy resolution, in plane scattering). We choose to consider only low temperature scattering i.e. where downscattering is dominating and a wavelength band of 3.1 Å to 4.76 Å.<sup>1</sup>

## 2 Kinematic flux calculations

It is possible to get an idea of how the two instruments will compare from simple kinematic considerations:

---

<sup>1</sup>When the flux simulations were done the natural length of long instruments at ESS was 170 m corresponding to a wavelengthband of 1.66 Å. In the meantime the numbers have been changed to 165 m and 1.7 Å. The results are however still valid for the new settings.

- CAMEA uses the full 71 ms pulse while the cold chopper can for similar resolution use 8 pulses of approximately 25  $\mu$ s (in Rep Rate Multiplication mode). This gives CAMEA a factor  $\sim 360$ .
- The reflectivity of the CAMEA analysers are on average about 50% if all 30 detectors are counted and beam attenuation is included. This gives the Cold Chopper a factor 2.
- Camea has 33% dark angles giving the cold chopper a factor 1.5.
- Camea have 30 detectors with a 1.4% resolution giving a total covered EF bandwidth of about 2 meV. The cold Chopper goes from 0.2  $E_i$  to  $E_i$  giving on average a 4 meV energy band. This gives a factor 2 to the cold chopper.
- We have so far only disregarded upscattered neutrons from the cold chopper. Approximately half information from the sample lies in the upscattering giving the cold chopper a factor 2.
- As we only regard downscattering CAMEA will get almost no signal from the analysers with the coarsest resolution (highest count rate) whereas the cold chopper will get the highest signal from the shortest wavelength. The exact effect of this needs simulation but a factor 2 is estimated.

Combining these factors one find that CAMEA will win with a factor 15 if only in-plane scattering is considered. But if out of plane scattering is also included The  $\pm 30^\circ$  coverage of the cold chopper will mean that the two instruments are comparable. However this is just an approximate calculation that amongst others does not take into account that

- the flux varies with the wavelength
- or there are small gaps between the analyser crystals.

Here, in order to reach a more accurate number, simulations have been performed.

### 3 Flux simulations

In order to compare the flux and coverage of the two instruments we performed a simulation with as equal settings as possible.

Both instruments used the same source, guide, chopper settings before the monochromating chopper, and same sample. The incoming and outgoing energy resolutions were chosen to match the outgoing resolution of CAMEA, and the bandwidth chosen were 3.1 to 4.76  $\text{\AA}$ . This resulted in a factor 380 in favour of CAMEA at the incoming flux.

For simplicity the secondary spectrometers were simulated individually. The ESS source was set to focus directly on the sample. A sample with a scattering cross section of  $\frac{d\sigma^2}{d\Omega dE} = \frac{k_f}{k_i} s(q, \omega)$  with constant  $s(q, \omega)$  was chosen as to not

favour one instrument that eg. happened to match a certain excitation curve. The signal just before the analysers was compared to the signal in the detectors to measure the fraction of the beam from the sample that each detector records. Afterwards the data was corrected for beam attenuation through the analysers and an average graphite reflectivity of 70% was chosen. Finally dark angles and the smaller vertical coverage of the backmost analysers of CAMEA were included. Only down scattering was considered.

### 3.1 Results

Comparing the two instruments gives a factor 22 to the CAMEA instrument if a  $\pm 2^\circ$  opening angle is considered. If one considers the full  $\pm 30^\circ$  detector coverage, the two instruments are almost equal CAMEA having 50 % more counts. It is thus clear that CAMEA in its key performance is more powerful than the cold chopper. This is however not a full and fair comparison as other experimental considerations lead to the cold chopper being the best choice in many cases.

## 4 Background

The two instruments deal with background in very different ways. The cold chopper will almost only allow useful neutrons on the sample but is not able to distinguish neutrons coming from the sample region from each other. CAMEA will have a much higher flux on the sample and relies on shielding and analyser crystals to sort away background neutrons. If a sample is placed completely alone in vacuum the cold chopper will probably be able to reach a lower background level since there will not be any background from the analysers. On the other hand it is easier to install vertical collimation on CAMEA so if there is a strongly scattering sample environment around the sample the cold chopper suffers far more than CAMEA.

Another important issue is the distribution of the background. Any neutron scattered from the sample surroundings of the cold chopper will get additional flight path and thus appear as inelastic background. On CAMEA the tens of cm difference in flight path will be small compared to the 165 m primary flight path so the extra background will fall within the elastic line. This is not the case for direct time-of-flight.

Heavy sample surroundings will cause an increased background in neutron scattering experiments. Two examples of such problems can be seen in figure 1 and shows how scattering from sample surroundings on time-of-flight spectrometers can pollute the inelastic region. We will in the following treat the background in two groups: Single and multiple scattering events.

### 4.1 Single scattering events.

These can be reduced by applying collimation however, if the sample environment has strong scatterers close to the sample it is impossible to shield it entirely,

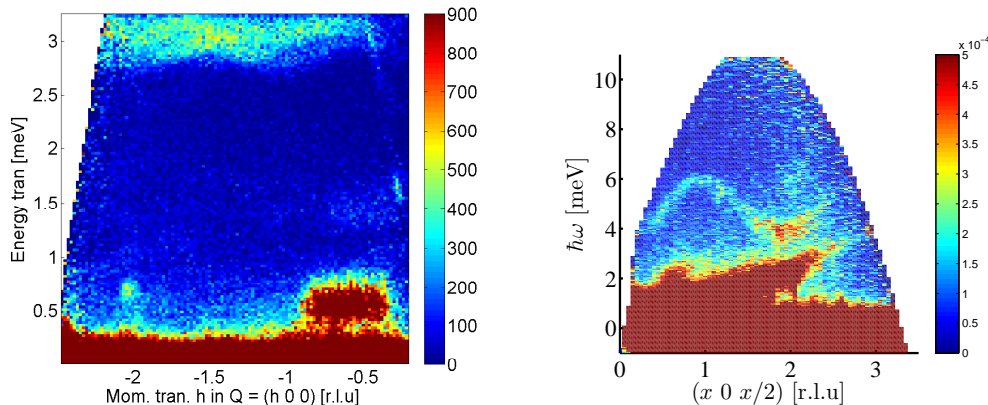


Figure 1: Examples of background from sample surroundings. Left: LET data of  $\text{SrCu}_2(\text{BO}_3)_2$  in an orange cryostat ( $E_i=12$  meV). Right: CNCS data on  $\text{CoCl}_2 \cdot 2\text{D}_2\text{O}$  with the 16 T magnet 'Fat Sam' that has a radius of 40.5 cm ( $E_i=12$  meV). The signals close to the elastic line are from the sample surroundings and stronger than the inelastic signal from the sample. In both cases the background can be reduced by the right choice of collimation/cryostat.

although the limited opening angle of CAMEA can help shielding material above or below the sample. The signal will however look sample like - i.e. Bragg peaks, Debye Scherrer cones and phonon dispersions and these can be mapped out by measuring without a sample.

## 4.2 Multiple scattering events

Although the cross section for multiple scattering is low, sufficient amounts of material in the sample surroundings can cause the elastic signal from these events to shadow inelastic scattering. Collimation can limit the problem but there is no way to shield for example the events shown in figure 2 by external collimation. The exact distribution of such background will depend on the precise layout of the sample surroundings but it is possible to calculate limits on the background distribution. Assuming that the multiple scattering respectively adds or subtract a distance  $\Delta l$  from the flight path the recorded of the neutron energy ( $E'$ ) will be:

$$E' = E \left( \frac{l}{l \pm \Delta l} \right)^2 \quad (1)$$

where  $l$  is the flight path used for time-of-flight measurements and  $E$  is the actual energy of the neutron. Since CAMEA uses analysers to determine  $E_f$  the distance in question will be the 165m primary flight path while it for direct time-of-flight will be the  $\sim 4$  m secondary flight path. This leads to the distribution seen in figure 3 left.

The extreme values for  $\Delta l$  that will make it through a radial collimator can be found from figure 2. The minimum will be  $\Delta l = R(\sqrt{2(1 - \cos(2\theta))} - 2)$ , where  $R$

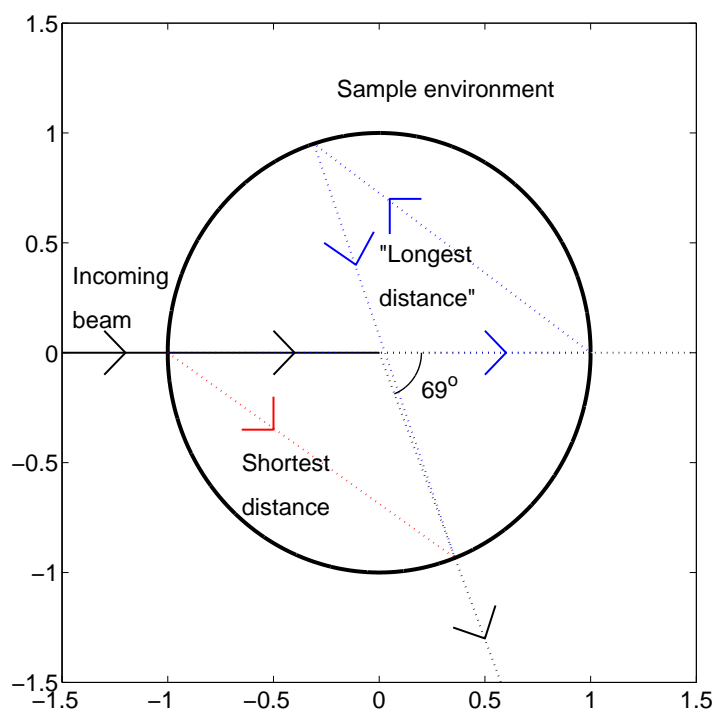


Figure 2: The longest (blue) and shortest (red) paths a neutron can travel to a detector at  $2\theta$  with maximum 2 scattering events if radial collimation removes neutrons that do not come from the sample direction.

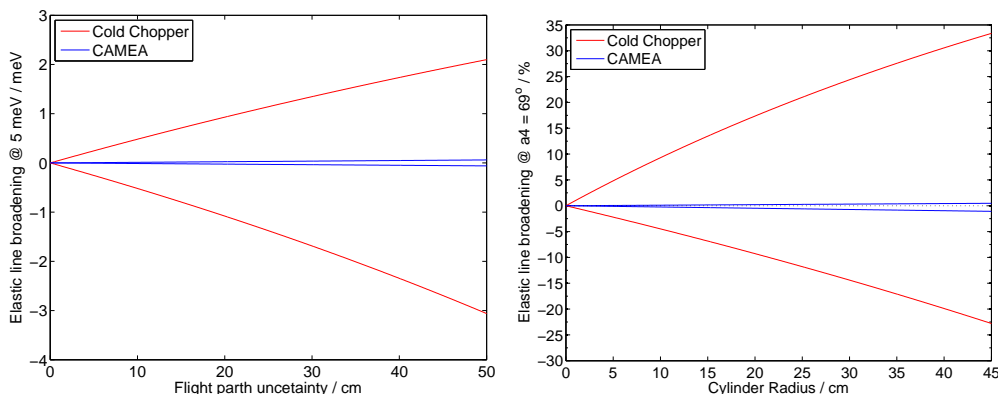


Figure 3: Boundaries for multiple scattering in the sample surroundings with maximum two scattering events pr. neutron. Left: calculated from a the travel path uncertainties. Right: Calculated from the longest  $\Delta l$  possible withing a cylinder of a given radius, as described in figure 2.

is the radius of the sample environments and  $2\theta$  is the recorded scattering angle. The maximum is in principle infinite but discarding events with more than two scatterings as higher order we reach a limit of:  $\Delta l = R * (\sqrt{2(1 - \cos(2\theta))} + 2)$ . At CAMEA the minimum path will be recorded as down scattering, while the maximum will appears as up scattering, while it is opposite for direct time-of-flight. These boundaries for multiple scattering from sample surroundings are displayed in figure 3 right for the centre of the CAMEA detector ( $2\theta = 69^\circ$ ). It can be seen that in the down scattering region where CAMEA is designed to deliver its optimal performance the extend of the scattering is less than  $\Delta E/E \approx 0.5\%$ . So multiple scattering will be contained in the elastic line, while it for direct time-of-flight can cause problems for low lying excitations and quasi elastic scattering with  $\Delta E/E \approx 30\%$ . On the up scattering side the maximum deviation can get close to 1% so in the most extreme cases it might cause a small widening of the elastic line on CAMEA while it can again ruin inelastic data on direct time-of-flight machines with  $\Delta E/E \approx 25\%$ .

It is important to note that the above equation do not predict that big inelastic regions will be overshadowed by multiple scattering events. It merely places a limit on what region can potentially be overshadowed by double scattering. Figure 1 does however confirm that the effect can be a real issue on direct time-of-flight spectrometers.

For direct time-of-flight one can obtain better results than shown in figure 1 by applying radial collimation outside the sample environment, reduce the sample environment in the beam, or incorporate radial collimation in the sample environments. This makes measurements with specialised light and medium level environments achievable but the bigger the amount of material the harder it becomes. For certain kinds of environments such as very strong magnets or pressure cells it is impossible to reduce the environments at beam height enough, or to add a radial collimator in the presure cell case. In these cases it will be easier to measure low lying excitations and quasi-elastic scattering on CAMEA.

Especially if the inelastic signal is weak, for example because a small sample is used.

It is possible to subtract parts of this background by measuring without the sample but if the multiple scattering event involved the sample, subtraction will be inaccurate. This can however only happen for  $\Delta l > 0$  so it is possible to map out all contribution from multiple scatterings without the sample on the down scattering side on CAMEA and up scattering side on direct ToF. Note that in the examples from figure 1 the background is much stronger than the inelastic signal from the sample so even if it is mapped out it might not be possible to reliably retrieve any actual data hidden below it.

We have assumed elastic scattering background events. Multiple scattering from sample surroundings including inelastic scattering can of course also occur but the cross section is substantially smaller and the events cannot be given the same meaningful limits as in the elastic case.

This further emphasises that CAMEA is an extremely strong instrument in the presence of complex sample environments but it will not be able to compete with the cold chopper at all settings.

## 5 Other experimental issues

### 5.1 Coverage

The cold chopper spectrometer looks at the elastic line with all RRM frames whereas the amount of analysers looking at it in CAMEA will be different. Usually only the high  $E_f$  frames will be recording the elastic line; the others will be concentrating on the down scattering region. This means that CAMEA will have a worse resolution at the elastic line but a much higher coverage in the inelastic than the elastics while the cold Chopper will have the highest coverage at the elastic line and lowest in the deep inelastics. (It is possible for CAMEA to have high coverage and good resolution at the elastic line too. By choosing a wavelength band that will enable the 2.5 meV analyser to record elastic scattering a resolution of 20  $\mu\text{eV}$  can be achieved but in that case the covered area will shift towards the upscattering region.) This difference makes the cold chopper even better at quasi elastics and emphasises the CAMEA strength in low temperature inelastic measurements.

### 5.2 High Resolution

CAMEA can reach a  $\frac{\Delta E}{E}$  resolution of just above 1.1% at 5 meV by using unmatched primary and secondary resolutions but will lose a substantial part of its flux doing so (the matched value is  $\frac{\Delta E}{E} = 1.4\%$ ). The cold chopper can not only reach these levels with a smaller loss by matching the resolutions. It will also be able to surpass it, making far more accurate measurements.



### 5.3 Time Resolution

Both CAMEA and the cold chopper can in principle have good time-resolution for time dependent experiments. However the monochromating chopper of the cold chopper means that the time where a certain energy transfer is recorded will be comparable to the time resolution of  $30 \mu\text{s}$  while it will be 100 times longer (3 ms) than the time resolution on CAMEA. This means that CAMEA will be able to resolve many processes with constant experimental settings while this can only be reached by running a stroboscopic measurement with a different frequency than the ESS pulse at a cold chopper instrument. The later will make for much longer experiments and together with the lower count rates makes many experiments unrealistically long on a cold chopper instrument while manageable on CAMEA.

### 5.4 Thermal Measurements

If we consider up-scattering the cold chopper will at first glance win a lot since the outgoing bands can be increased to any energy for almost no cost in time and it will thus be possible to reach any energy coverage. Of course much of this gain is insubstantial since the resolution will worsen considerably. None the less the Cold Chopper Spectrometer will gain compared to CAMEA in conditions where up-scattering is relevant.

### 5.5 Bragg peaks

The high intensity of CAMEA means that some Bragg peaks will be strong enough to harm the detectors if they are not protected for example by reducing the efficiency of the detectors that are illuminated by a Bragg peak. The problem will be much smaller at the cold chopper spectrometer. The primary focus of a spectrometer is however not to measure high intensity Bragg peaks so the problem will be small for practical measurements.

## 6 Conclusion

The Cold chopper spectrometer has an impressively large achievable parameter space compared to most other spectrometers and will be an excellent flexible spectrometer that can handle most challenges but will not be able to compete with more specialised instruments within their optimal field of operation.

CAMEA will have 22 times higher count rates and lower inelastic background when cold samples and extreme environments are needed. Both instruments thus have a clear role in an instrument suite.