CSPEC: An update on the spectrometer of the ESS

PASCALE DEEN CSPEC LEAD SCIENTIST (DARIA NOFERINI) SENIOR SCIENTIST FOR SPECTROSCOPY



development of the cold chopper



CSPEC: Scientific aims

Quasielastic scattering:

Translational dynamics

Diffusive dynamics

Rotational dynamics



J. Phys. Chem. C 121, 7088 (2017)





Materials: Glass forming, liquid dynamics, crystal growth, hydrogen storage, fuel cells.

Soft matter: Polymer nanocomposites, organic photovoltaics, polymer electrolytes

Biology: hydration water, protein structure-dynamics-function, cell membrane-protein, drug delivery Chemistry: ionic liquids, clays, complex fluids



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Quasielastic scattering:

Translational dynamics

Diffusive dynamics

Rotational dynamics

Low lying energy modes:

Spin dynamics

Critical scattering

Collective excitations

Quasiparticles











Materials: Glass forming, liquid dynamics, crystal growth, hydrogen storage, fuel cells.

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Magnons, phonons, polarons Topological states of matter: Majorana fermions. RVB states, Quantum spin liquids, emergent behaviour.



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Nature Physics 9, 435–441 (2013)





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Study of low lying excitations of materials with a focus on small samples, in-operando/kinetic behaviour Need 10-50 x current day signal/noise to perform adequately



CSPEC Specifications

- •The cold chopper spectrometer of the ESS (2 20 Å). •Cold neutrons (2-20 Ang) with $\Delta E/E = 1.5 \% @ 4 Å$ (Ei, $\Delta E = \infty < E_i < 0.2E_i$). •Focus flux on range of sample areas 4 x 2 cm² \rightarrow 1 x 1 cm².
- •Signal to noise = 10^5 (@5 Å, Vanadium).

- Polarisation analysis.
- Much improved coupling of neutron scattering with theory.





Study of low lying excitations of materials with a focus on small samples, in-operando/kinetic behaviour Need 10-50 x current day signal/noise to perform adequately

•Detector will provide angular range of $-30 < 2\theta < 140^{\circ}$ in the horizontal plane and +/- 26.5° in the vertical plane with a planar sample to detector distance = 3.5 m = 2.49 Str•Enhanced sample environment : in-situ/kinetic phenomena. < 1 min resolution.



CSPEC Instrument length



30 - 160 m instruments Question of science case, do I want to see many length scales, timescales or do I want to focus? Question of bandwidth





Long pulse versus short pulse spallation versus reactor



Brightness Reactor: Continuous Spallation: high but sparse (RRM)

Background Reactor: continuous Spallation: pulsed, clean in between ...

Lineshapes Reactor: Symmetric line shapes derived from chopper openings. Spallation: Short pulse instruments - Carpenter function Long pulse: choppers.





Chopper spectroscopy at ESS: <u>A1 + High</u> flux, low noise, symmetric lineshapes. Sample

Spallation



CSPEC broad parameters

Instrument Class	Spectroscopy Cold	
Moderator		
Primary flightpath (Moderator to M chopper)	158.5 m	
Secondary flightpath (M Chopper to detector)	5 m	
Wavelength range	1.72 Å	
Flux at sample (4 x 2 cm²), 5 MW (λ = 5 Å, ΔΕ/Ε =3%)	MW 3e6n/s/cm² (single pulse) x 5 - 10 with RRM cumulat MW 7.8e6n/s/cm² (focussed beam, single pulse)	
Flux at sample (1 x 1 cm ²⁾ , 5 MW (λ = 5 Å, ΔΕ/Ε =3%)		
Detector coverage	Complete: (H) -30° < 20 < 140°, (V) ±26.5° day 1 : (H) 5° < 20 < 90°, (V) ±26.5° · September 202	
Energy resolution	1.5% @ 4 Å	





CSPEC Overview





CSPEC within the ESS



Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment Volume 957, 21 March 2020, 163402



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CSPEC Guide

•Signal to noise = 10^5 (@5 Å, Vanadium). •Optimise to cold moderator.

•2 x LOS (Prompt pulse)







Detector feedthrough flanges



CSPEC Guide

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- •2 x LOS (Prompt pulse)





Detector feedthrough flanges



CSPEC Guide (McStas) Positional & divergence coverage (**4 x 2 cm²**). Tapered guide Clean divergence profiles



PSD < 10 % variation across 4 x 2 cm² Horizontally, the beam divergence extends to 1° for $\lambda i < 4$ Å, 1.5° for $\lambda i > 4$ Å.









CSPEC Guide (McStas) Positional & divergence coverage (**1 x 1 cm²**): elliptical guides x 2.5 in flux for 2 Å < λ < 10Å.



PSD < 10 % variation across 1 x 0.7 cm².

Divergence increases linearly from 1° for lambda = 3 Å and 3° for λ =10 A (width) Structure in divergence in vertical direction / consider experimental conditions.

















Elastic energy resolution across $\Delta \lambda = 1.7$ Å.



Across accessible bandwidth (1.72 Å) $3\text{\AA} = 0.023 < \Delta \text{E/E} < 0.039$ $8\text{\AA} = 0.01 < \Delta \text{E/E} < 0.012$ Add pulses, gain flux, if possible.







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Add pulses, gain flux, if possible.

(a) $1.12 \le E_i \le 1.61 \text{ meV}$



CSPEC Overview



Secondary spectrometer Detector tank





Incorporate: (a)Guide exchanger (4x2 - 1x1 cm²) (b)Gate valve (c)Radial Oscillating collimator (d)Detector collimation vanes (e)3He detectors -30 < 2θ < 140 (H), -26.5 < 2θ < 26.5



Secondary spectrometer Radial collimator













TABLE III. CSPEC radial collimator parameters.



Cave and control cabin









Cave and control cabin



Some reality CSPEC – HAII E01 – 160 m from moderator









Target and bunker area April 2020



Bunker wall April 2021

Bunker wall feedthrough

934,6)

Guide

Production of neutron guides by the TUM optics group

Guide vacuum housing

Guide vacuum housing

Alignment < 50 µm Vacuum tests/ check seals Acceptance of components

Guide vacuum housing

Primary spectrometer shielding PACADAR GROUP

Chopper cascade

AIRBUS

Secondary spectrometer in hall E01

Detector tank

Particular points:

- •100 m³
- Evacuation to 1e-04 mbar (huge stresses).
- Aluminium (PA).
- Collimation.
- •Internal Cd coating.
- Particular sample environment access.
- Access from side and top.
- Careful consideration for enhanced SE.
- Extraction of detector vessels.
- •35 T, 1 mm positional resolution
- Walls are 40 mm thick reinforcement 350 mm tall
- •2 mm Al. gate valve

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Radial oscillating collimator Improve signal to noise 10⁵ Oscillates with ~ 1 Hz

Secondary spectrometer

Detectors He3

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^{3}He + n = ^{3}H + p + 764 keV
```

3.5 m long, position sensitive pixels = 2.5 cm = 48000 pixels

Secondary spectrometer

Evidence for a three-dimensional quantum spin liquid in PbCuTe₂O₆

Shravani Chillal , Yasir Iqbal, Harald O. Jeschke, Jose A. Rodriguez-Rivera, Robert Bewley, Pascal Manuel, Dmitry Khalyavin, Paul Steffens, Ronny Thomale, A. T. M. Nazmul Islam, Johannes Reuther & Bella Lake

PHYSICAL REVIEW X 11, 021044 (2021)

Spinon Fermi Surface Spin Liquid in a Triangular Lattice Antiferromagnet NaYbSe₂

Peng-Ling Dai,^{1,||} Gaoning Zhang,^{2,||} Yaofeng Xie,³ Chunruo Duan,³ Yonghao Gao,⁴ Zihao Zhu,⁴ Erxi Feng,⁵ Zhen Tao,¹ Chien-Lung Huang,³ Huibo Cao[®],⁵ Andrey Podlesnyak[®],⁵ Garrett E. Granroth[®],⁵ Michelle S. Everett[®],⁵ Joerg C. Neuefeind[®],⁵ David Voneshen,^{6,7} Shun Wang,⁸ Guotai Tan[®],¹ Emilia Morosan,³ Xia Wang,² Hai-Qing Lin,⁹ Lei Shu,⁴ Gang Chen,^{10,4,*} Yanfeng Guo[®],^{2,†} Xingye Lu[®],^{1,‡} and Pengcheng Dai^{®,3,§}

Instrument readout streaming architecture

• 38 TiB in event information per experiment.

BrightnESS is funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 676548

brightness

MSlice/Horace/PACE

CSPEC Sample environment (BOT = Beam on target)

* In scope

BOT	HC= BOT + 3 months	FS= BOT + 6 months	SOUP=BOT + 12 months
Cryofurnace*	14 T magnet (access to)	High pressure (large samples)	Pump and probe setup*
He3 insert*	Automatic sample changer*	Humidity chamber	High pressure (small samples)
Sample stick rotation stage*		High temperature furnace (access to)	
6 T magnet*			

Dilution insert (From Pool) Uniaxial pressure cell (2 GPa) Further collaboration with university teams (Roskilde University, Malmö University, Copenhagen University, Lund University)

CSPEC core team

Engineer: Fernando Moreira (Lead, LLB), Matts Olson (TUM), Miguel Campos Ferro(LLB) Scientists: D. Noferini, P.P. Deen, G. Tucker (DMSC)

TUM: W. Lohstroh LLB: S. Longeville

A difficult project but a very collaborative/committed team

& ESS & TUM & LLB technical groups

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⁽⁰⁾ P. P. Deen^{1,2,a)}, S. Longeville³, ⁽⁰⁾ W. Lohstroh⁴, F. Moreira¹, G. Fabrèges³, L. Loaiza⁴, and ⁽⁰⁾ D. Noferini¹

https://europeanspallationsource.se/instruments/cspec

We welcome you all soon(ish). pascale.deen@ess.eu

Radial Oscillating Collimator

TABLE III. CSPEC radial collimator parameters.

Instrument readout streaming architecture 26880 voxels per detector vessel and 860 160 detector voxels •38 TiB in event information per experiment Result of an extensive test and evaluation phase involving many partners

BrightnESS is funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 676548

brightness

Detector tank

33 T

Walls are 40 mm thick - reinforcement 350 mm tall 3 mm gate valve

Aligned with air pads - achieve 1 mm positional resolution

Engineer: Fernando Moreira (Lead, LLB), Luis Loaiza (TUM), Gregoire Fabrèges (LLB) Scientists: P.P. Deen, D. Noferini, G. Tucker (DMSC)

TUM: W. Lohstroh LLB: S. Longeville

& ESS technical groups

CSPEC Specifications

Instrument Class
Moderator
Primary flightpath (Moderator to M chopper)
Secondary flightpath (M Chopper to detector)
Wavelength range
Flux at sample (4 x 2 cm²), 5 MW (λ = 5 Å, ΔΕ/Ε =3%)
Flux at sample (1 x 1 cm ²⁾ , 5 MW (λ = 5 Å, ΔΕ/Ε =3%)
Detector coverage
Energy resolution

Detector tank (sample to detector = 3.5 m, height = 3.5 m) Out to tender: reply 5th March (slight covid delay), 8 interested. Particular points:

- •Evacuation to 1e-04 mbar (huge stresses)
- •Aluminium / Stainless steel with muR < 1.01
- Particular sample environment access
- Careful consideration for enhanced SE
- •Extraction of detector vessels.

Pelican

Polarisation Analysis System

Overall polarisation efficiency: Spin flipper efficiency: Polariser efficience: ³He analyser efficience: ³He analyser lifetime: 10

Pelican Dehong Yu.

- One touch $\lambda/2$
- Transition from LAMP to Mantid
- New sample environment:

7 T Superconductor Magnet

- Achieved up to 7 T magnetic field with variable sample temperature from 300 K down to 50 mK.
- Very low stray field: 5 gauss at 1 m diameter.
- Easy operate: one command
- Open up new scientific opportunities for spin dynamics under high magnetic field.

Single crystal measurements and data processing.

High Pressure – up to 2 GPa

- Achieved up to 2 GPa pressure with sample • temperature from 300 K down to 100 K.
- Several user experiments performed successfully.
- Open up new scientific opportunities for material dynamics under high pressure, for example, pressure induced order to disorder phase transition, responsible for caloric effect in plastic crystals; Protein dynamics for deep sea life under hundreds of MPa pressure, ...

Installation campaign of guides/ housing. September 2022

Installation: 3 to 4 campaigns, 10 days each. Outside bunker: 2 campaigns.

In-hunker + choppers: 1 or 2 campaigns.

Sample Environment

- Standard orange cryostat and -furnace 1.5...550 K
- Dilution inserts 40 mK
- Dedicated furnace 1000 °C
- Liquid and clamp pressure cells
- Simultaneous dielectric + spectroscopy (under pressure)
- User provided equipment ...

Sanz et al., Rev. Sci. Instr. 89, 023904 (2018)

Connection to the Capillary

Neutron Beam

Cd foil for shielding

NEUTRONS FOR SOCIETY

5

59

(2) 160 m & cold neutrons & spallation source = less noise. S/N 10^{5} .

CSPEC The Cold Chopper spectrometer of the ESS

	R2	2lpha	$2b_0$	$\gamma~^{o}$
m	$708 \mathrm{mm}$	0.8 o	$48.85~\mathrm{mm}$	2.38°

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(a) $1.12 \le E_i \le 1.61 \text{ meV}$