Spectroscopy division: Overview rescoping of instruments.
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In this overview we present the most important needs for high performance of the spectroscopy instrument. Additional needs are presented in the individual instrument rescoping documents. Sample environment needs are not considered in this document.

Instrument	Rescoping option	A: Scientific Impact (5: high, 1: low)	B: Manpower (1:high, 5:low)	C: Technical Risk (1:high, 5:low)	B: Cost	FOM: A*B*C
VESPA	T0 chopper	5	Some (Chopper group) 4	5	**0.85 M€**	100
VESPA	Increase analyser modules	4	Can be included and delivered within current instrument construction: 5	4	**3.6 M€ for 10 (0.36 each)**	80
CSPEC	^{3}He full detector coverage (2.5 bar)	5	Minimal: 5	5	**2.025 M€**	125
CSPEC	^{3}He full detector coverage (5 bar)	2	Minimal: 5	5	**+4.375 M€**	50
T-REX	Full detector coverage	5	Significant (Detector group) 1	3	**>5 M€**	15
T-REX	Extra blades for P chopper	2	Julich chopper group: 3	2	**0.5 M€**	12
MIRACLES	Complete Analyser/collimator/detector coverage Si (1 1 1) & (3 1 1)	3	Can be included and delivered within current instrument construction: 3	1	**1.67 M€**	9

VESPA

(1) T0 Chopper: **0.85 M€**

Resources needed: Requires significant resources from the chopper team.

The current SNR of TOSCA and VISION are estimated to 3×10^{-3}, and the Signal to Noise Ratio (SNR) target for next generation NVS instruments, TOSCA+ and VESPA, should be 10^{-4} or better. A T0 chopper will be essential to optimise the SNR on VESPA. VESPA is a straight guide instrument that views the thermal moderator. Previous instruments with such a guide configuration have observed a significant improvement in SNR with the introduction of a T0 chopper to remove the fast neutron prompt pulse. A particular, and published, example is that of 4SEASON, see Figure 1, showing that a T0 chopper can improve the SNR by an up to order of magnitude.

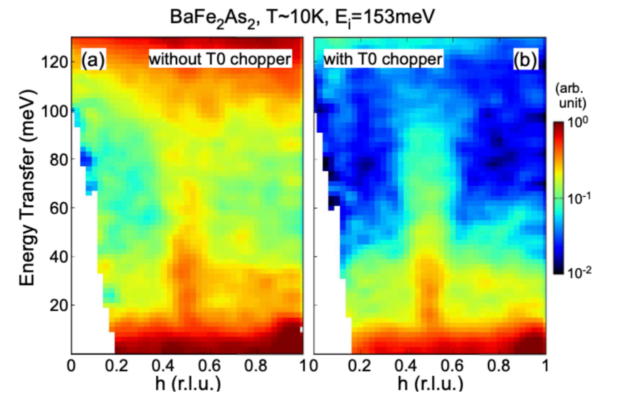

Figure 1: The effect of a T0 chopper on straight guide instrument 4SEASONS [1].

VISION, the vibrational spectrometer of SNS, studied the effect of a T0 chopper with test measurements of the empty cryostat while progressively dephasing their T0 chopper up to 30 μs from its nominal phase, private communications. Their results indicate that, in the TOF range where the pulse is generated, and where γ and epithermal neutrons can be directly detected by the detectors, the background increases by a factor 17. Note that these catastrophic degradations of the background occur when the T0 chopper is dephased by only 30 μs: the background increase would be worse if the T0 chopper was to be parked open. The ESS will have a long pulse and significantly larger source power than existing MW spallation facilities, and as such the background issues due to high energy neutrons can be expected to be significantly worse. In the absence of T0 chopper, the elastic line and the high energy region of the spectra, corresponding to the TOF range 0-10 ms, are expected to be unusable.

(2) Increase analyser modules: 10 x 0.36 = **3.6 M€**

Resources needed: The instrument team can implement these upgrades as part of the current instrument build.

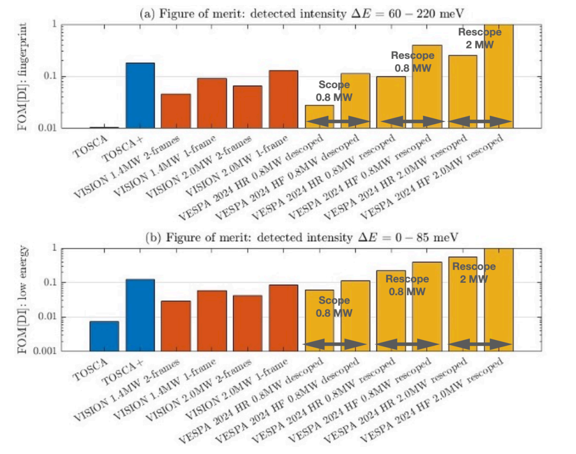

Figure 2: Normalised FOM of VESPA and other NVS instruments, for (a) the fingerprint region of the spectra and (b) at low-energy.

As most experiments are flux limited, a suitable figure of merit (FOM) is to consider a quantity proportional to the detected intensity:

$$\mathrm{FOM} = \Phi \cdot \frac{\Omega}{4\pi} \cdot T_{\mathrm{Be}} \cdot \eta \cdot \Delta\theta \cdot R$$

where Φ is the peak flux (brightness) on a 1×1 cm^2 area in n/s/cm^2, integrated in energy over the fingerprint or low-energy regions, Ω is the solid angle coverage of the analysers in sr, T_{Be} is the transmission of the beryllium filter in %, η is the detection efficiency of the detectors in %, $\Delta\theta$ is the mosaic spread of the analyser crystals in degrees, and R is the peak reflectivity of the analyser crystals in %.

The FOM metrics, normalised to the completed VESPA in high-flux (HF) setting and with 2.0 MW source power, are reported in Figure 2. The day 1 performance of a descoped VESPA with reduced source power are only 11% of that of the complete instrument at nominal power. In the fingerprint region, the high-flux setting of a descoped VESPA has comparable performance to those of VISION, while the high-resolution setting, which has an energy resolution comparable to that of VISION, has about 3 times less flux. Rescoping the instrument by fully completing the spectroscopy banks corresponds to a gain of 3.5 in detected intensity and makes the high-resolution setting on par with VISION. Note that both a fully rescoped instrument and the 2.0 MW source power are required to provide a significant improvement in flux compared to existing instrument.

In the low energy range, because of the large cold neutron brightness of ESS, even a descoped VESPA in high-resolution mode has comparable performance to those of the existing NVS instruments.

A fully rescoped instrument will make VESPA world leading, enabling significantly more sensitive measurements and, most importantly, in-situ studies that can access very weak hydrogenous content in the investigation of, for example, solids and liquids, soft matter, complex fluids, and biomaterials.

CSPEC

(1) ^{3}He completion (2.5 bar): **2.025 M€**

Resources needed: Only the procurement of ^{3}He *is needed.*

Cold chopper spectroscopy has seen enormous success in the last 20 years due the access of a broad 4 dimensional S(**Q**, ω) that can be mapped directly to theoretical developments. The broad overview, both for S(Q, ω) and S(**Q**, ω), significantly helps to restrict theoretical models and determine subtle variations in diffusive parameters and exchange interactions. The scope of the CSPEC detector, see Figure 3, provides 58% of the completed detector coverage with a ^{3}He pressure of 2.5 bar. This means that the broad **Q** coverage is compromised. In addition, the neutron detection efficiency is significantly reduced, with 2.5

bar, for λ< 6 Å, providing less than 2 x detection efficiency when compared to the world leading instruments, IN5 (5 bar), CNCS (6 bar), LET (10 bar) and AMATERAS (10 bar).
Figure 3 shows the day 1 scope coverage and the detector regions that need to be rescoped, these include a low negative 2θ region (in yellow) and the extended Q region (in turquoise).

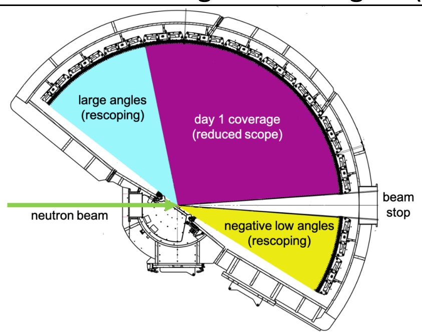

Figure 3: Detector coverage of the CSPEC instrument showing the scope of the instrument and the requested rescoping.

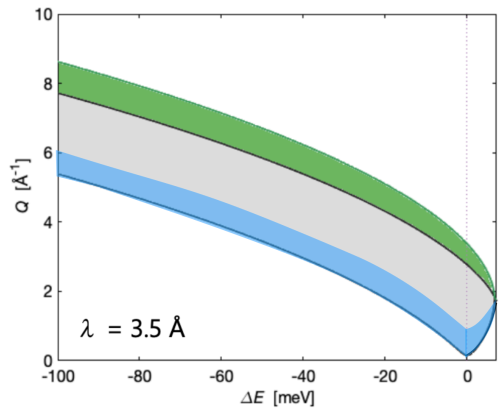

Figure 4: CSPEC S(Q, ω), for λ_i = 3.5 Å, showing full detector scope, with the scope reduction in blue (negative low angles) and green (large angles).

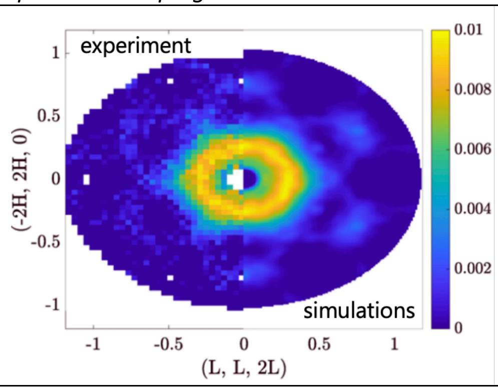

Figure 5: Single crystal magnetic S(Q, ω = ΔE) scattering of Yb3Ga5O12,) as measured on the old chopper spectrometer of the SNS, CNCS, with λi = 7.265 Å. Comparison of experimental data and RMC fit (left and right, respectively).

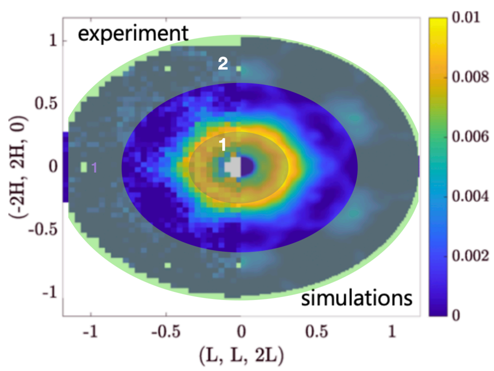

Figure 6: Data from Figure 5 with regions in green representing the regions where the CSPEC detector will be rescoped. Region 1 is the negative low angle region and region 2 is the large angle region.

Figure 4 shows the effect of this descoping on S(Q, ω) for λ=3.5 Å. Figure 5 shows a typical S(**Q**, ω) scattering profile measured to determine the low lying excitations in a hyperkagome frustrated magnet as measured on CNCS (SNS)[2]. Figure 6 marks the effect of the CSPEC detector descoping on such a data set. Region 1 will have limited detector coverage and thus detection efficiency is reduced by a factor of 2 and region 2 is not accessible with the current detector scope of CSPEC.

The FOM for time-of-flight spectroscopy is given by

$$\mathrm{FOM} = \Phi \cdot \Omega \cdot E$$

where Φ is the peak flux (brightness) in n/s/cm^2, Ω is the solid angle coverage of the detectors and E is the detector efficiency. Different scenarios are presented in Figure 7 comparing the world leading instruments, IN5, LET, CNCS and AMATERAS with CSPEC, current scope and full scope, 0.8 and 2 MW and 2.5 and 5 bar ^{3}He. In single pulse mode, the mode most commonly employed on current day spectrometers, it is clear that CSPEC will not be world leading until full detector coverage is provided with 2 MW ESS power. Increasing the detector efficiency further is not essential for early science. However, ensuring that the RRM mode is effectively employed will be essential since large gains in FOM can be made in this mode.

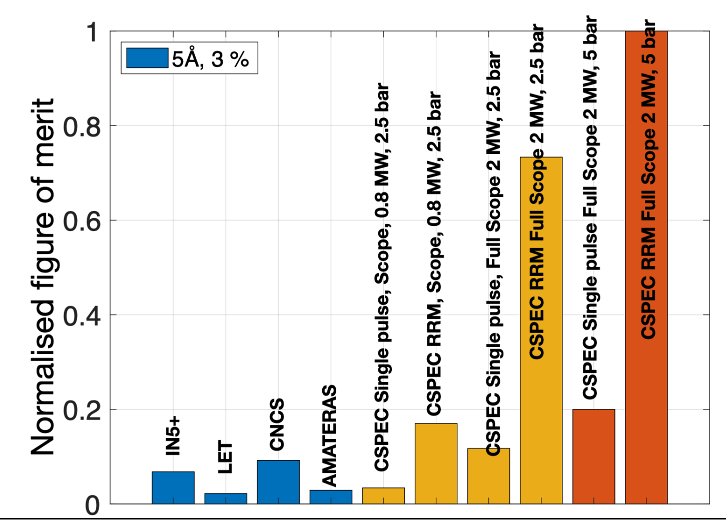

Figure 7: Comparison of the normalised FOM for tof spectrometers with the recently upgraded IN5, LET, CNCS (2 MW) and AMATERAS compared to CSPEC single pulse and RRM for 0.8 MW and 2 MW ESS power and 2.5 and 5 bar ^{3}He pressure.

The request is therefore that the CSPEC detector coverage shall be completed with 2.5 bar ^{3}He. Any further increase in gas pressure can be considered once the instrument is operational.

T-REX

(1) Complete detector coverage from 40 – 100 %. **2 M€ for detector boxes + detectors (cost to be provided by the detector group)**

Resources needed: Significant resources needed from the detector group – however these will be as a continuation of the current project and can possible be outsourced to a company.

Similar to the cold chopper spectroscopy, thermal chopper spectroscopy also benefits from scattering profiles across broad swathes of S(**Q**, ω).

The T-REX detector was descoped to 40% of its full coverage, see Figure 8, with like CSPEC, a descoping of a low Q negative detector region and a high Q region. We show a constant-energy slice of magnon scattering in a honeycomb ferromagnet at T = 1.7 K, measured with an incoming energy of 15 meV as measured on the recently commissioned instrument thermal chopper spectrometer of the ILL PANTHER, Figure 9. Superposed on Figure 9, Figure 10, are the regions that are affected by the descoping of detector on T-REX. In pink is the low Q region that will, in comparison to comparable instruments, have 50 % detection intensity. In green is the low Q region that will not be accessible with the current detector scope. Upgrading the detector can be done step by step whenever a new detector module, each covering 18° horizontal angle, is ready as integration time and cost allows.

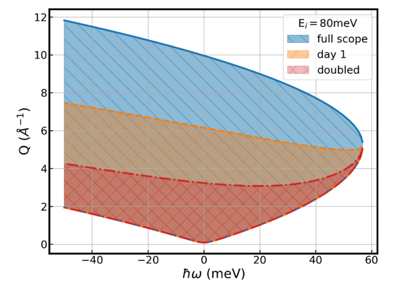

Figure 8: T-REX S(Q, ω), for λ_i = 1.01 Å, showing full detector scope, with the scope reduction in red (negative low angles) and blue (large angles).

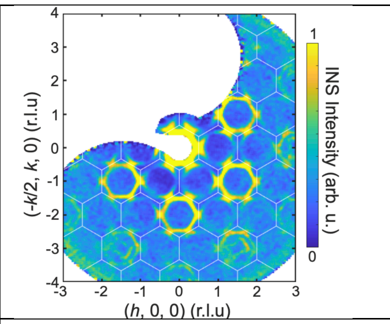

Figure 9: Constant-energy slice of magnon scattering in a honeycomb ferromagnet at T = 1.7 K, measured with an incoming energy of 15 meV. The data are integrated over energy transfers between 4 and 5 meV [3].

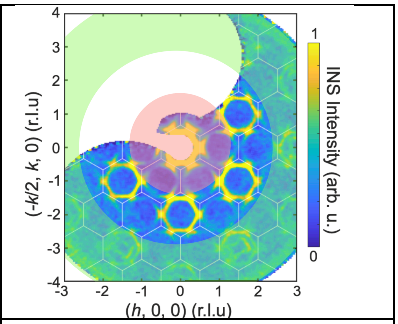

Figure 10: Data from Figure 9 with regions in pink and green representing the regions where the CSPEC detector will be rescoped. Pink region is the negative low angle region and the green region is the large angle region.

The normalised FOM for T-REX, presented in Figures 11 and 12, are given by

$$\text{FOM} = \Phi \cdot \Omega$$

where Φ is the peak flux (brightness) in n/s/cm^2, Ω is the solid angle coverage of the detectors. The full detector coverage is therefore needed to provide a significant improvement over existing instruments at 2MW ESS power.

Figure 11 shows the normalised FOM for thermal chopper spectrometers, Ei = 50 meV, ΔE/E = 5%, compared to T-REX with initial detector scope and 2 MW ESS power. Figure 12 shows the normalised FOM for thermal chopper spectrometers, Ei = 50 meV, ΔE/E = 5%, compared to T-REX with full detector coverage and 2 MW ESS power. It is again clear that it is essential for T-REX to have its full detector coverage and that full use of RRM modes must be available.

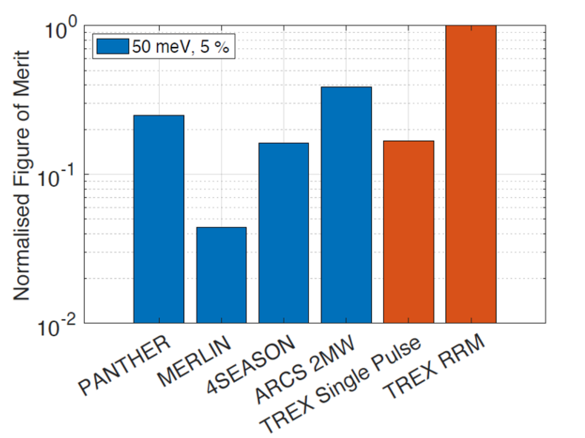

Figure 11: Normalised FOM for thermal chopper spectrometers compared to T-REX scope and 2 MW ESS Power.

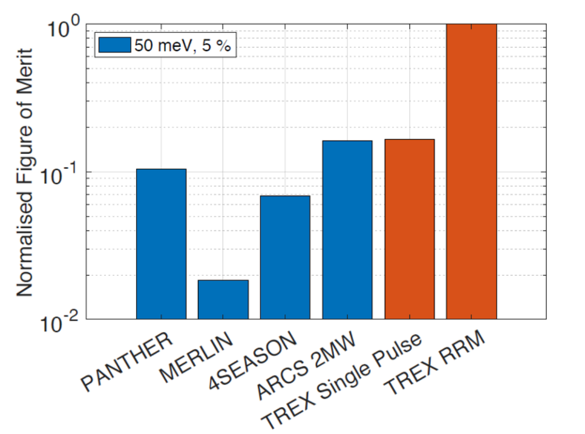

Figure 12: Normalised FOM for thermal chopper spectrometers compared to T-REX full scope and 2 MW ESS Power.

(2) Additional 2 discs for pulse shaping choppers. 0.5 M€ (current estimate)
Resources needed: Julich resources.

The P-chopper at 108m is cutting the long ESS pulse into sub-pulses up to 24 RRM (repetition rate multiplication) pulses and controls the incident wavelength resolution of these pulses. In day-1 scope, the chopper system is equipped with two chopper discs separated by 10cm along the neutron path. The chopper housing is already designed and built to host up to 4 discs in 2 pairs in over/under configuration, in day-1 scope only the two upper discs exist. All discs feature two openings of 35° and 20° for high-flux and high-resolution measurements, respectively. An upgrade to four discs would allow T-REX to decouple the energy resolution of the primary spectrometer from the repetition rate of the chopper by allowing advanced pulse shaping options. Essentially, the triangular transmission function of a two-disc assembly can be changed to a trapezoidal or rectangular shape, therefore cutting tails that worsen the resolution. This is especially useful in cases of deep inelastic scattering, where the resolution of the primary spectrometer can be matched to the already very good resolution of the secondary spectrometer providing a unique capability.

This is an upgrade that can be facilitated at a later stage.

MIRACLES

(1) Rescope: Complete the analyser bank with Si (1 1 1) and (3 1 1) analysers (plus detectors and radial collimator) to the right side. **1.67 M€**

Resources: The upgrade can be done without any disruption of the operation program, since all the integration, installation and adjustment features have already been manufactured, in anticipation to this completion effort.

MIRACLES will, within scope, provides analyser coverage with Si (1 1 1) crystals, on one side of the MIRACLES detector tank, that provides momentum transfer up to approximately 2 $Å^{-1}$. Rescoping the instrument will extend the Q-range up to 3.8 $Å^{-1}$ using Si (3 1 1) analyser crystals, already a possibility on comparative backscattering instruments such as BASIS (SNS) and DNA (JParc). Extending the Q-range of the instrument will enable more detailed analysis over broader spatial scales often performed using several instruments. In-operando studies, as needed for example for rapidly screening battery materials, will particularly benefit from the extended Q-range. An example is shown in Figure 13 which shows a study on the reorientational dynamics of metal borohydrides using the high flux back scattering spectrometer (HFBS), the time-of-flight disc chopper (DCS) and the neutron spin echo (NSE) instruments at NIST. Rescoping MIRACLES with Si (3 1 1) would extend the Q range and will provide information up to 3.8 $Å^{-1}$, see blue region in Figure 13, in a single measurement thereby enabling the determination of different reorientational dynamics in complex materials. This rescoping is considered essential for MIRACLES to be competitive with current world leading instruments.

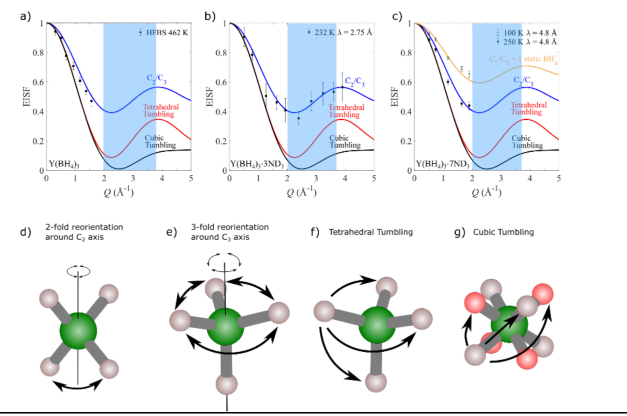

Figure 13: Figures from [4] EISFs determined from QENS spectra for (a) Y(BH4)3, (b) Y(BH4)3·3ND3, and (c) Y(BH4)3·7ND3 at different temperatures compared to EISF models for each respective system. (d-g) Representations of common reorientational motions for a tetrahedral anion.

Polarisation analysis on all instruments. Polarisation analysis (PA) provides tremendous opportunities for spectroscopy instruments. This has been exemplified by the successes on the chopper spectrometer LET of ISIS which has recently been equiped with neutron polarization analysis using a combination of a supermirror polarizer and ^{3}He wide-angle analyser system [5]. A particular example is that of a neutron spectroscopy PA study on water relaxation that shows significant coherent scattering of water from meso to intermolecular scales calling into doubt decades of work that considered most of the scattering profiles to be derived from incoherent contributions only. All spectroscopy instruments, except VESPA, have future proofed their instrument design to enable PA. T-REX will incorporate PA from day 1 but MIRACLES, CSPEC and BIFROST will require further technical developments that can be delivered once the instruments are operational. We therefore do not consider PA within this rescoping exercise.

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[2] L. Sandberg *et* al. *PHYSICAL REVIEW B* **104**, 064425 (2021)
[3] B. Fåk *et* al. *EPJ Web of Conferences* **272**, 02001 (2022)
[4] J. B. Grinderslev *et* al. *J. Phys. Chem. C*, **128**, 4431–4439 (2024)
[5] A. Arbe *et* al. *Phys. Rev. Research* **2** 2022015(R) (2020)