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Published in:
Review of Scientific Instruments

DOI:
10.1063/5.0059907

Publication date:
2021

Document version
Publisher’s PDF, also known as Version of record

Citation for published version (APA):
Deen, P. P., Longeville, S., Lohstroh, W., Moreira, F., Fabrèges, C., Loaiza, L., & Noferini, D. (2021). CSPEC: The cold chopper spectrometer of the ESS, a detailed overview prior to commissioning. Review of Scientific Instruments, 92, [105104]. https://doi.org/10.1063/5.0059907
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Cite as: Rev. Sci. Instrum. 92, 105104 (2021); https://doi.org/10.1063/5.0059907
Submitted: 14 June 2021 • Accepted: 13 September 2021 • Published Online: 07 October 2021

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Cite as: Rev. Sci. Instrum. 92, 105104 (2021); doi: 10.1063/5.0059907
Submitted: 14 June 2021 • Accepted: 13 September 2021 •
Published Online: 7 October 2021

P. P. Deen,1,2,a) S. Longeville,3 W. Lohstroh,4 F. Moreira,1 G. Fabrèges,3 L. Loaiza,4 and D. Noferini1

AFFILIATIONS
1 European Spallation Source, Tunavägen 24, 22363 Lund, Sweden
2 Nanoscience Center, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen Ø, Denmark
3 Laboratoire Léon Brillouin, Université de Paris-Saclay, CEA/CNRS UMR 12, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France
4 Heinz Maier-Leibnitz Zentrum, Technische Universität München, 85748 Garching, Germany
a) Author to whom correspondence should be addressed: pascale.deen@ess.eu

ABSTRACT
CSPEC is the cold chopper spectrometer of the European Spallation Source (ESS) and will come online with the ESS beam on the target. CSPEC will be the first cold chopper spectrometer on a long pulsed spallation source, which provides great opportunities in terms of signal to noise and novel measuring schemes. We provide a detailed overview of the instrument, scientific design considerations, and engineering requirements.

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I. MEASURING DYNAMICS IN MATERIALS
The properties and functionality of materials are derived from where atoms are and how they move. Understanding atomic positions and movement is, therefore, essential to test, in a stringent manner, theoretical models of materials. Dynamic behavior in materials can vary enormously. Collective modes such as phonons and magnons, with picosecond timescales, can determine thermal and electrical conductivity of materials. Quantum fluctuations give rise to new states of matter in the nanosecond to picosecond regime. Rotational and translational diffusion are important for many bio-physical processes in the picosecond to microsecond regime. A chopper spectrometer can access a broad range of timescales from picosecond to nanosecond fluctuations, with the associative spatial scales, and is thus a workhorse instrument for understanding material properties. In this paper, we provide the scientific and technical requirements that have led to the design and construction of the cold chopper spectrometer of the European Spallation Source (ESS), CSPEC.

Inelastic neutron scattering (INS) encompasses broad energy and spatial domains and is generally subdivided into two distinct regimes: first, a measure of the energy transfer of neutrons interacting with matter with scattering processes at small energy scales, quasielastic neutron scattering (QENS), and second, generally at higher energy transfers through the creation and annihilation of elementary excitations, inelastic neutron scattering (INS). The resultant double partial differential cross section, for both QENS and INS, is proportional to the dynamic structure factor $S(Q, \omega)$ and depends on the wavevector transfer between the sample and neutrons, $Q$, and the neutron energy transfer between the sample and neutrons, $\omega$.

Neutron scattering is particularly effective since $S(Q, \omega)$ can be derived within the Born approximation, which can be expressed directly in terms of space and time dependent correlations. Indeed, $S(Q, \omega)$ represents the space and time Fourier transform of the probability of finding atoms or spins, $i$, separated by a particular distance to atoms or spins, $j$, at a particular time $t$, $r_i(t)$. As such, one directly compares the experimental signatures, $S(Q, \omega)$, with complex theoretical models of the material probed.

A direct geometry spectrometer is a workhorse instrument for any neutron scattering research facility providing an unparalleled overview of $S(Q, \omega)$ with simultaneous insight into spatial and dynamic correlations over a wide region of reciprocal space. Direct geometry chopper spectrometers exist at reactor sources, for instance, INS (ILL), TOFTOF (FRM2), and DCS (NIST), and short pulse spallation sources, such as LET (ISIS), CNCS (SNS), and AMATERAS (J-PARC). Here, cold chopper spectrometers are
singled out to make a direct relevant comparison with CSPEC. Each instrument aims to optimize signal to noise within a neutron energy range that permits the scattering, from the sample, of neutrons with nearly infinite energy gain to those with energy losses down to 20% of the incident neutron energy. A reactor source chopper spectrometer is usually designed to optimize the flux for a single incident wavelength, while a spallation source instrument is able to provide a broad incident wavelength band via the use of repetition rate multiplication (RRM). To date, the relative flux on the sample between reactor and spallation source chopper spectrometers depends on the peak brilliance of the facility and the ratio of the frequency of the neutron pulse on the sample (50–300 Hz, typically) on a reactor source to the frequency of that on the spallation source (25–60 Hz). Through the use of repetition rate multiplication (RRM), a range of monochromatic neutron pulses with various wavelengths impinge on the sample within each spallation period. On current day chopper spectrometers, these adjacent incident pulses cannot be accumulated due to their widely varying incident energies. In contrast, on CSPEC, scattered neutrons with closely matched incident energies can be accumulated to improve the flux on the sample. The noise at the various facilities can vary significantly. A reactor source chopper spectrometer is always affected by the continuous operation of the reactor, providing a time independent neutron background, while a spallation source instrument will observe a burst of high energy neutrons from the prompt pulse of the spallation process, as the proton pulse collides with the target to produce neutrons, but is clean in between.

CSPEC, the cold chopper spectrometer of the ESS, is optimized to harness the significant peak and average flux of the European Spallation Source while taking advantage of the low noise levels that accompany spallation. CSPEC has been developed to study life sciences, energy, and functional materials in addition to emergent sciences, energy, and functional materials in addition to emergent techniques, such as cold or thermal neutrons, is given by

\[
E = \frac{p^2}{2m_n} = \frac{h^2 k^2}{2m_n},
\]

where \(h\) is the reduced Planck’s constant, \(k = \frac{2\pi}{\lambda}\), and \(m_n = 1.675 \times 10^{-27}\) kg is the neutron mass. The CSPEC guide extracts neutrons from the ESS 20 K parahydrogen moderator. The kinetic energy of the neutrons equals 1.72 meV for \(T = 20\) K, given by \(k_B T\) with \(k_B = 1.381 \times 10^{-23}\) JK\(^{-1}\). This energy, via the de Broglie relation, provides a frequency of 0.42 THz directly relevant to the kinetic energies and fluctuations found in materials.

A time of flight chopper spectrometer probes the dynamic energy scale of a sample using the time of flight of nearly monochromatic neutrons interacting with the sample and scattered into the detector. The energy resolution of the instrument will determine the lowest energy transfers that can be probed. The energy resolution, \(\Delta E\), is determined by the wavelength uncertainty, \(\Delta \lambda\), which in turn is derived by the time of flight uncertainty, \(\Delta t\), given by

\[
E[\text{meV}] = \frac{81.81}{\lambda^3[\text{Å}^3]} \times \frac{\hbar \pi}{m_n \text{[kg]} L_{SD}\text{[m]}},
\]

with \(L_{SD}\) being the sample to detector distance, providing the relationship

\[
f[\mu\text{s}] = 252.79\lambda[\text{Å}] L_{SD}\text{[m]}.
\]

As such, the energy resolution at the elastic line is defined by

\[
\frac{\Delta E}{E_i} = 2\frac{\Delta \lambda}{\lambda_i} = \sqrt{\frac{E_i[\text{meV}] \Delta t_{\text{det}}[\mu\text{s}]}{1142 L_{SD}\text{[m]}}},
\]

considering \(\Delta \lambda\) extracted from Eq. (3) and \(\lambda_i\) derived from Eq. (2).

The time of flight uncertainty on the detector, \(\Delta t_{\text{det}}\), is derived from the primary and secondary spectrometer uncertainties, as shown in Fig. 1. The primary spectrometer time uncertainties include \(\Delta t_1\), the uncertainty on the detector due to the pulse shaping (PS) chopper, and \(\Delta t_2\), the uncertainty on the detector due to the monochromating (M) chopper. A third uncertainty, \(\Delta t_3\), is related to the uncertainty in the length of the secondary flight path caused by the finite sample size and detector thickness. The uncertainties are independent and can thus be added in quadrature,

\[
\Delta t_{\text{det}} = \sqrt{\Delta t_1^2 + \Delta t_2^2 + \Delta t_3^2}.
\]

\(\Delta t_1\) and \(\Delta t_2\) are related to the opening times of the PS and M choppers, respectively, through the geometry to the instrument distances, \(L_0\), the moderator to monochromatic chopper distance; L1, the pulse shaping chopper to monochromatic chopper distance; and L2, the monochromatic chopper to detector distance, as shown in Fig. 1(a),

\[
\Delta t_1 = \frac{L_2}{L_1}, \quad \Delta t_2 = \frac{L_2 + L_0}{L_0}.
\]

The flux on the sample, \(\Phi\), for a particular energy resolution at a particular incident wavelength, \(\lambda_i\), can then be calculated according to

\[
\Phi = B\Delta \Omega \Delta \lambda \Delta R P,
\]

with B being the source brilliance; \(\Delta \Omega\) being the divergence accepted in the horizontal and vertical directions; R being the duty cycle, the fraction of time for which the beam is on the sample; and P being the transport of the guide. R for a single pulse is given by \(t_2/\text{ESS period (71 ms)}\).

The European Spallation Source is a long pulsed source with a frequency \(F = 14\) Hz repetition rate, as shown in Fig. 1(b). The wavelength band, \(\Delta \lambda\), extracted on a spallation source instrument is inversely proportional to the instrument length according to Eq. (3). Utilization of the available source brilliance in the wavelength band is optimized through RRM. RRM is a common method in many short pulsed spallation source chopper spectrometers, with a typically short moderator to detector distance, 20–30 m. On these
instruments, the use of RRM results in 4–5 incident monochromatic wavelengths with a broad variation in wavelengths, typically from $2 < \lambda < 10$ Å, across a single time frame, $\sim \Delta \lambda_i$, as shown in Fig. 1(b). The moderator to detector distance in CSPEC is 163.5 m, thereby providing a short 1.72 Å wavelength band, $\Delta \lambda_2$, as shown in Fig. 1(b), with the possibility to closely match incident wavelengths across the 71 ms (1/14 Hz) period of the ESS. It is easy to see that closely matched wavelengths make it possible, in certain circumstances determined by energy and wavevector transfer resolution requirements, to accumulate pulses and thereby significantly increase the flux on the sample. It should be noted, as shown in Fig. 1(b), that a short instrument will measure cold neutrons in the same time frame as the spallation pulse, while on a long instrument, the measuring period is a later time frame. The use of RRM on CSPEC is described in greater detail later in the text.

III. QUASIELASTIC SCATTERING

Quasielastic neutron scattering is due to processes occurring with a distribution of energies, such as stochastic rotational motions, reorientations, and translational diffusion, on the picosecond to microsecond timescales.16 The aforementioned motions are typically found in hydrogenous materials, soft-matter, biological systems, and glassy compounds. Typically, these materials have short range spatial correlations, and as such, the Q-resolution can be degraded to improve the flux or focus the neutron beam on a smaller sample with a resultant degradation of divergence and thus Q-profiles. In contrast, it is advantageous to have a freely tunable energy resolution to adjust the experimental time window to the timescales of the motions of interest. The data that one extracts in a quasielastic experiment around zero energy transfer need to be deconvoluted from the experimental shape of the elastic line and the resolution function, and any deviation from a triangular or Gaussian energy resolution function makes it difficult to extract the information required. It is imperative that the signal to noise is optimized and the background is minimized and well understood. The CSPEC demand for a signal to noise of $10^5$ at 5 Å comes from the need to observe weak broad signals, in Q and E, that are relevant in condensed matter. These signals often lie within the background noise and are thus difficult to extract. A high signal to noise will provide the required access.

The neutron beam spot size, at the sample position, for quasielastic scattering of non-single crystal materials must be able to vary from $4 \times 2$ cm$^2$, thereby optimizing the scattering intensities of dilute but abundant samples, down to $1 \times 1$ cm$^2$ for compounds with small sample volumes. RRM will allow the cumulative use of adjacent incident pulses for the incident energy $\lambda_i > 6$ Å, with small variations in the energy and momentum transfer, to increase the flux.

The comments made in Sec. III remain true for quasielastic scattering from a single crystal except that the Q-resolution, which is closely matched to the energy transfer, must remain adequate to determine the lifetimes and spatial correlations across the entire S(Q, $\omega$). The scientific interest in quasielastic scattering of single crystals is rooted firmly in hard condensed matter, typically magnetism or functional materials. Novel materials in these scientific domains are difficult to synthesize and result in small crystals as small as mm$^3$. It is therefore important to be able to focus the neutron beam to a small spot size while maintaining a clean divergence profile that can adequately probe S(Q, $\omega$).

IV. INELASTIC NEUTRON SCATTERING

Inelastic neutron scattering occurs due to processes with discrete energy steps. These include local excitations such as crystal field levels, collective excitations such as phonons and spin waves, and higher energy vibrational modes such as stretching modes and librations.

An understanding of crystal field levels can be adequately gained by scattering from a powdered sample since no variation in energy transfer with wavevector transfer is expected.17,18 In contrast, collective excitations, with very distinct variations in energy and wavevector transfer, from powdered samples can also provide useful, albeit limited, information by comparing computational modeling methods such as density functional theory or linear spin wave theory with powder averaged S(Q, $\omega$). This is particularly useful for compounds that cannot be synthesized as large single crystals. However, inelastic neutron scattering from single crystal samples provides the most exacting and accurate information via a four
dimensional $S(Q, \omega)$. This is exemplified by the very active scientific field of research focused on novel states of matter such as those proposed by the Kitaev spin model on a honeycomb lattice. These materials harbor Majorana bound states as its excitations and are expected to be used as a component in topological quantum computers. The magnetic excitations of these novel states are low lying, in energy, and highly unusual. Subtle variations in $S(Q, \omega)$ must be determined to quantify and understand the details of the exchange interactions that lead to these novel states. To gain optimal information from the scattering profiles, it will be imperative to have direct access to theoretical models convoluted with the instrumental resolution. A focusing nose, optimizing the flux for mm to cm sized samples, will increase signal to noise. Signal to noise can be increased further by accumulating 6–10 incident wavelengths via RRM if the energy and $Q$-resolutions permit.

V. KINETIC MEASUREMENTS

A combination of the high flux and the multi-energy mode, via RRM, makes CSPEC most suitable for experiments that investigate time-resolved kinetic phenomena, including pump-probe experiments and out of equilibrium behavior. The high flux via RRM will enable monitoring of transient phenomena with a time resolution of minutes. For cyclic processes, time-resolved stroboscopic measurements will benefit both from the high flux and the multi-energy mode to probe the dynamic response of a compound to an external trigger with a time resolution of the order of milliseconds.

VI. INSTRUMENTAL DETAILS

The scientific requirements for CSPEC, as outlined Secs. III and IV, lead to the following specifications:

- CSPEC shall extract a wavelength range of 2–20 Å.
- The CSPEC guide shall extract the flux with ±1° divergence at 3 Å and more, if possible for higher wavelengths.
- CSPEC shall measure in repetition rate multiplication configuration for all measurement modes.
- CSPEC shall be capable of energy resolutions down to and better than $\Delta E/E_i = 1.5\%$ for wavelengths greater than 4 Å.
- CSPEC shall be capable of the momentum transfer resolution $\Delta Q/Q = 2\%$.
- CSPEC shall provide a signal to noise of $10^5$ at 5 Å. Signal to noise is defined as the peak of the intensity at the elastic line of a vanadium sample vs noise probed at a time of flight when the background level has been reached.
- The chopper cascade shall ensure that for each impinging pulse on the sample with energy $E_i$, neutrons with a final energy, $E_f$, $0.2E_i < E_f < \infty$ shall be measured.
- The neutron beam at the sample position shall illuminate a sample area ranging from $4 \times 2$ cm$^2$ to $1 \times 1$ cm$^2$ (height × width).
- The detectors provide a detectable angular range of $5^\circ < 2\theta < 140^\circ$ with a sample to detector distance of 3.5 m in the azimuthal plane and a vertical detectable range of ±26.5°.
- CSPEC shall probe magnetic excitations in magnetic fields up to 12 T.
- The design of the instrument will accommodate the sample environment equipment required to match the science case.
- Sample environment within the CSPEC scope for the wide range of scientific cases studied on CSPEC should be consistent with the demands of signal to noise.
- The systems design shall provide the space and flexibility necessary to host and drive future developments, for instance, further focusing optics for smaller sample sizes, possibly integrated into the sample environment, further in situ sample environment such as secondary characterization [RAMAN or nuclear magnetic resonance (NMR)], XYZ polarization analysis.

A cartoon overview of the resultant instrument is shown in Fig. 2, showing the optics, chopper cascade, instrument shutter, cave, sample environment, detector tank, and detector position.

VII. INSTRUMENT PARAMETERS

A. Chopper cascade

The chopper cascade ensures clean incident monochromatic neutron bursts at the sample position with incident energies $E_i$ and scattered with a final energy, $E_f$, $0.2E_i < E_f < \infty$, measured at the

![FIG. 2. Cartoon overview of the CSPEC instrument showing ESS buildings: Monolith, bunker, D03, E02 and E01, and various CSPEC components and relevant distances. Components in white are upgrade features: polarization analysis and completion of detector coverage. BW = bandwidth, PS = pulse shaping, and M = monochromating choppers. Reproduced with permission from Andersen et al., ‘The instrument suite of the European Spallation Source,’ Nucl. Instrum. Methods Phys. Res., Sect. A 957, 163402 (2020). Copyright 2020 Author(s), licensed under a Creative Commons Attribution (CC BY) license.](image)
detector position. An energy resolution of $\Delta E/E_0 = 1.5\%$ will be achieved for wavelengths equal to or greater than 4 Å. The chopper cascade that will provide these specifications is presented in Fig. 3 and Table I. The bandwidth choppers, BW1, BW2, and BW3, have been designed to extract a 1.72 Å wavelength bandwidth around the central wavelength $\lambda_{\text{c}}$, ensuring maximum flux from the time independent part of the ESS pulse structure. The BW chopper openings will be triangular. The energy resolution chopper cascade, the PS and M choppers, are based on a relative distance and frequency of 2/3 such that the M choppers are positioned at a distance $L = x/3$ with the PS choppers positioned at 2x/3. To ensure an optimal pulse transmission through the chopper cascade, the M and PS choppers have one and three transmission windows, respectively, and rotate at frequencies of $F_M = 2F_{\text{PS}}$, where $F_M$ = frequency of the M chopper and $F_{\text{PS}}$ = frequency of the PS chopper. The RRM chopper prevents frame overlap between the various incident pulses and runs at a frequency $F_{\text{M}}/n$, $n =$ integer and a multiple of the ESS source frequency. The chopper openings for the high speed choppers will be rectangular providing a clean scattering profile for the edges, in TOF, of the incident beam.

B. Guide profile

Chopper spectroscopy is a flux intensive technique with success based on optimizing signal to noise. As such, the CSPEC guide must transport cold neutrons with a broad divergence, signal, while limiting high energy fast particles, noise, derived from proton pulse spallation on the target. Liouville’s theorem states that an increase in the flux per area, beyond the flux extracted from the moderator, is accompanied by an increase in the spread of the beam divergence. The space density of the neutron flux extracted from the moderator must be transported to the sample, ensuring that the final divergence and flux profile are consistent with the instrument specifications. The divergence profiles of the neutron beam are derived from geometric considerations of the beam extracted from the moderator, the horizontal and vertical guide profiles, and the wavelength dependence of the critical angle, $\theta_c$, of neutron reflection of Ni/Ti supermirror guides,

$$\theta_c[\text{deg}] = 0.099m_{\text{mirror}}\lambda[A],$$

in which $m_{\text{mirror}}$ represents the increase in the critical angle of a Ni/Ti supermirror relative to that of a Ni thin film.\(^2\)

High energy particles from the prompt pulse are ejected after the proton beam hits the target and, as such, is a time dependent feature that is observed in all spallation instruments. The prompt pulse has been shown to extend up to 3 ms beyond the proton pulse on the target with a slow exponential decay consistent with the moderation of fast particles through the facility and instrument structures.\(^3\) In the case of the ESS, the proton pulse on target extends 3 ms, and therefore, there will be a prompt pulse across 6 ms in time. Limiting high energy particle transport through the instrument is achieved by curving the guide away from the line of sight (LOS) of the target.\(^4\)

The CSPEC guide starts at 1.9 m from the 3 cm tall moderator using the port axis W3. The W3 port axis is positioned between the thermal and cold moderators. The guide is rotated away from the W3 axis, as shown in Fig. 4, to view only the cold H$_2$ moderator and thus extract $2 < \lambda < 20$ Å. The first 2 m of guide sections is funneled from 0.043 × 0.045 m$^2$ (height × width) → 0.055 × 0.07 m to extract an optimal flux and reduce the divergence profile transmitted beyond the first guide sections. Transporting a reduced divergence will limit the supermirror m-values required for subsequent guide pieces. Limiting the m-value of supermirror guides limits shielding requirements, since the interaction of neutrons with Ni/Ti guides results in high energy gammas, and vastly reduces guide costs. The first guide section, 1.9–56.4 m, is curved with a radius of curvature (ROC) equal to 1600 and 4000 m in the vertical and horizontal direction, respectively. Vertically, an s-bender guide curves the guide

| Name     | Pos. (m) | Angle (°) | Num | F (Hz) | Ø (m) |
|----------|----------|-----------|-----|--------|-------|
| BW1 (SB) | 14.95    | 40.7      | 1   | 14     | 0.7   |
| BW2 (SB) | 20.47    | 41.9      | 1   | 14     | 0.7   |
| BW3 (SB) | 104.59   | 193       | 1   | 14     | 0.7   |

| Name     | Pos. (m) | Width × height (mm) | Num | F (Hz) | Ø (m) |
|----------|----------|---------------------|-----|--------|-------|
| PS (CR)  | 105.67   | 114.66 × 73.89      | 3   | 168    | 0.7   |
| RRM (SB) | 158.45   | 22.6 × 49.0          | 1   | 336    | 0.7   |
| M (CR)   | 158.5    | 22.58 × 49.0         | 1   | 336    | 0.7   |

FIG. 3. Time–distance diagram defining the chopper cascade on CSPEC.

\(^{23}\) Liouville’s theorem states that an increase in the flux per area, beyond the flux extracted from the moderator, is accompanied by an increase in the spread of the beam divergence. The space density of the neutron flux extracted from the moderator must be transported to the sample, ensuring that the final divergence and flux profile are consistent with the instrument specifications. The divergence profiles of the neutron beam are derived from geometric considerations of the beam extracted from the moderator, the horizontal and vertical guide profiles, and the wavelength dependence of the critical angle, $\theta_c$, of neutron reflection of Ni/Ti supermirror guides,

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FIG. 3. Time–distance diagram defining the chopper cascade on CSPEC.
twice out of line of sight (LOS) of the target and moderator. Horizontally, the guide is curved to return the instrument on the W3 instrument axis and to the correct position within the instrument hall, as shown in Fig. 5. The distance that an instrument will lose line of sight of the moderator is determined by geometric arguments such that

$$\text{LOS} = \sqrt{8wR},$$  \hspace{1cm} (9)

where \(w\) is the width or height of the curved guide and \(R\) is the radius of curvature in the horizontal or vertical direction. The minimum wavelength that is transported by a curved guide is given by \(\lambda_c\),

$$\lambda_c = \frac{575}{m_{\text{mirror}}} \sqrt{\frac{2wR}{m}}.$$  \hspace{1cm} (10)

Table II provides the relevant critical parameters for the CSPEC curved guide.

Beyond the curved guide section, an elliptically opening funnel, opening from \(0.055 \times 0.07\) m (height \(\times\) width) to \(0.111 \times 0.115\) m (height \(\times\) width), extends across 14 m and reduces the divergence profile of the beam for the next stretch of the guide such that \(m = 2\) supermirrors can be employed. The following 24 m section is a straight section before an elliptical funnel in the vertical direction, which reduces the height of the beam to 0.074 m at the PS chopper position with \(m\)-values slightly increasing to \(m = 2.5\). The final guide section, from the PS to M chopper positions, is again elliptically focused to achieve the required height and width, \(0.049 \times 0.023\) m (height \(\times\) width), and to achieve the specified time resolution. \(M\)-values increase to \(m = 3.5\) at the chopper position. The final guide section beyond the M chopper is an exchangeable guide piece that allows both a beam area at the sample position of \(4 \times 2\) cm\(^2\) and a \(1 \times 1\) cm\(^2\) (height \(\times\) width), via an unfocussed tapered elliptical nose and a focusing elliptical nose. The focusing nose provides an increase of 2.5 in flux/cm\(^2\) across \(2 < \lambda < 10\) Å. Focusing the beam onto the relevant sample area will further reduce background effects that are derived from scattering of incident neutrons onto instrument components, e.g., slits, often resulting in small angle scattering and spurious multiple scattering effects.

The wavelength dependence of the beam flux and divergence profiles for the unfocussed guide and focused guide are shown in Figs. 6 and 7, derived from McStas ray tracing simulations.\(^7\) The beam profiles for the unfocussed beam are uniform for each wavelength with less than 10% variation across the required beam area, \(4 \times 2\) cm\(^2\). The unfocussed guide provides continuous divergence profiles in both the horizontal and vertical directions. Horizontally, the beam divergence extends to \(\pm 1^\circ\) for \(\lambda < 4\) Å and \(\pm 1.5^\circ\) for \(\lambda > 4\) Å. Vertically, the wavelength dependence of the beam...
TABLE II. CSPEC guide parameters for the curved section.

| Vertical Width (m) | ROC (m) | LOS (m) | \( \lambda_c \) (Å) | \( m_{\text{mirror}} \) |
|-------------------|---------|---------|---------------------|---------------------|
| 0.07              | 1600    | 29.93   | 1.36                | 4–3                 |

| Horizontal Width (m) | ROC (m) | LOS (m) | \( \lambda_c \) (Å) | \( m_{\text{mirror}} \) |
|----------------------|---------|---------|---------------------|---------------------|
| 0.055                | 4000    | 41.95   | 0.972               | 3.5–2.5             |

FIG. 6. Wavelength dependence of the flux and divergence at the sample position for the unfocussed guide nose showing (a) beam height, (b) beam height divergence, (c) beam width, and (d) beam width divergence.

FIG. 7. Wavelength dependence of the flux and divergence at the sample position for the focused guide nose showing (a) beam height, (b) beam height divergence, (c) beam width, and (d) beam width divergence.
divergence increases linearly with \( \pm 1^\circ \) for \( \lambda = 3 \text{ Å} \) and \( \pm 3^\circ \) for \( \lambda = 10 \text{ Å} \).

The beam profiles for the focused beam spot are uniform for each wavelength with less than 10% variation across 1 \( \times \) 0.7 cm\(^2\). The focused guide provides continuous divergence profiles in the horizontal directions with a linear wavelength variation from \( \pm 1.5^\circ \) for \( \lambda < 3 \text{ Å} \) to \( \pm 4^\circ \) for \( \lambda = 10 \text{ Å} \). Vertically, the beam divergence shows three peaks, derived from the stringent focusing requirements. This profile will be observed in the Bragg peaks of single crystal samples as well as within well-defined excitations for the vertical scattering direction. It will therefore be important to align crystals in suitable directions, making use of the increased flux when possible. In addition, it will be essential to consider the convolution of the data with the instrumental resolution to extract relevant information.

**C. Repetition rate multiplication on CSPEC**

In this section, we will provide an overview of the possibilities afforded by RRM on CSPEC. The energy resolution is defined by the M chopper, which is linked to the PS chopper as stated previously, \( F_M = 2 F_{PS} \). It is essential that the choppers are phased to the ESS source, 14 Hz, and as such, only multiples of the ESS source that are wholly divisible by 2 \( \times \) 14 can be employed, i.e., 28:28:336. The bandwidth of CSPEC is \( \Delta \lambda = 1.72 \text{ Å} \) and incident wavelengths, \( \lambda_i \), in the range of \( \lambda_i = \lambda / 2 < \lambda_i < \lambda_i + \Delta \lambda / 2 \) will impinge on the sample within one ESS time period. The energy resolution of the elastic line as a function of the incident wavelength and M chopper frequency, determined via McStas simulations, can be described by a power law function, as shown in Fig. 8. It can be seen that \( \Delta E / E_i \) for low \( \lambda_i \) varies greatly, while \( \Delta E / E_i \) for higher wavelengths are nearly equivalent across \( \lambda_i \), as shown in Fig. 8.

It is up to the experimental team to determine how many pulses they are able to accommodate within their wavevector and energy transfer resolution. Furthermore, the number of pulses that can be accommodated will depend on the energy loss acceptable within the experiment. A quasielastic experiment can accommodate an energy loss such that \( E_f = 0.8 E_i \), while an inelastic experiment may need \( E_f = 0.2 E_i \), as explained diagrammatically in Fig. 9. Figure 9 shows time of flight diagrams from the sample to detector (considering the largest sample to detector distance = 3.913 m) and the adjacent pulses within an ESS period for (a) \( \lambda_i = 3 \text{ Å} \), with the M and RRM choppers both running at 224 Hz and \( E_f = 0.8 E_i \), and (b) \( \lambda_i = 3 \text{ Å} \), with the M running at 224 Hz and RRM running at 112 Hz to achieve \( E_f = 0.2 E_i \). Frame overlap between adjacent pulses is not an issue in Fig. 9(a), and all possible incident pulses are transmitted, 14 pulses. In the case of an increased dynamic range, with \( E_f = 0.2 E_i \), the RRM chopper removes half of the pulses to reduce frame overlap, and the number of pulses transmitted is reduced to 7, as shown in Fig. 9(b). The variation of the energy resolution across the CSPEC bandwidth for 3 Å is \( 
\begin{align*}
0 &< \Delta E / E_i < 0.023 , \\
0.023 &< \Delta E / E_i < 0.039 , \\
0.039 &< \Delta E / E_i < 0.093 , \\
0.093 &< \Delta E / E_i < 0.122 , \\
0.122 &< \Delta E / E_i < 0.161 .
\end{align*}
\)

which may not be scientifically suitable for accumulation. However, for the bandwidth around 8 Å, the energy resolution varies from \( 0.01 < \Delta E / E_i < 0.012 \) and can be more easily accommodated into a single dataset, as shown in Fig. 8.

**D. Experimental area**

The CSPEC sample environment area is optimized for the broad range of science that a cold chopper spectrometer addresses. Figure 10 shows a preliminary engineering drawing of the detector tank inclusive of the sample pot. The sample environment area is accessible via a side door and a top flange. Top access is envisaged for conventional cryostats and magnets as the sample environment...
FIG. 10. (a) Overview of the detector tank with particular components outlined. (b) Vertical cut through the detector tank. (c) Horizontal cut through the detector tank with an overview of the detector array in the detector tank. Letters in Figures (a) and (b): (a) incident neutron beam, (b) sample environment pot from the top view of a person, (c) radial collimator, (d) detector collimation vanes, (e) detector vessel with the zoomed image of the two detector columns within a vessel, and (f) beam dump. The zoomed image of Figure (c) shows the 2 detector columns separated by a neutron absorbing vane.

while side access is envisaged for more specialized sample environments. The sample pot diameter is 1 m to provide maximum access. Auxiliary sample environment ports have been added to provide access for further utilities. Figure 10 shows a cut through the detector tank and reveals, from left to right, the guide exchanger, the sample environment pot, the 4 mm thick aluminum gate valve, the oscillating radial collimator, detector collimation vanes, detectors, and the beam stop. In this image, a detector is being removed for maintenance. The 4 mm thick aluminum gate valve is designed to easily separate the sample environment pot from the evacuated detector area, in the closed position, such that the sample environment pot can provide a different environment to the evacuated detector tank, if an experiment requires it. In normal operation, the gate valve will be in the open position and can provide an unimpeded neutron scattering path from the sample to detector.

The detector tank must be consistent with the magnetic field sample environment requirements and the requirements of neutron polarization to be implemented shortly after CSPEC comes online. In order to pursue polarization analysis, the magnetic environment that the incident neutrons are affected by must be limited to avoid any depolarization.25 The requirement is such that within the sample pot and up to 1.45 m radius from the sample point, the base material, welding seams, and all built in components shall have an as-built relative magnetic permeability $\mu_r < 1.01$.

E. Radial collimator

A radial collimator is a series of septa placed radially, separated by an angle of $2\alpha$, at a distance $R_1$ from the center of the sample with a length extending to a distance $R_2$ from the center of the sample, as shown in Fig. 11. The septa absorb scattering from a spatial and angular region that extends beyond the sample, $> b_0$, and for a scattering angle $> \gamma$. A radial collimator is essential equipment to improve the signal to noise of the experiment. $b_0$ and $\gamma$ are chosen not only to accommodate the beam on sample and the sample size but also to limit scattering from external radiation shields or outer housings that are important components for sample environments, but not of scientific interest. The radial collimator on CSPEC will provide quite tight collimation to limit any secondary scattering effects from sample environments and will be needed to reach the CSPEC specification of a signal to noise of $10^5$.

The CSPEC sample pot diameter must provide sufficient space for a wide range of experiments, and this affects the $R_1$ parameter of the radial collimator. The minimum radius of the collimator and thus $R_1$, directly beyond the Al gate valve, is 504 mm. Septa thicknesses are not considered in the following considerations.

Geometric considerations following Fig. 11 result in the following relationships:

$$b_0 = \frac{2\alpha R_1 R_2}{R_2 - R_1}, \quad (11)$$

$$\gamma = \theta + \alpha = \alpha + \tan^{-1} \left( \frac{2R_1 \sin(\alpha)}{R_2 - R_1} \right). \quad (12)$$
Consistency with the CSPEC requirements provides the following radial collimator parameters shown in Table III.

The radial collimator will oscillate providing a time averaged scattering profile that is not affected by the septa widths. As such, the radial collimator must withstand a 0.1 Hz oscillation with a ±1° oscillation of variable amplitude. The absorbing material must provide a transmission less than 10⁻³. This will be possible by coating thin Mylar foils (micrometer thickness) with either (99%⁷B)⁴B₁₀C or Gd₂O₃ in an ultrahigh vacuum compatible binder.

### F. Detector technology

The detector technology for chopper spectroscopy has historically been based on ³He absorption technology and has defined the standard for thermal neutron scattering. Indeed, ³He-based detectors have many of the required characteristics for thermal neutron scattering, which include high uniformity of response, high neutron counting efficiency, and low gamma-sensitivity. The technology is very mature and robust. However, the recent ⁴He crisis made it necessary to consider novel technologies for neutron scattering research. A novel detector technology for CSPEC is based on thin film converters of boron-10 carbide, ⁴B₁₀C. These new technologies are complex to implement, and significant tests have been completed to conform to the CSPEC requirements, which include the following:

- Intensity as a function of time of flight for an incoherent scatterer, measured at 2 K, in the region 3σ < λ < 5σ shall be ≤2.5 times that for ³He detectors (essential) and should be equivalent to that for ³He detectors (desirable).
- Detection efficiency shall be ≥60 at 4 Å.
- Count rate capability shall be 50 times greater than ³He detectors and should be 100 times greater than ⁴He detectors.
- The dark noise across all detectors shall be less than 0.35 Hz/m² and should be less than 0.14 Hz/m².
- The scattering signal to noise shall be 10⁵ at 5 Å and should be 10⁶ at 5 Å. The signal is defined as the peak neutron intensity on the detectors by an incoherent scatterer and compared to the noise defined as the neutron intensity at a time when the signal has decayed to background levels.
- Gamma efficiency shall be ≤10⁻³.

It is beyond the scope of this paper to review the ⁴B₁₀C detector development, which is addressed in a number of different papers and references within. Geometrically, the detector geometry is distinctly different to a ³He detector.

A detector column on CSPEC is 3.5 m tall with the detector area subdivided into voxels of 2.5 × 2.5 × 1 cm³, providing the required wavevector transfer. Uniquely, for a thermal neutron detector optimized for time of flight spectroscopy, the detector has a significant depth, with 16 cm deep voxels to increase detection efficiency.

The thickness of the boron layers, coating the voxels, have been optimized with respect to the CSPEC wavelength range. Each detector vessel, housing 2 detector columns, will provide 6 (wide) × 16 (deep) × 140 (high) × 2 (columns) equaling 26 880 voxels per detector vessel and 860 160 detector voxels for the complete detector array, 2.49 Str and 30.6 m². The extraction of S(Q, ω) from such a large detector array is bringing about a paradigm shift for data analysis. The details will be published in future works.

Figure 10(c) shows a top view of the detector tank with the 32 detector vessels placed at the edge of the evacuated detector tank, as shown in Fig. 10(c): (a) the incident neutron beam, (b) the sample environment pot from the top view of a person, (c) the radial collimator, (d) detector collimation vanes, (e) the detector vessel with the zoomed image of the two detector columns within a vessel, and (f) the beam dump. The two detector columns in each vessel are separated by a neutron absorbing vane, and each detector vessel is separated from the next detector column by a collimation vane. Each detector vessel can be aligned to the sample position to ensure optimal scattering.

### G. Conclusion

In conclusion, an overview of the cold chopper spectrometer of the ESS, CSPEC, has been provided. We show the relevant instrument parameters from the moderator to detector tank with emphasis on extracting cold neutrons at a long pulsed spallation source. The instrument specifications and relevant solutions to achieve those specifications are outlined. It will be of great interest to provide a direct comparison of the expected performance to true experimental performance once CSPEC is operational in the coming years.

### ACKNOWLEDGMENTS

We thank Peter Link, TUM, for the development and manufacture of the CSPEC optics in addition to fruitful discussions thereof. CSPEC is a German/French collaboration supported equally by the German and French in-kind contributions to the ESS.

### AUTHOR DECLARATIONS

**Conflict of Interest**

The authors have no conflicts to disclose.

### DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Rev. Sci. Instrum. 92, 105104 (2021); doi: 10.1063/5.0059907

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