Choosing the right spectrometer

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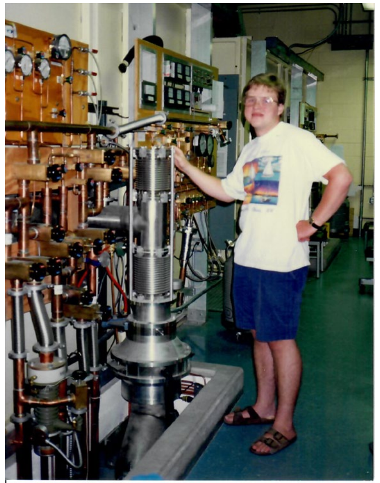
ARCS Instrument Scientist

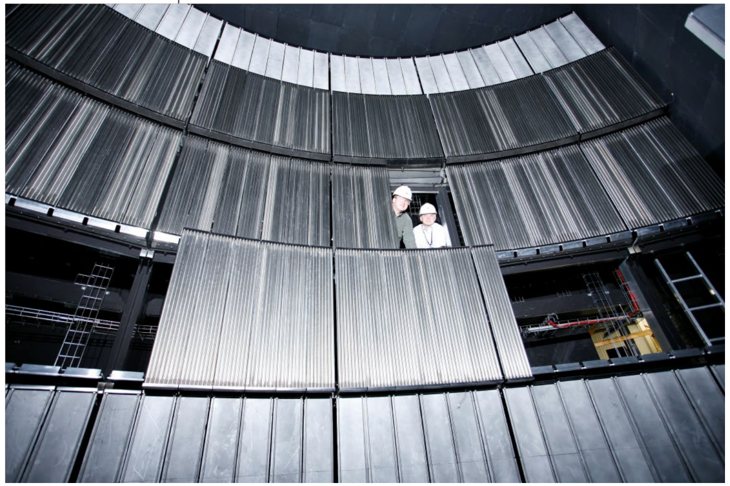
Neutron Scattering Division

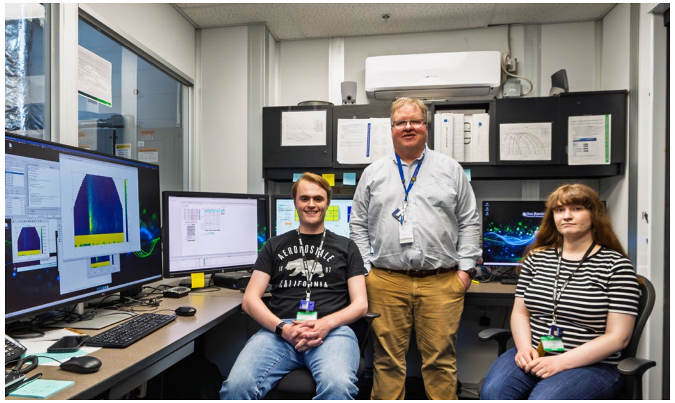
Neutron School 2026

Career Path

- University of Florida 1993-1998
  - PhD in Ultralow temperature Condensed Matter Physics, Working on Haldane spin chains Advisor M. W. Meisel
- ORNL Neutron Scattering group 1998-2000
  - Post Doc, Working on low D quantum spin systems, Advisor S. E. Nagler
- Spallation Neutron Source 2000-2013
  - Instrument Scientist, working on direct geometry spectrometer design, science design and operation of SEQUOIA
- Neutron Data Science Group 2013-2019
  - Lead a group of 12 in the development of reduction and visualization software for neutron scattering
- ARCS Instrument Scientist 2019-
  - Support users and operation of the instrument







Overview

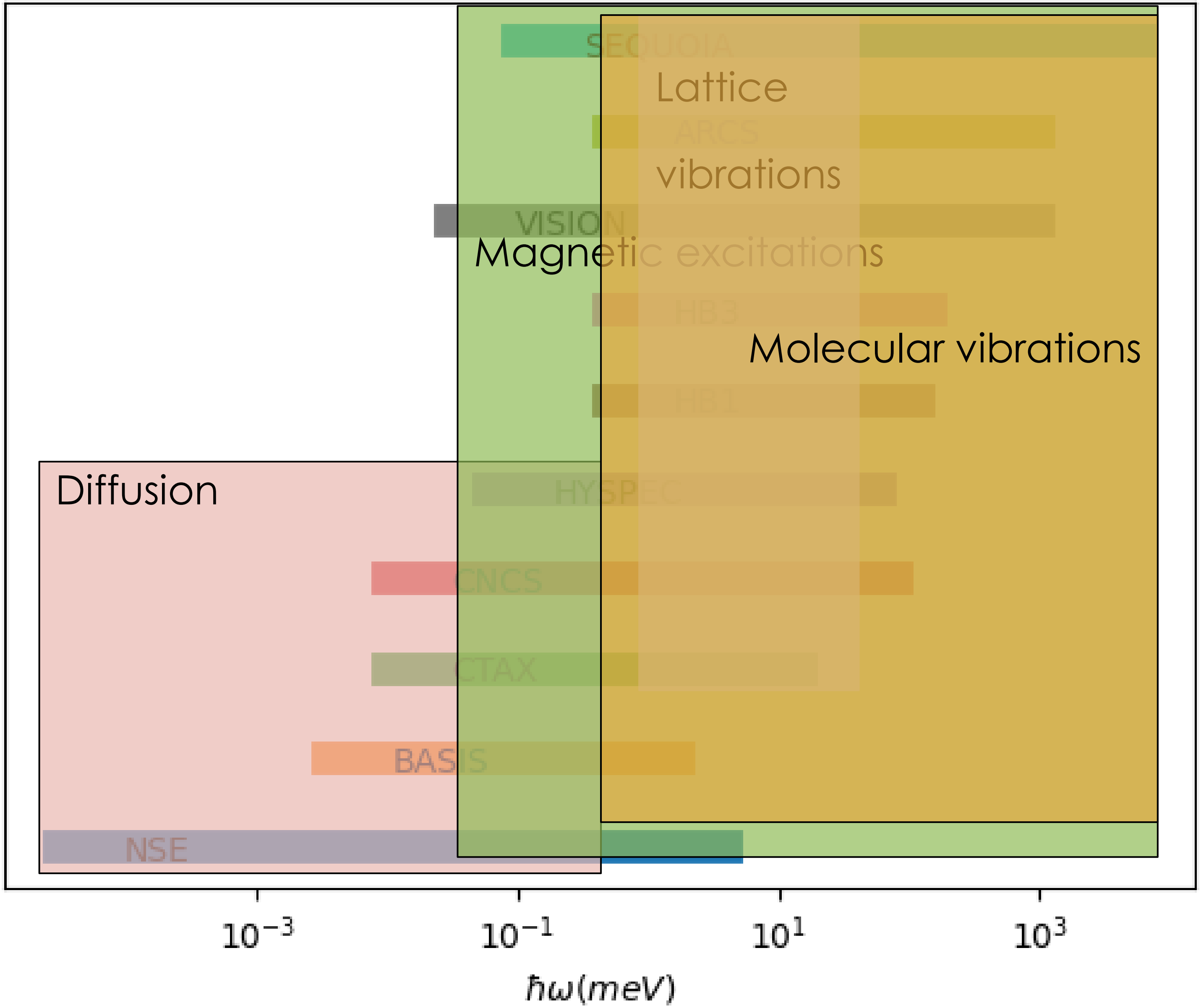
- Introduction
- Energy Range
- Q Dependence
- DGS vs. TAS Flux considerations
- Polarization considerations
- Sample planning
- Background considerations
- Resolution considerations
- Summary

Introduction

- Spectroscopy is checking if energy is gained or lost during the neutron's interaction with the sample.
- Spectrometers at ORNL
  - PTAX- HB1, TAX-HB3, CTAX, Veritas - HB1A (mostly used for diffraction)
  - BASIS, CNCS, HYSPEC, NSE, VISION, ARCS, SEQUOIA
- How do I choose the best instrument for my science?
  - Instrument Scientists are here to help. Consult them at all stages of your experiment planning.
- This talk provides some general guiding principles to help choose a spectrometer; starting with the most straightforward and moving to more subtle.

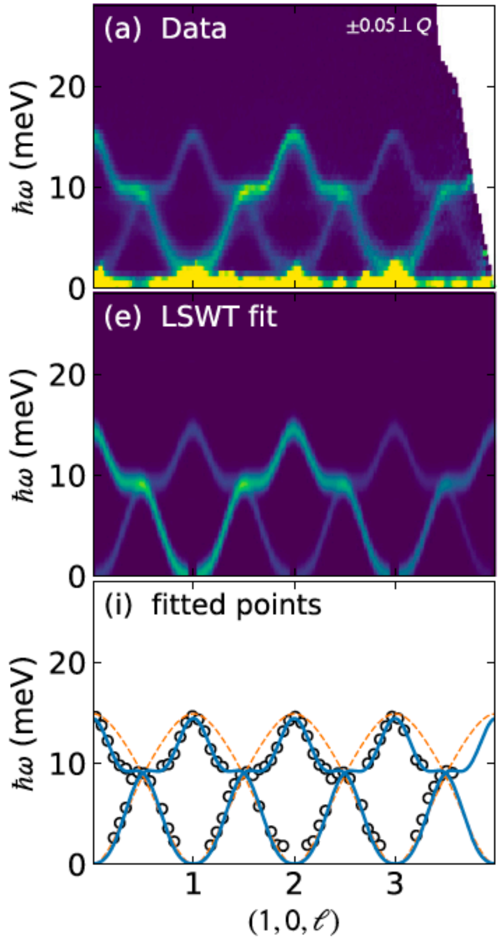
What Energy scale?

- Coldest neutron instruments for Diffusion
- Lattice and magnetic excitations cover lots of instruments
- Highest Energy instruments for molecular vibrations
- A complimentary measurement can help guide instrument choice
  - Specific heat, magnetic susceptibility, NMR, FTIR/Ramen
- Instrument scientist guidance is helpful



Will My data vary Quickly in Q?

- Yes
  - Phonons, Magnons
  - ARCS, SEQUOIA, CNCS, HYSPEC, HB1,HB3,CTAX
- No
  - Molecular vibrations, diffusion
  - Vision, Basis, NSE



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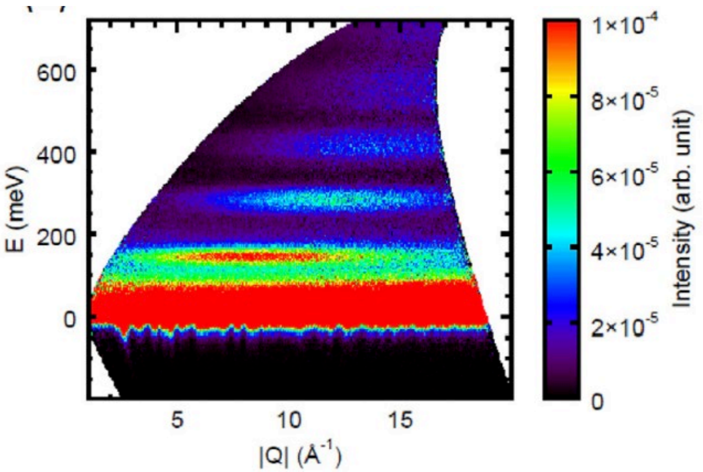

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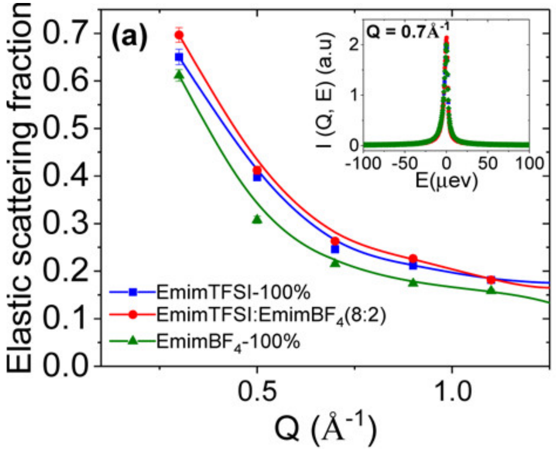
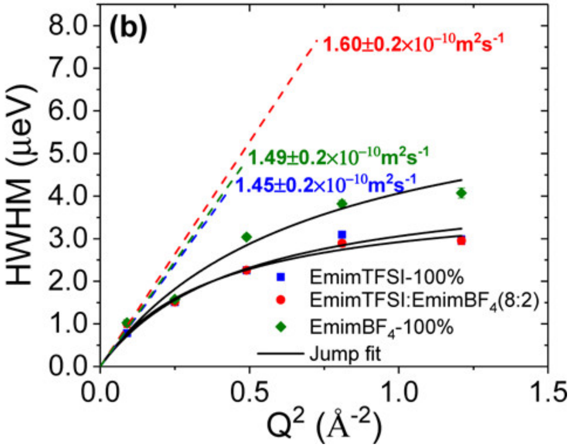
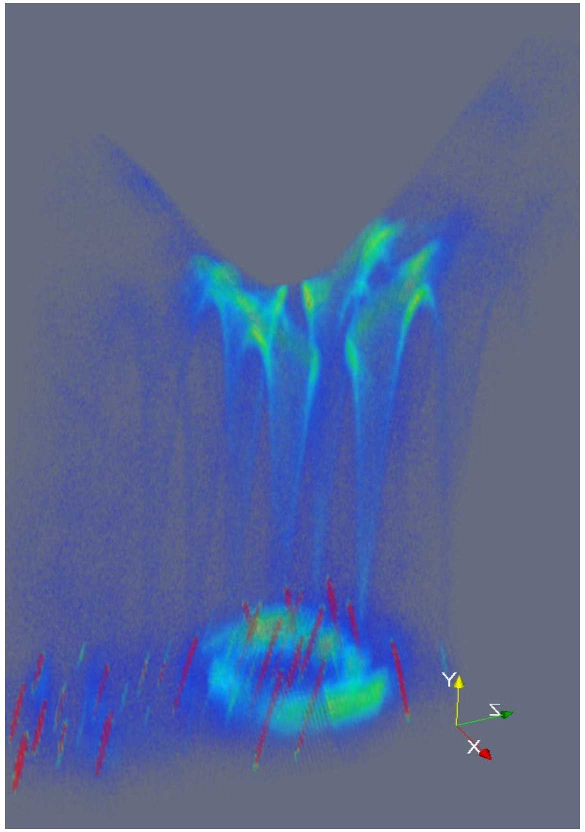




N. C. Osti et al. J. Phys. Chem. C, **122**, 10476 (2018)

Magnetic and Lattice excitations

- TAS instruments most neutrons in a single Q, ω voxel
  - HB1,HB3,CTAX
- DGS Instruments, fastest to map Q, ω space
  - CNCS, HYSPEC, ARCS, SEQUOIA



S. E. Hahn *et al.*
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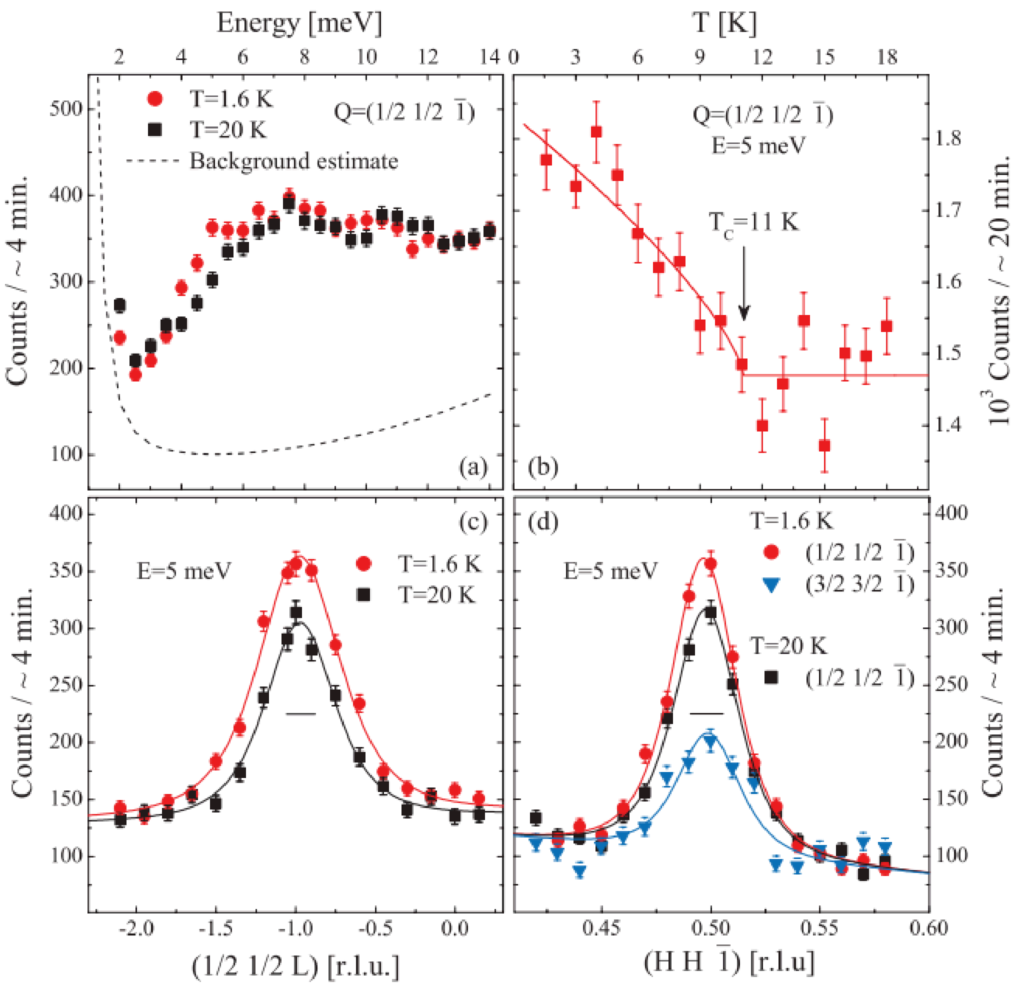


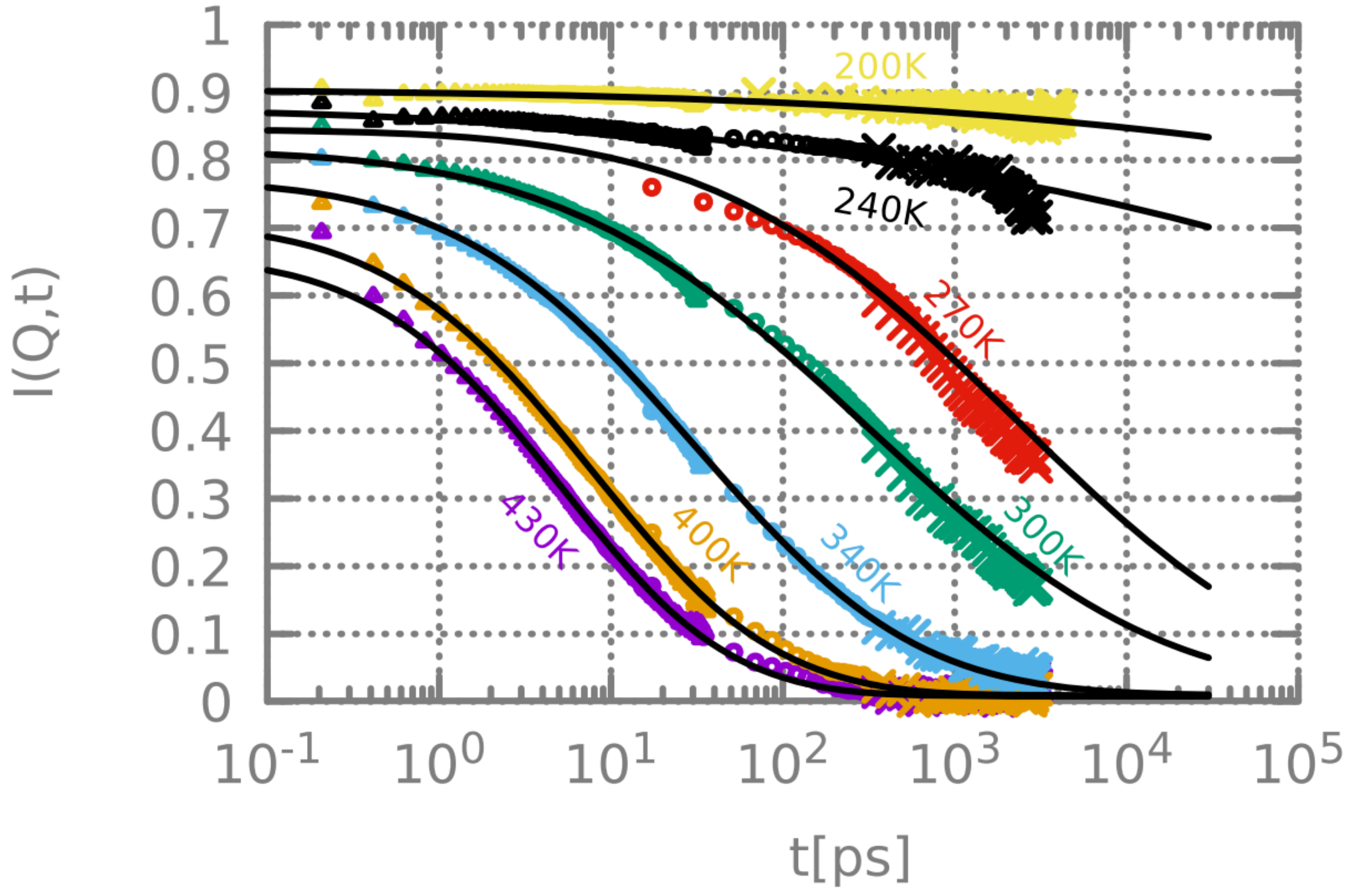
A. D. Christianson, *et al.*
Phys. Rev. Lett. **103**, 087002 (2008)

Groups of instruments

- Energy range, Q resolution and mode allow you to narrow the choice to a few instruments
  - Broad mappings of lattice or magnetic excitations – CNCS, HYSPEC, ARCS, SEQUOIA
  - Diffusive motions – CNCS, BASIS, NSE
  - Localized study of lattice or magnetic excitations – HB1, HB3, CTAX
  - Molecular vibrations – VISION, SEQUOIA, ARCS
- Talking with the Instrument Scientists on one of these instruments is the best way to move forward

More than one instrument may be required

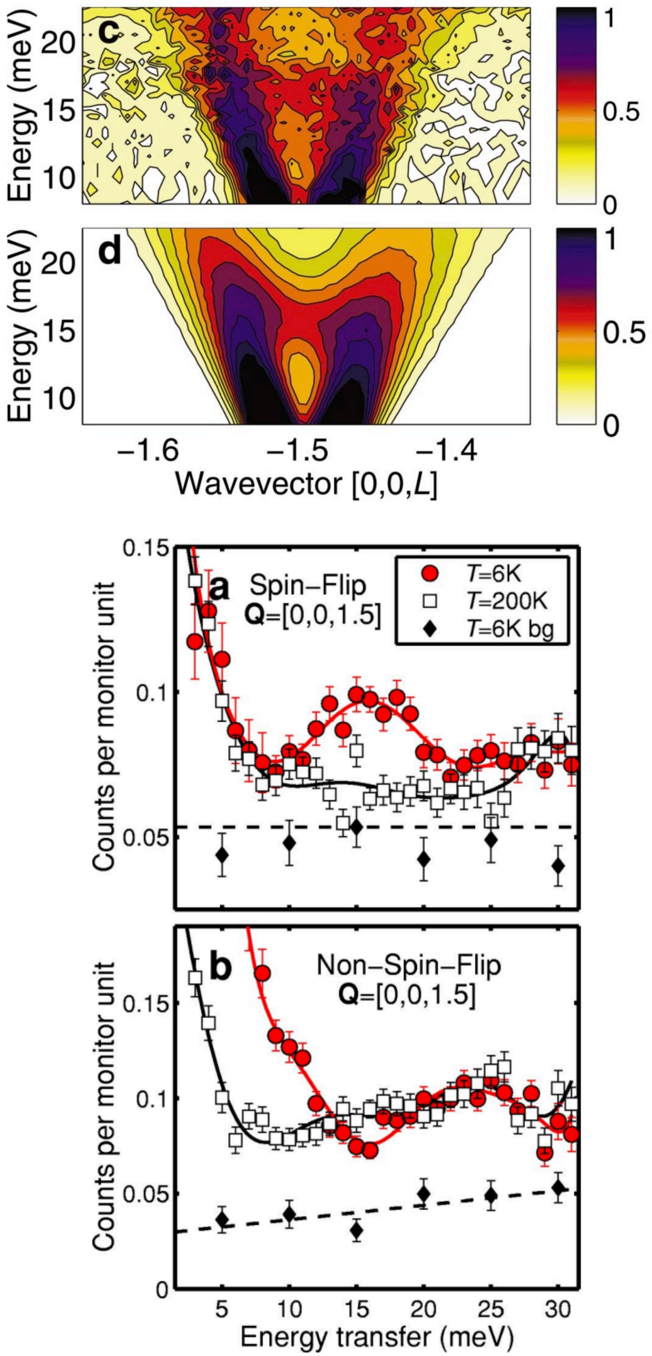
- Study of fractal diffusion in polymer fuel cell
- Many time scales
- Required 3 instruments
  - CNCS (△)
  - BASIS (O)
  - Spheres (×) (MLZ)
- Usually start with coarsest resolution



Hopfenmüller *et al.* J. Chem. Phys. **148**, 204906 (2018).

Does the Beam Need to be polarized?

- Separating Magnetic and Lattice Modes
- Identifying type of spin excitation (Transverse vs. Longitudinal)
- Used for timing in Spin Echo
- Things to think about.
  - Flux on sample is < 50% of unpolarized flux
  - Polarized beams are limited to cold (HYSPEC and NSE) and Thermal (HB1 and HYSPEC beams)
  - Usually a complimentary, unpolarized measurement should be done first.
- Polarized instruments
  HB1, HYSPEC, NSE



B. Lake, D. A. Tennant, S. E Nagler, Phys. Rev. B **71**, 134412 (2005)

Sample Size

- Rule of thumb
  - Your sample should be the size of your 👍
  - We are bending this rule
- 10% scatterer
  - Means 1% multiple scattering
  - For the High density polyethylene this is 3mm

$$0.10 = e^{-\sigma_s \rho t}$$

Scattering lengths and cross sections for various isotopes evaluated at 2200 m s^{-1}

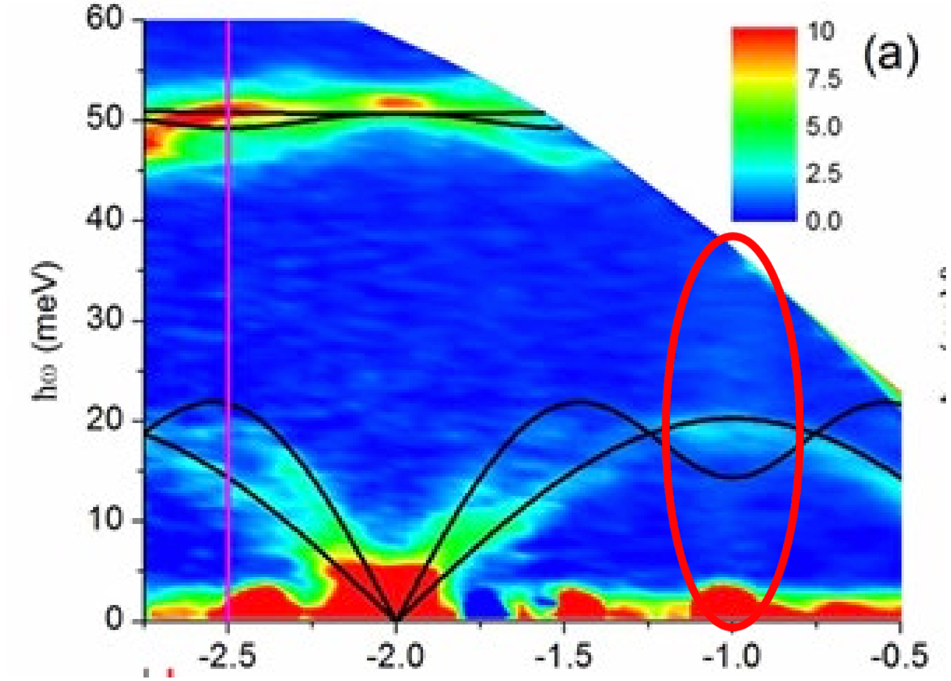
	Z	A	I(π)	abundance %	b_c fm	b_+ fm	b_- fm	σ_c barn	σ_i barn	σ_s barn	σ_a barn
n	0	1	1/2		-37.0(6)	0	-37.0(6)	43.010(20)		43.010(20)	0
H	1				-3.7409(11)			1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2	99.986(8)	-3.7395(11)	10.817(5)	-47.420(14)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1	0.015(8)	6.6681(27)	9.530(30)	0.97(6)	5.592(7)	2.050(30)	7.640(30)	0.000519(7)
		3	1/2		4.792(27)	4.18(15)	6.6(4)	2.890(30)	0.14(4)	3.03(5)	6e-06

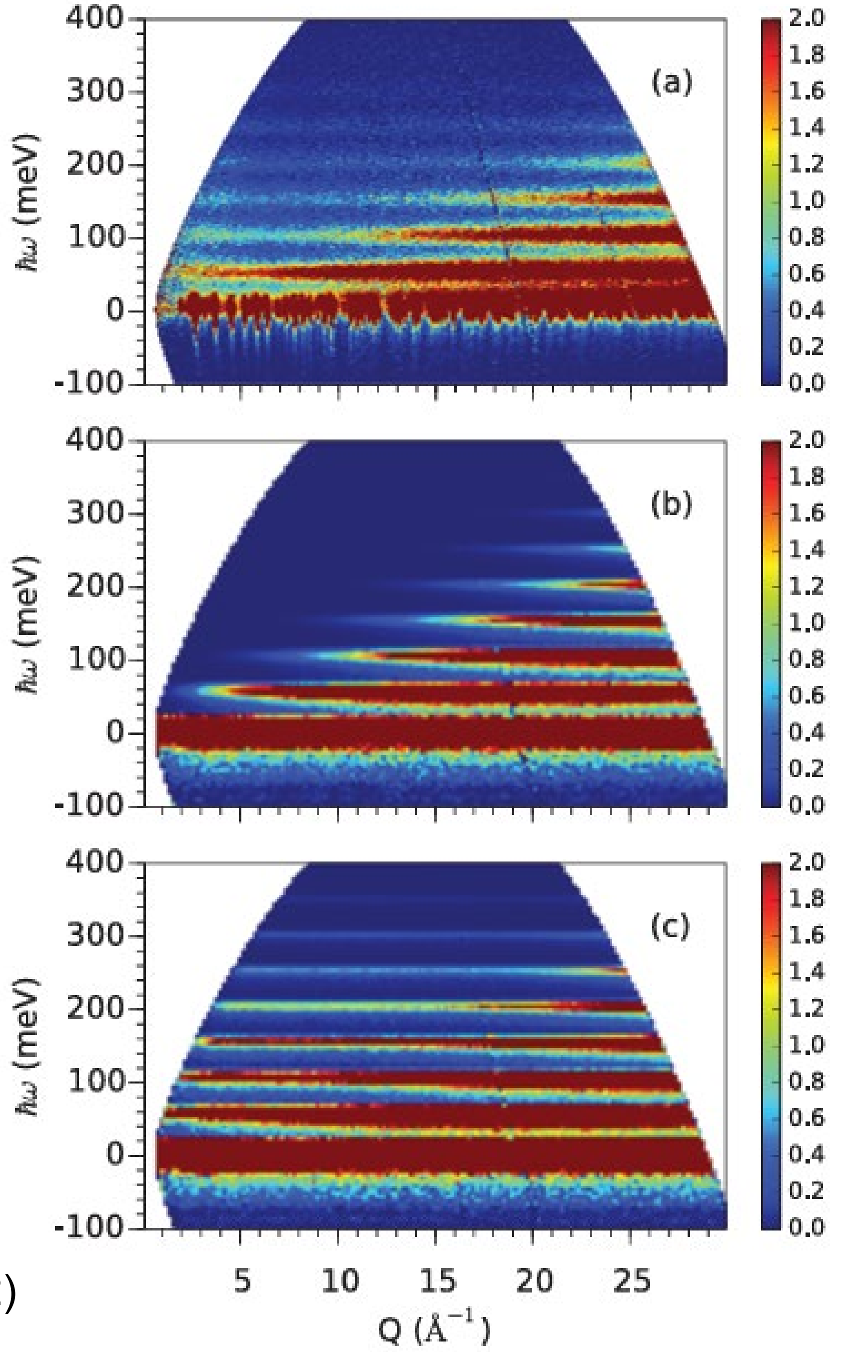
https://www.ncnr.nist.gov/resources/n-lengths/

Neutron News, Vol. 3, No. 3, 1992, pp. 29-37

UN and multiple scattering

- Sample sized to see weak itinerant magnetism
- Incoherent to optic multiple scattering clearly evident.

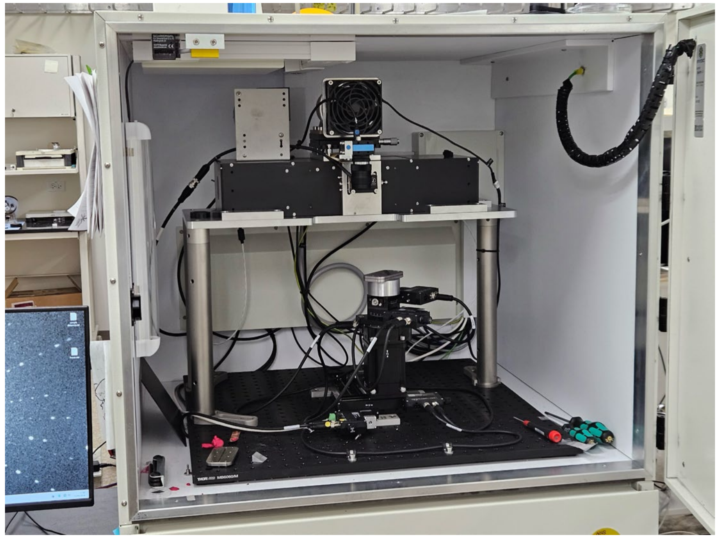


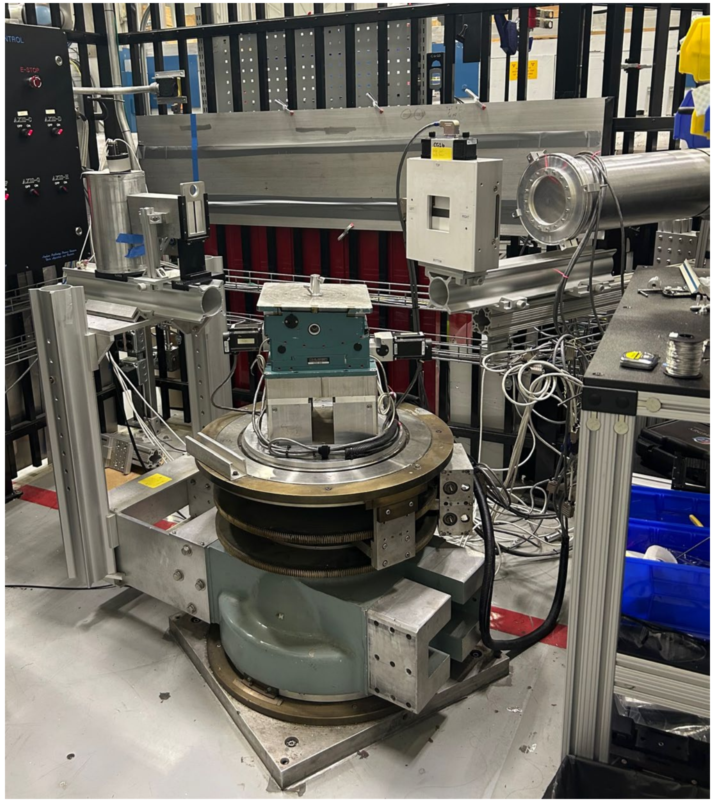


A.A. Aczel *et al.* Nature Communications **3**, 1124 (2012)
J.Y.Y. Lin *et al.,* Physical Review B, **89,** 144302 (2014)

Sample Orientation

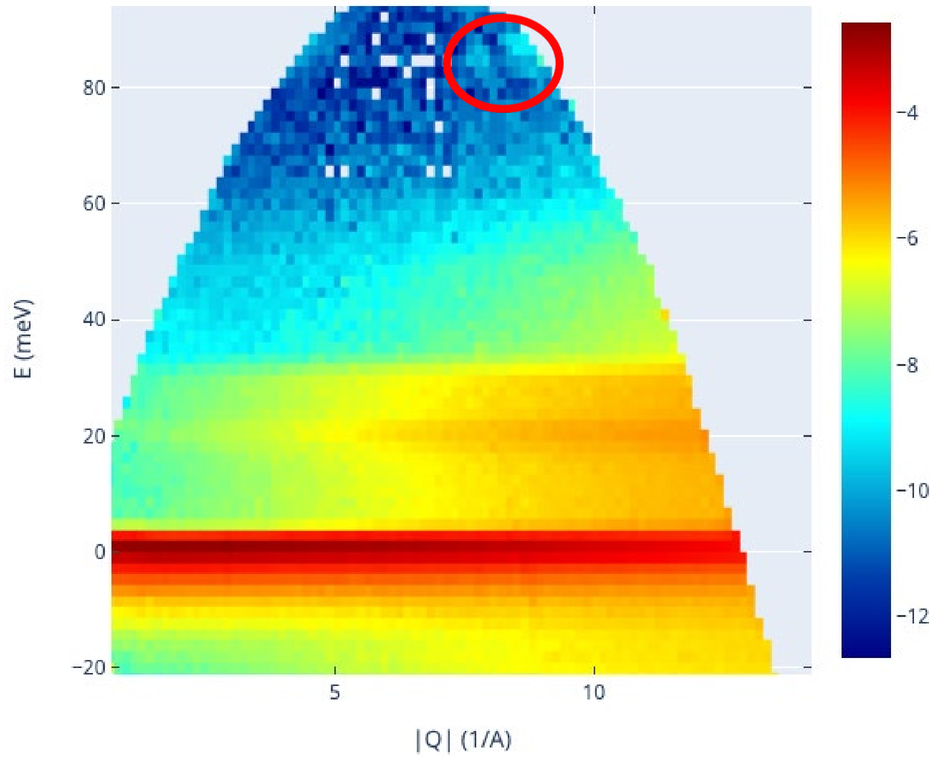
- Orientation of single crystals
  - For triple axis you must be in the scattering plane
    - Orient with xray Laue or neutrons at HFIR
    - You can request time in IPTS
  - DGS instruments with large detector arrays are more forgiving, but you count more efficiently if you know your orientation
  - Special Sample environment may place more restrictions.



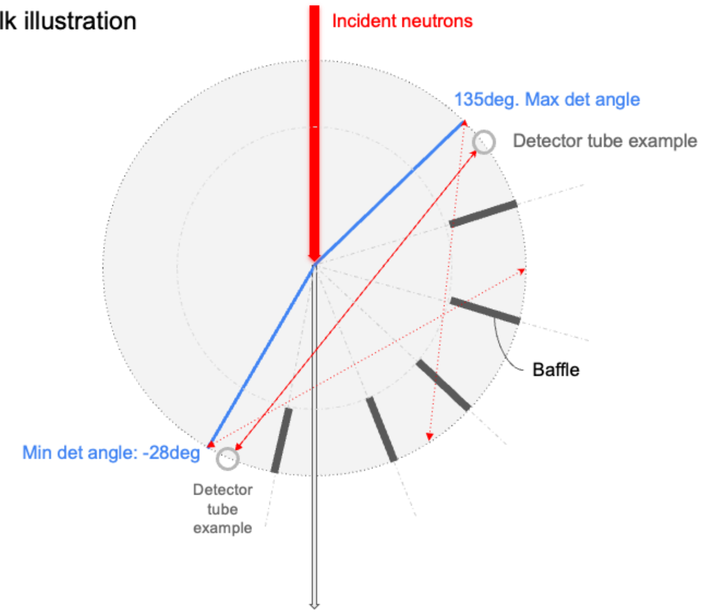


Background Considerations

- For triple axis spectrometers
  - Background tends to be flat, but larger than DGS instruments
  - Spurions are straightforward to calculate and identify
- For TOF instruments
  - Background tends to be low but structured
  - Usually appears at wrong time of flight
  - Sometimes structured background is hard to distinguish from signal.
  - Example Tube to Tube scattering on ARCS

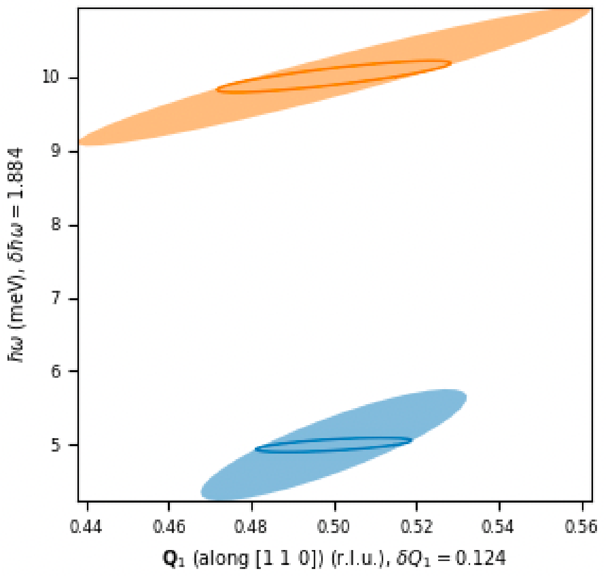


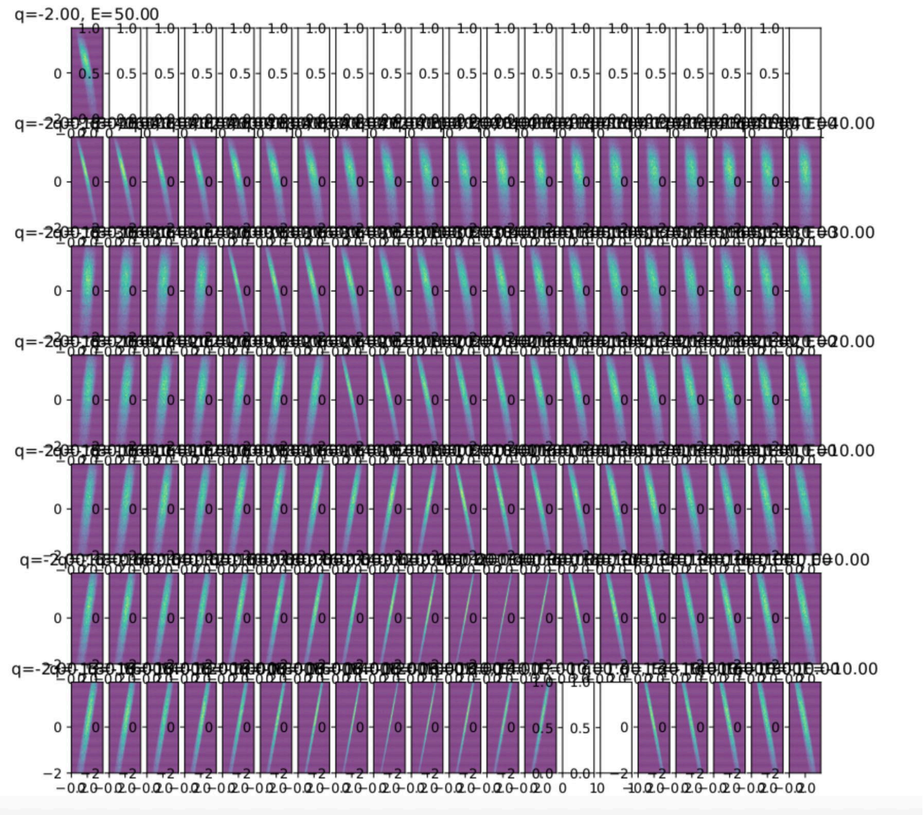
Cross talk illustration



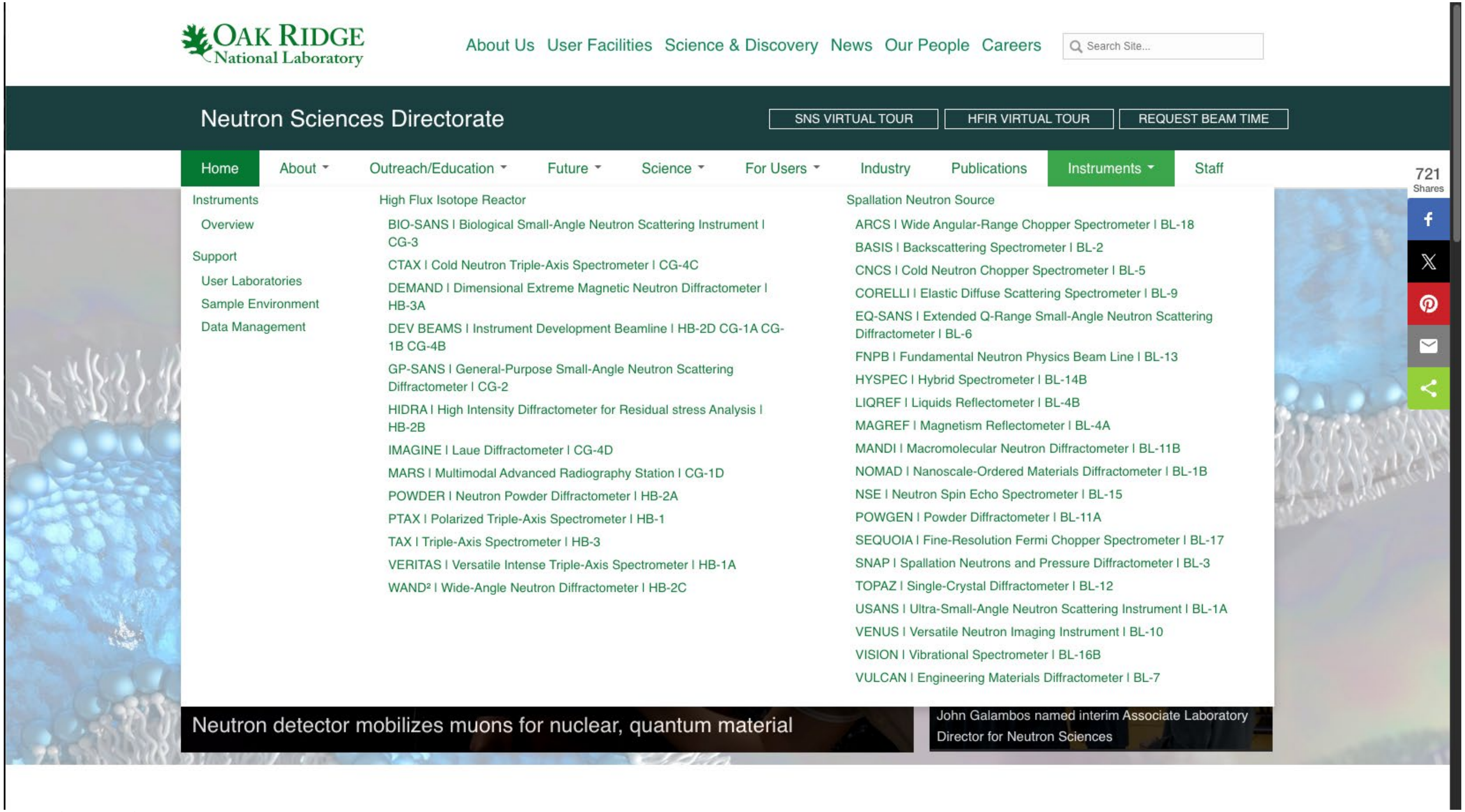
Resolution

- Finest resolution instruments are at spallation source
- Finest resolution is often not the best configuration
  - It comes with longer counting times or reduced Q,ω space coverage
- A TAS provides tunable resolution with
  - Collimation, focusing and Wollaston Prism options,
  - Change orientation with W vs. anti W configuration
- DGS instruments
  - Chopper speed and slit choice is used to tune resolution
  - Resolution orientation is fixed.
- Resolution choices are subtle (talk to the instrument staff)





Neutrons.ornl.gov is the easiest way to contact your instrument staff



Direct Geometry Spectroscopy

ARCS


Doug Abernathy


Garrett Granroth


Camille Bernal-Choban

CNCS


Daniel Pajerowski


Andrey Podlesnyak

Software


David Dhalbom


Andrei Savici

SEQUOIA


Matt Stone


Sasha Kolesnikov


Colin Sarkis

HYSPEC


Barry Winn


Ovi Garlea

Triple Axis Spectroscopy

HB3

Songxue Chi

Ellie Clements

CTAX

Tao Hong

Hodaka Kikuchi

HB1A

Wei Tian

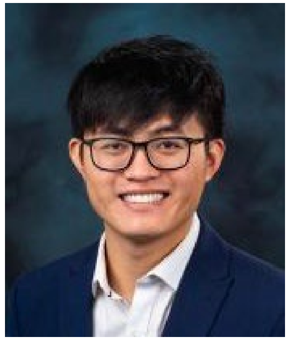
Adam Aczel

HB1

Masa Matsuda

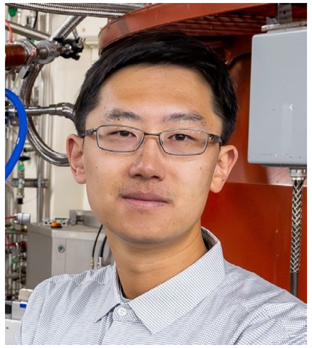
Avishek Maity

Wollaston Prisms



Fankang Li

Software

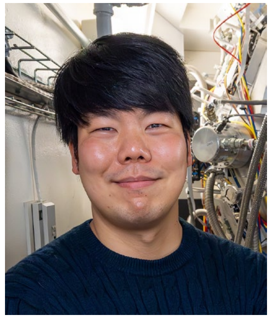


Kyle Ma

Indirect Spectroscopy and NSE

Vision

Murillo Martins



Hyun June Moon

BASIS

Niina Jalarvo

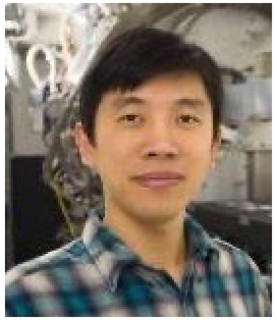
Naresh Osti

NSE

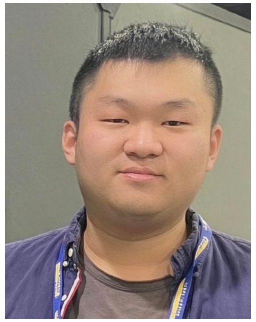
Laura Stingaciu

Piotr Zolnierczuk

Software



Yongqiang (YQ) Chen



Bowen Han

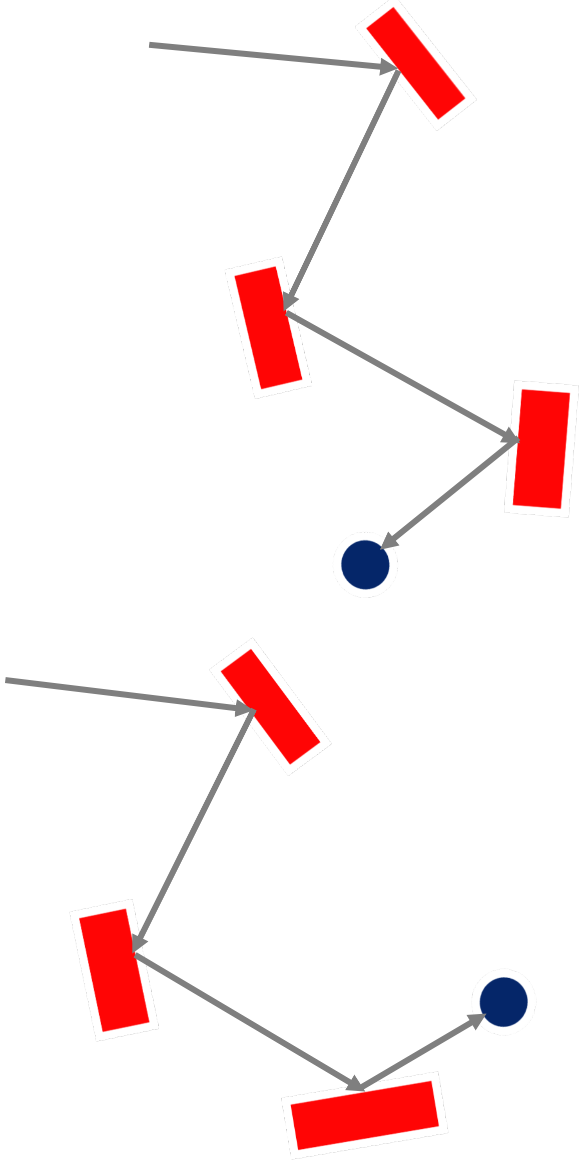
(Green: Supports Polarization Analysis)	Cold Moderator / 2 meV < Ei < 100 meV	Thermal Moderator / 5 meV < Ei < 2000 meV	
1-3% elastic E resolution / less flux	CNCS	SEQUOIA	Direct Geometry Spectrometers
3-5% elastic E resolution / high flux	**HYSPEC**	ARCS	
Highest time-averaged flux, localized & finite Q, ω	CTAX	HB1A, **HB1**, HB3	Triple-Axis Spectrometers
Fine energy resolution with flat dispersion / high throughput	BASIS, NSE	VISION	Indirect Geometry Spectrometers

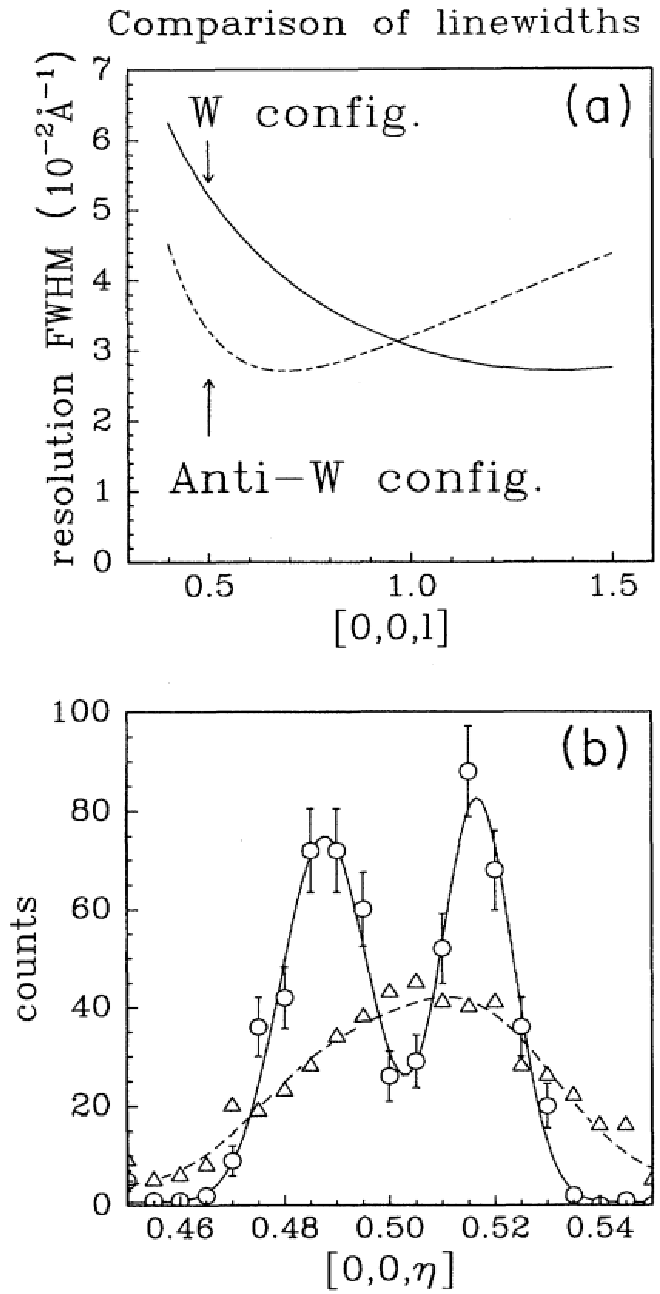
Summary

- Energy scale and Q dependence can narrow down what spectrometer to use
- Polarization is a powerful technique, but can be complex
- Sample size and orientation is important
- Resolution, and background considerations are tricky
- Ask Instrument staff for help

TAS Resolution Example

- Chain coupling in $KCuF_3$
- At small l
  - Anti- W configuration cuts the excitation in a focusing condition
  - W configuration does not
- Performed on TAS at HFBR

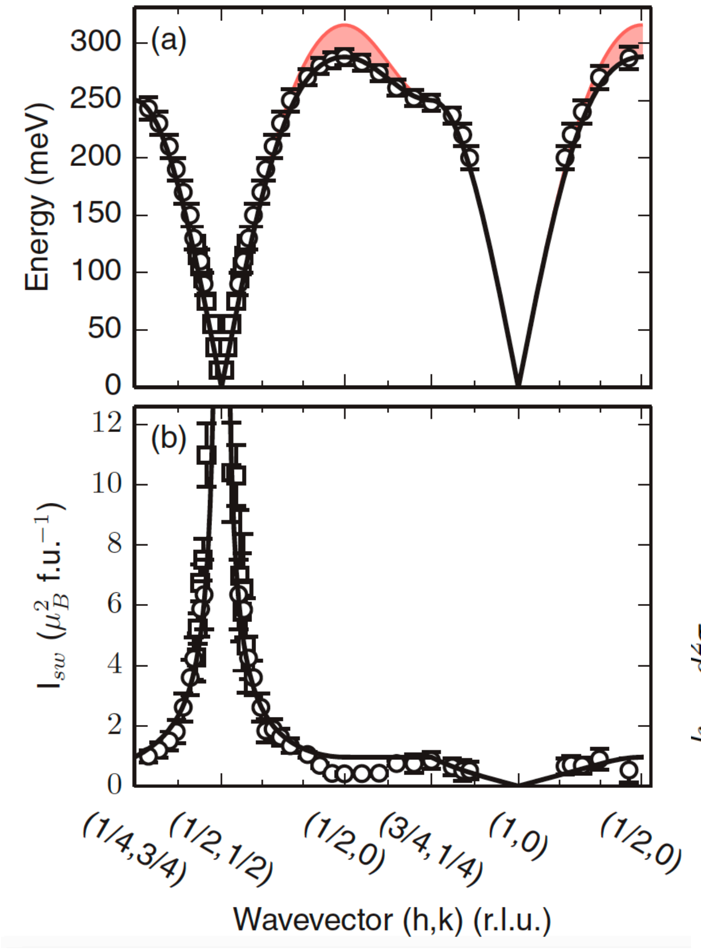


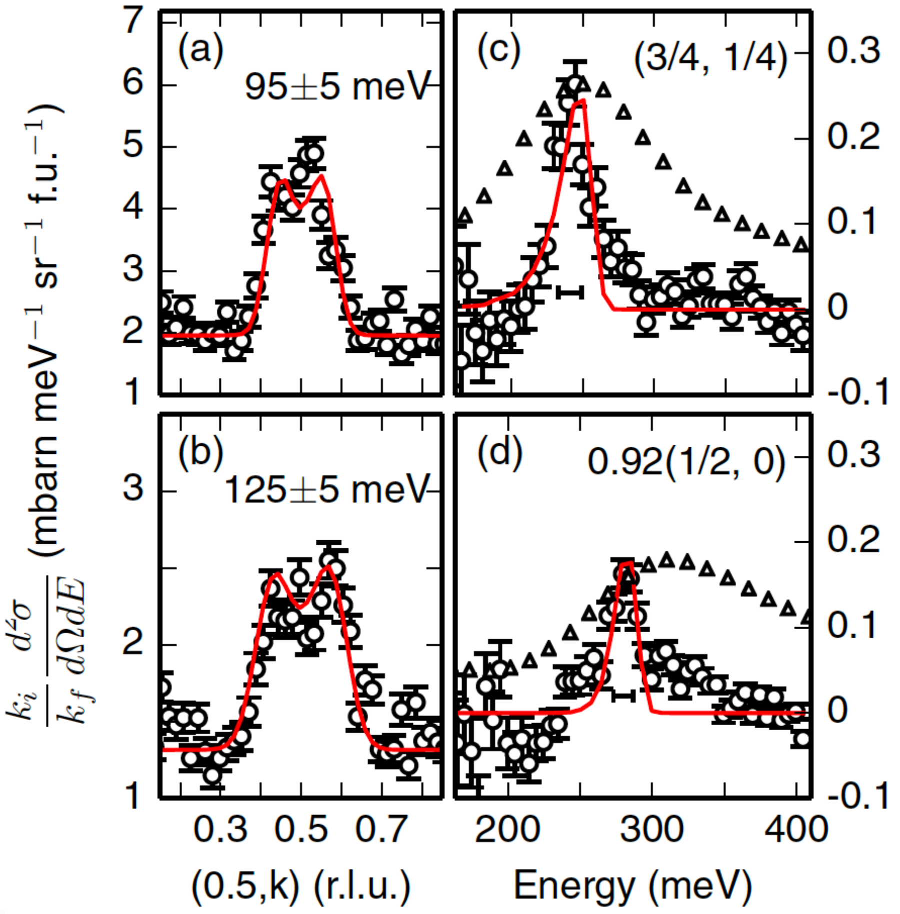


D. A. Tennant, *et al.* Phys. Rev. B **52**, 13381 (1995)

DGS Resolution example

- Zone Boundary Modes in $Sr_2CuO_2Cl_2$
- Resolution of SEQUOIA allowed fine measurement at zone boundary
- Energy Range and Flux Unique to SEQUOIA





K. Plumb *et al.* Phys. Rev. B **89**, 180410(R) (2014)