

# Choosing the right spectrometer

Garrett E. Granroth  
ARCS Instrument Scientist  
Neutron Scattering Division  
Neutron School 2026

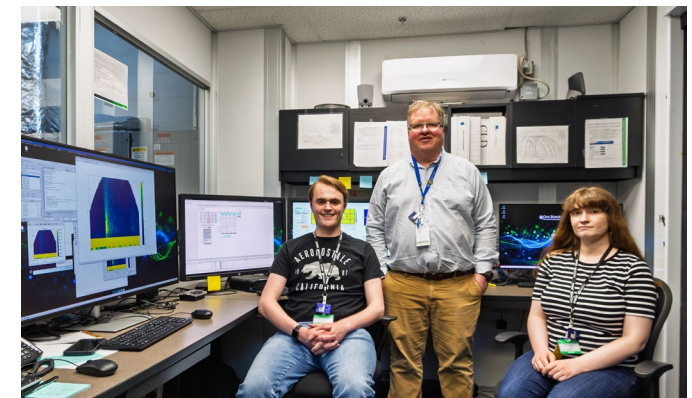
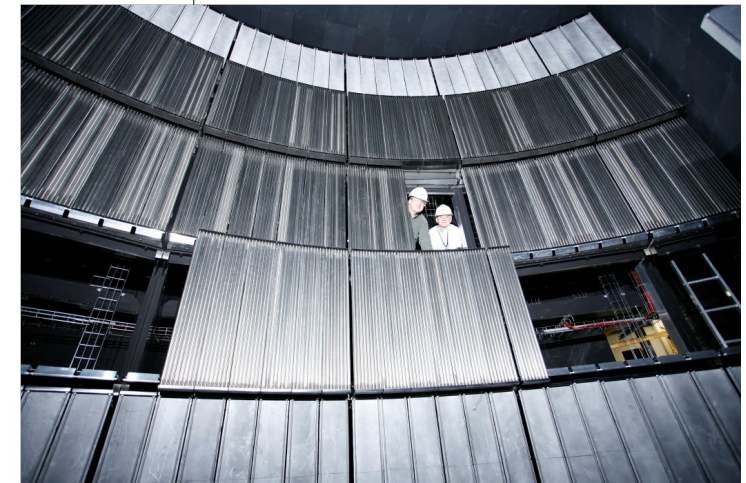
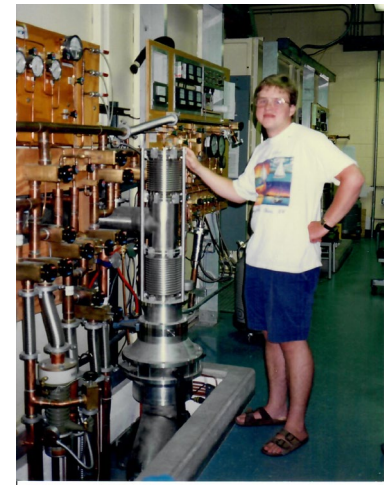
ORNL is managed by UT-Battelle, LLC for the US Department of Energy



U.S. DEPARTMENT OF  
**ENERGY**

# 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

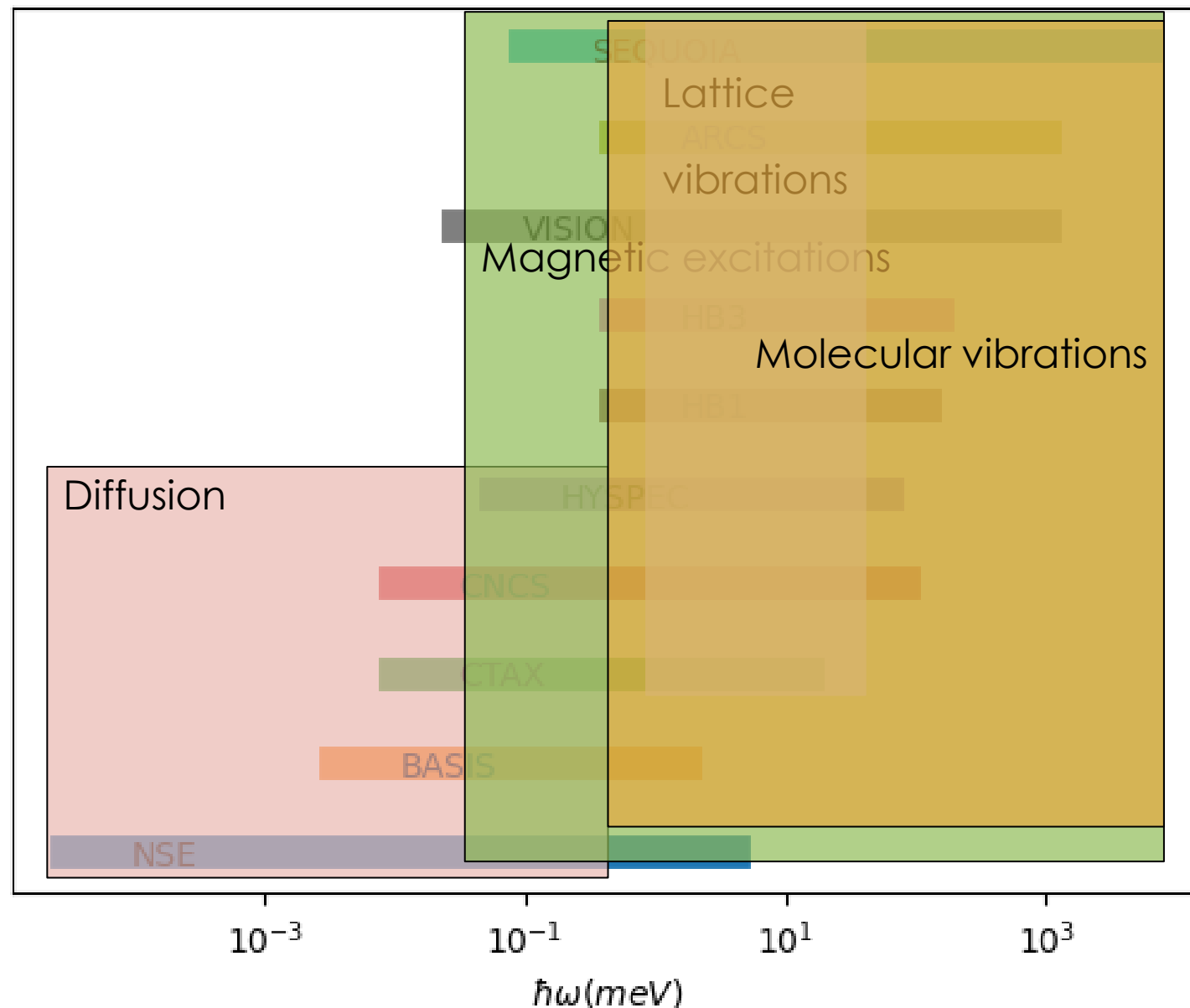
- Introduction
- Energy Range
- Q Dependence
- DGS vs. TAS Flux considerations
- Polarization considerations
- Sample planning
- Background considerations
- Resolution considerations
- Summary

# 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.

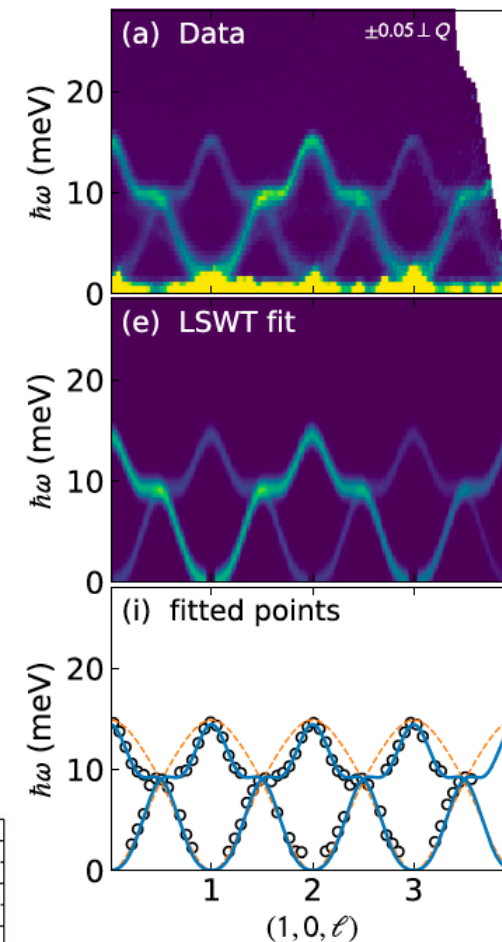
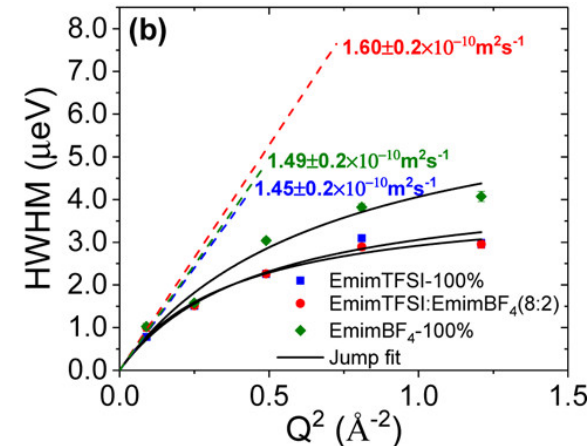
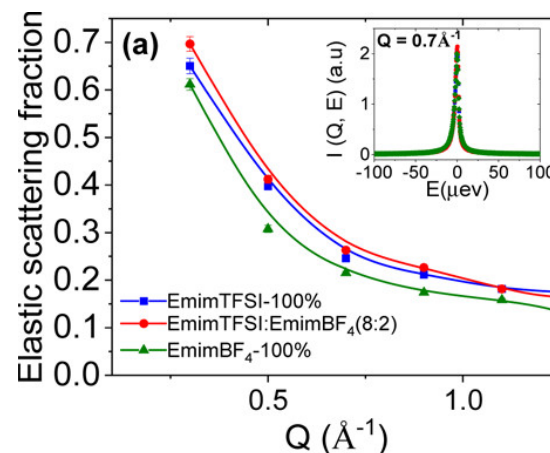
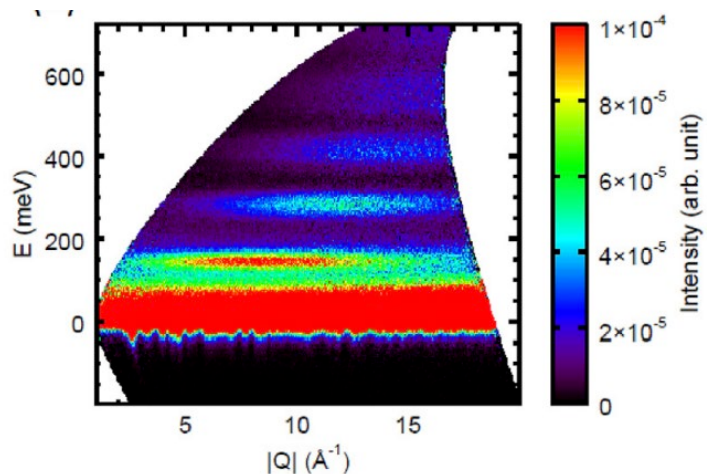
# What Energy scale?

- 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/Raman
- 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



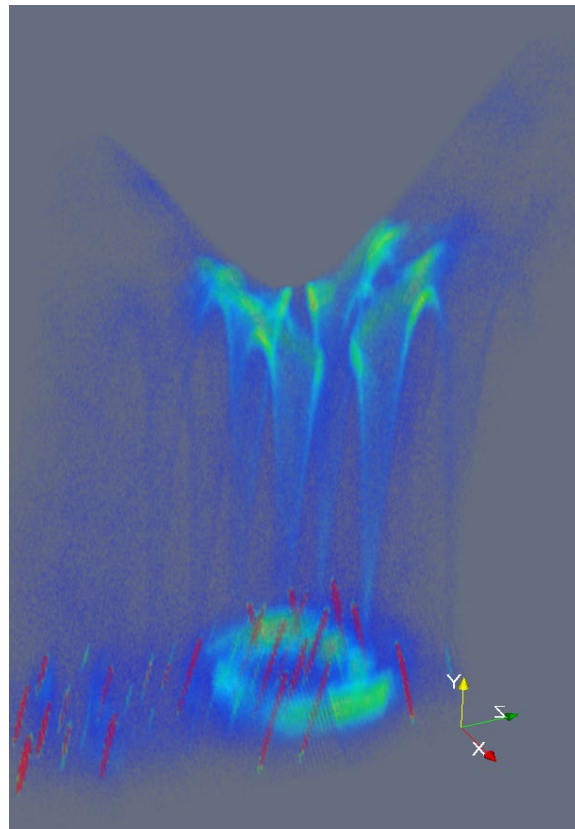
A. Sheie *et al.* *Phys. Rev. B* **105**, 104402 (2022)

T.R. Prisk *et al.* *J. Alloys Comps.* **818** 152832 (2020)

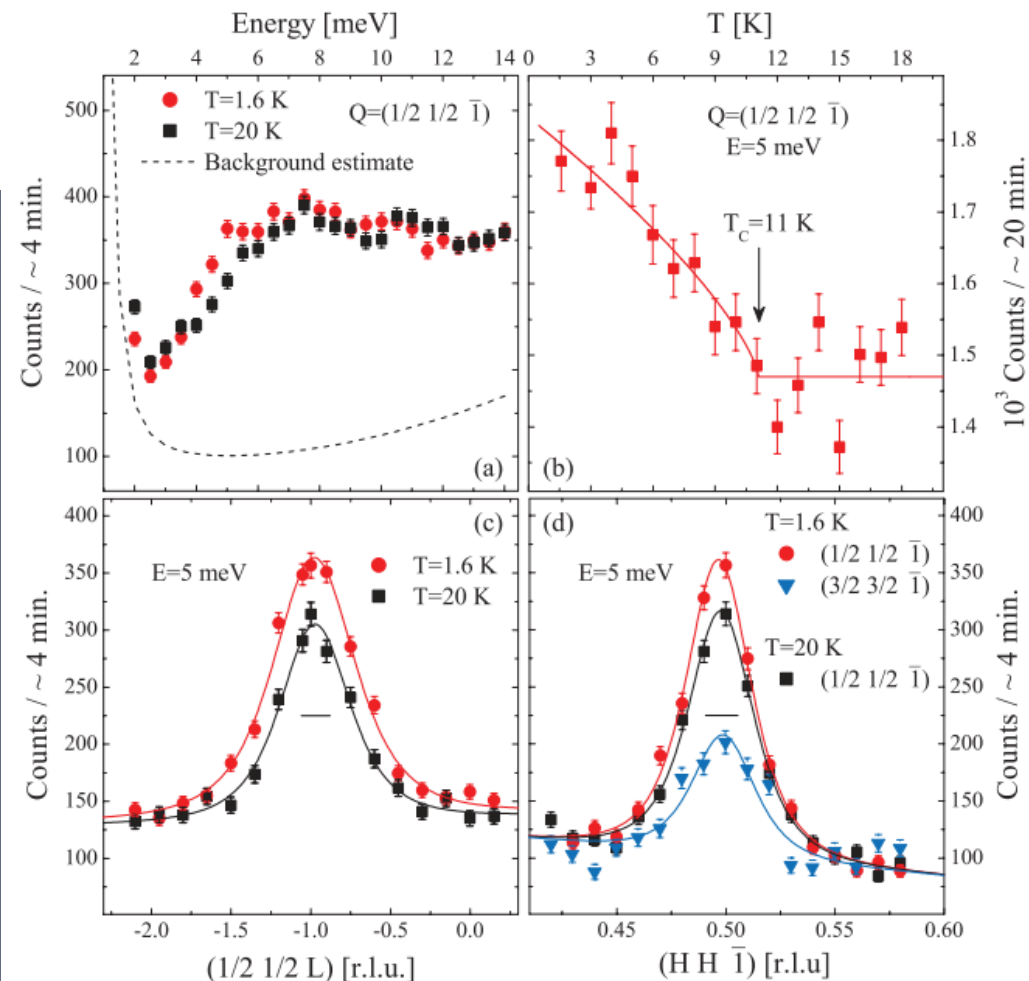
N. C. Osti *et al.* *J. Phys. Chem. C*, **122**, 10476 (2018)

# Magnetic and Lattice excitations

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



S. E. Hahn *et al.*  
Phys. Rev. B **89**, 014420 (2014)



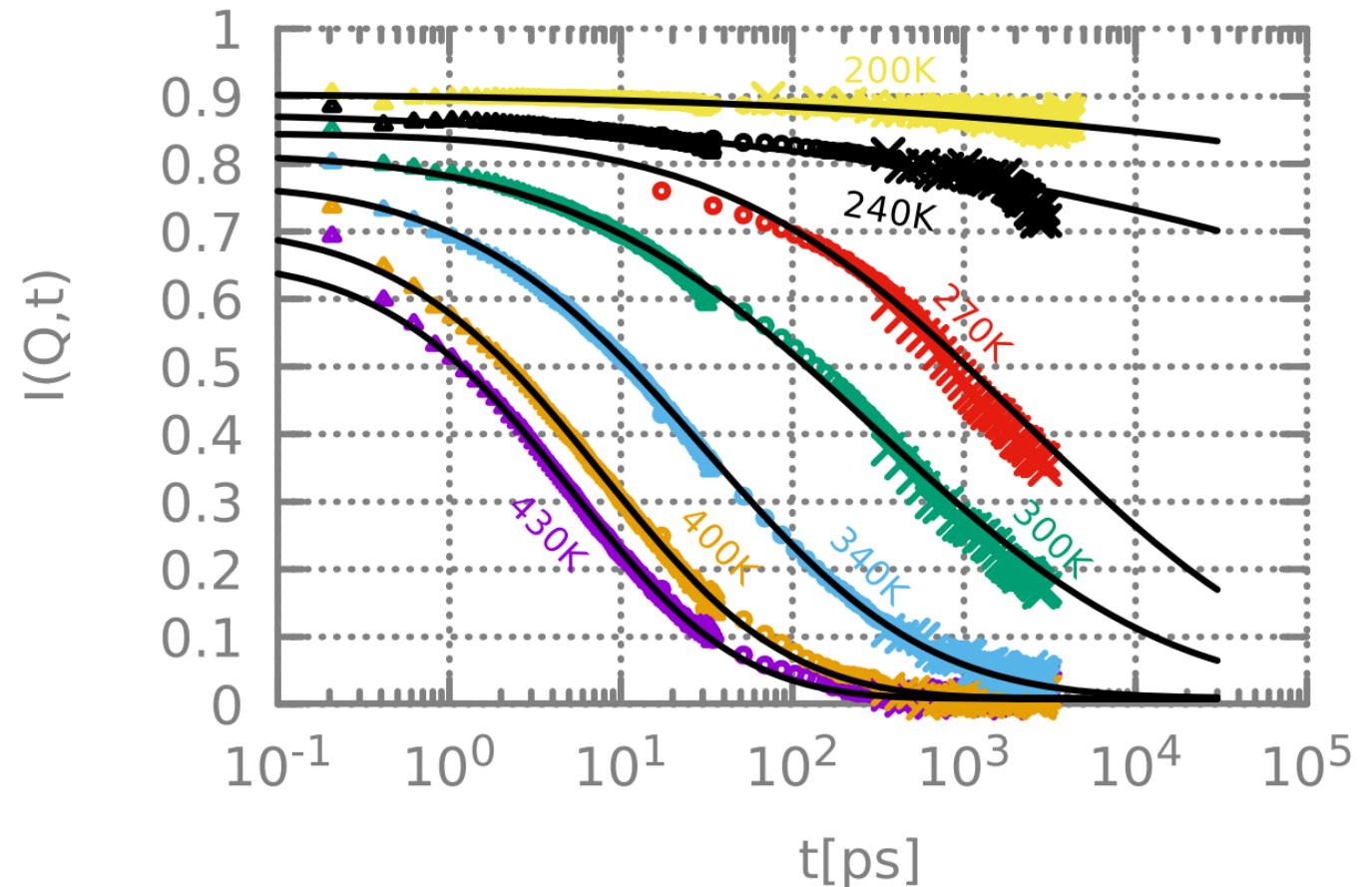
A. D. Christianson, *et al.*  
Phys. Rev. Lett. **103**, 087002 (2008)

# 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

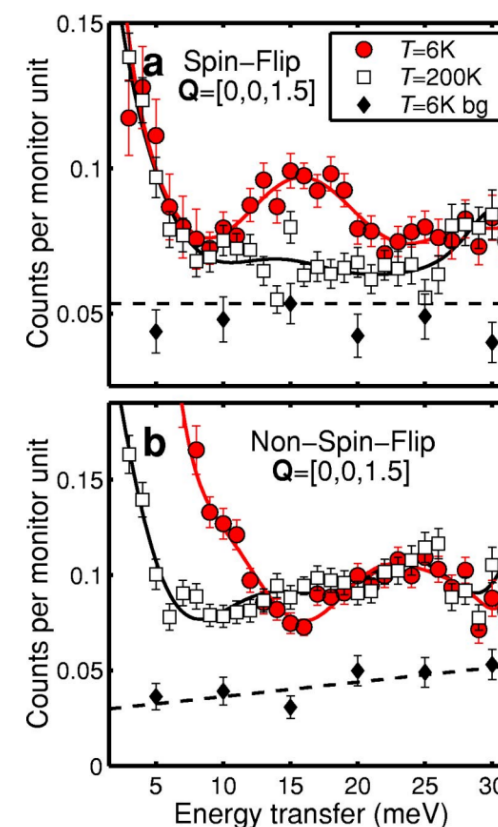
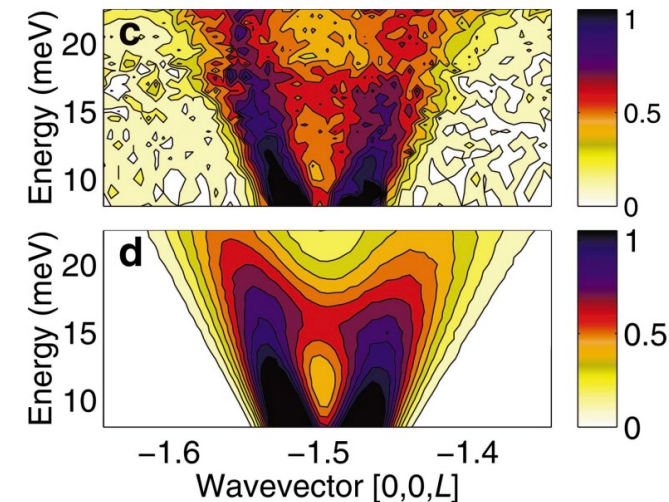
- Study of fractal diffusion in polymer fuel cell
- Many time scales
- Required 3 instruments
  - CNCS ( $\Delta$ )
  - BASIS (O)
  - Spheres ( $\times$ ) (MLZ)
- Usually start with coarsest resolution



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



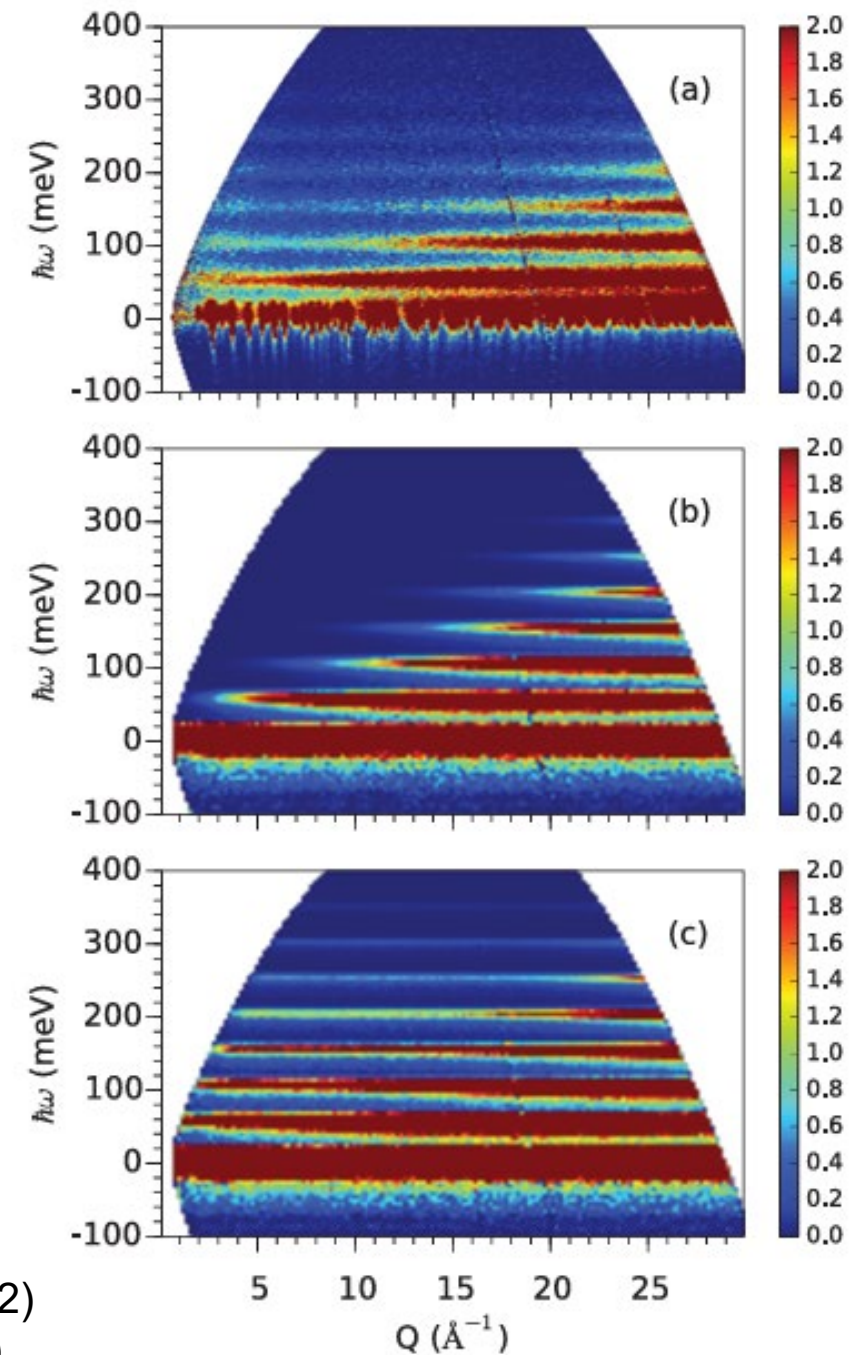
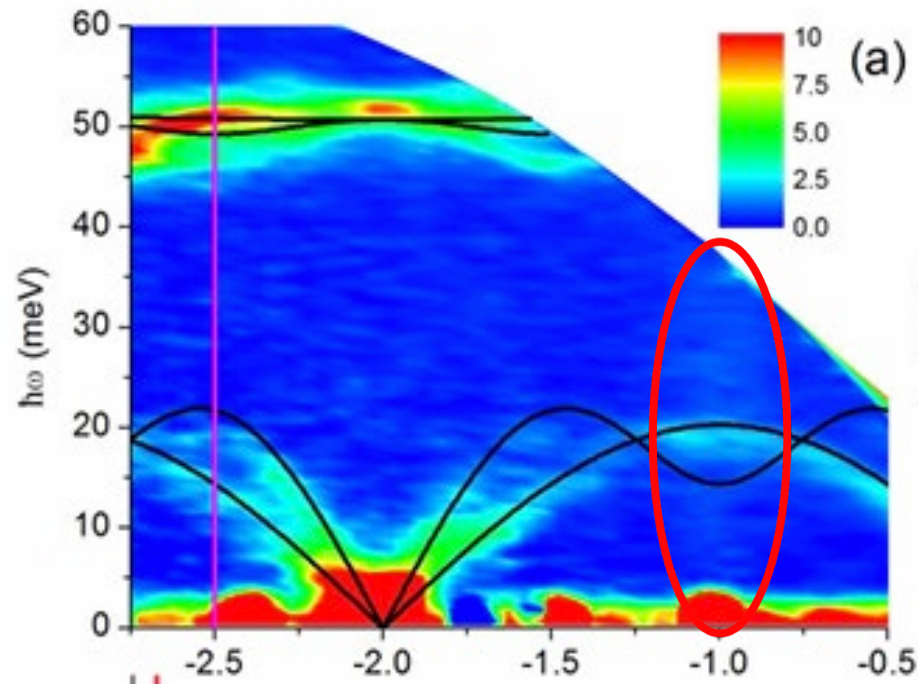
$$0.10 = e^{-\sigma_s \rho t}$$

Scattering lengths and cross sections for various isotopes evaluated at 2200 m s<sup>-1</sup>

|   | Z | A | I(π) | abundance % | b <sub>c</sub> fm | b <sub>+</sub> fm | b <sub>-</sub> fm | σ <sub>c</sub> barn | σ <sub>i</sub> barn | σ <sub>s</sub> barn | σ <sub>a</sub> 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               |

# UN and multiple scattering

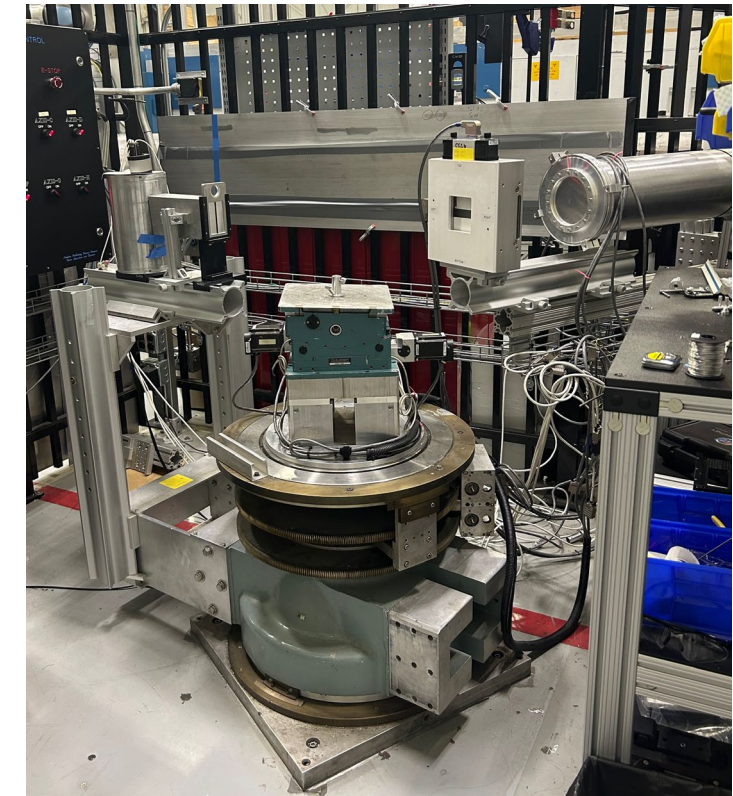
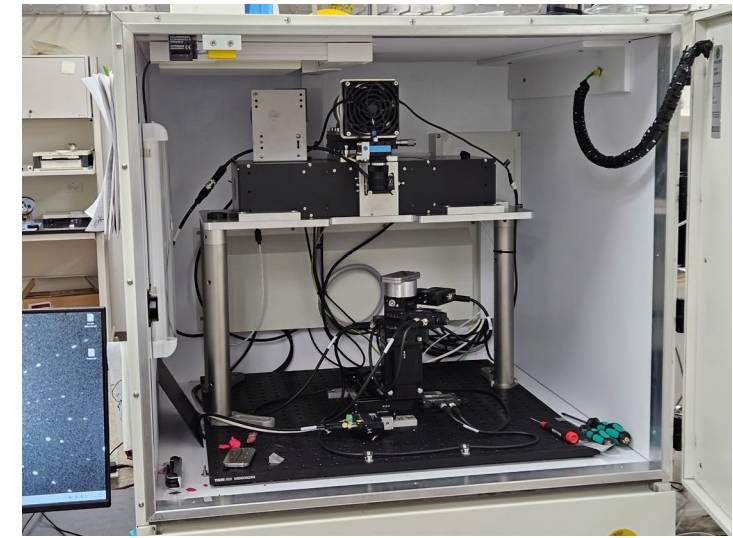
- Sample sized to see weak itinerant magnetism
- Incoherent to optic multiple scattering clearly evident.



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

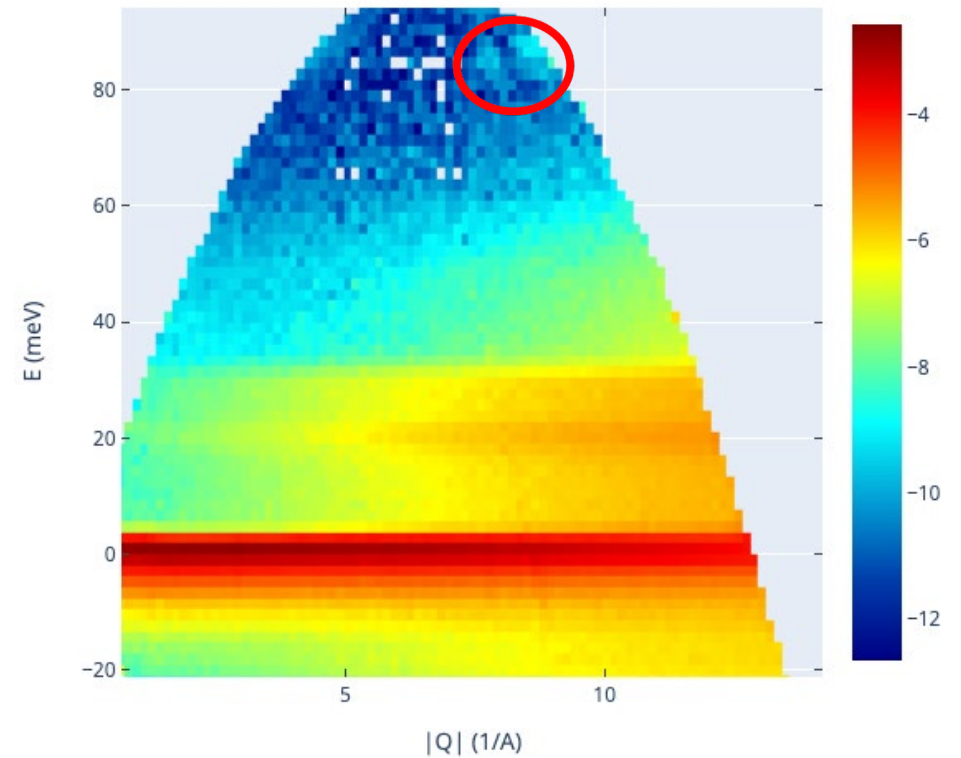
# Sample Orientation

- 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.

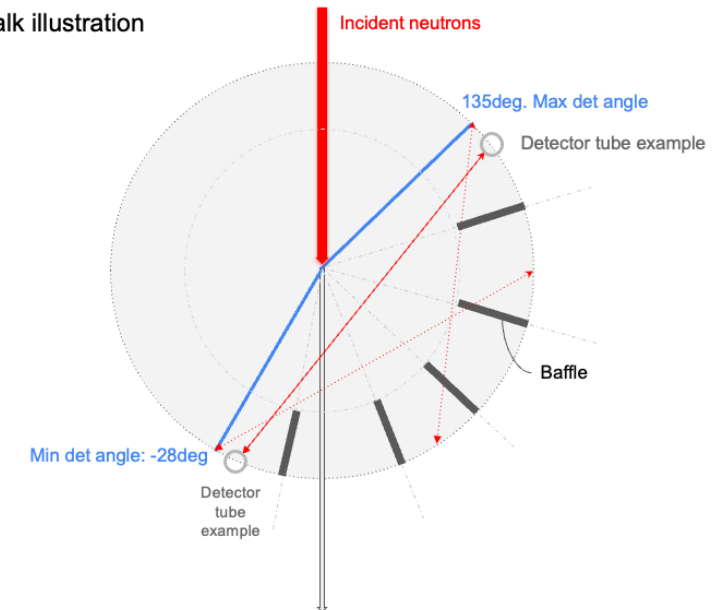


# Background Considerations

- 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

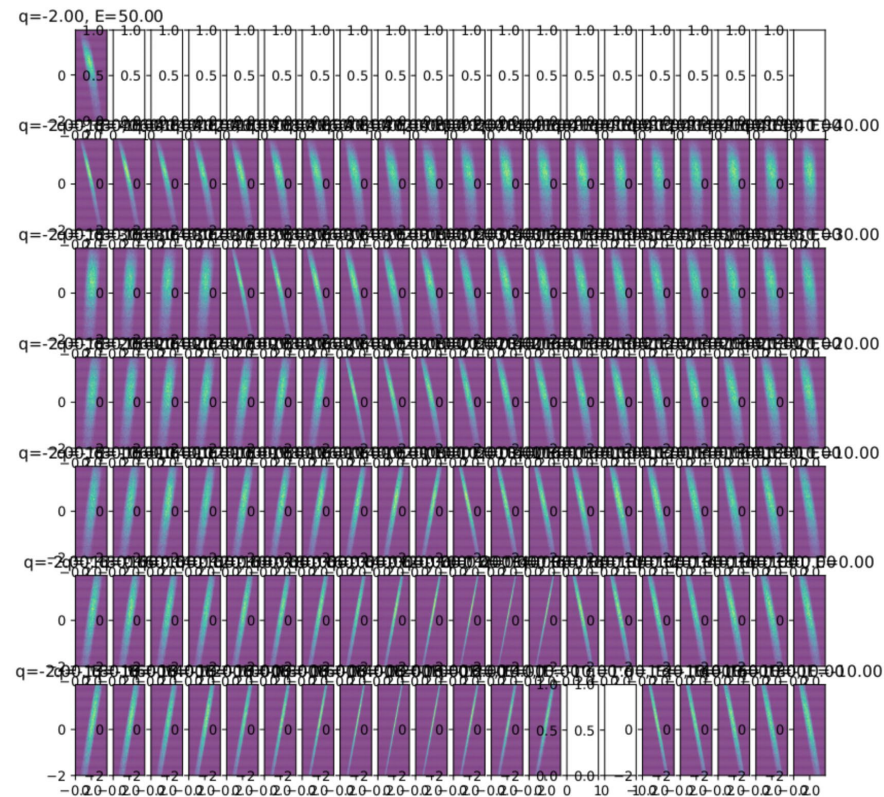
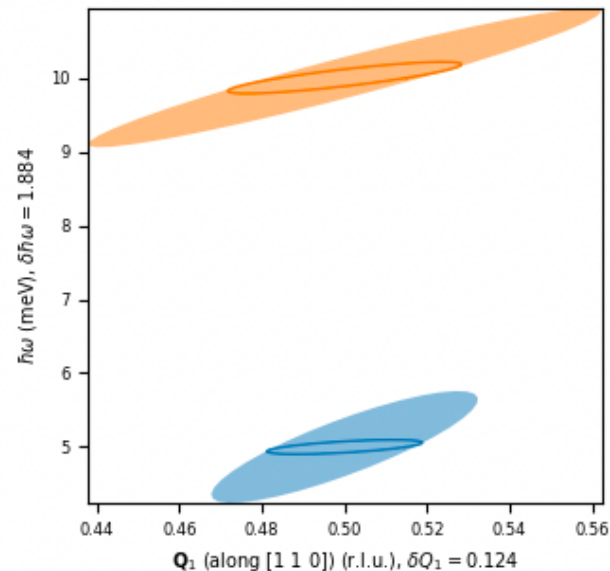


Cross talk illustration

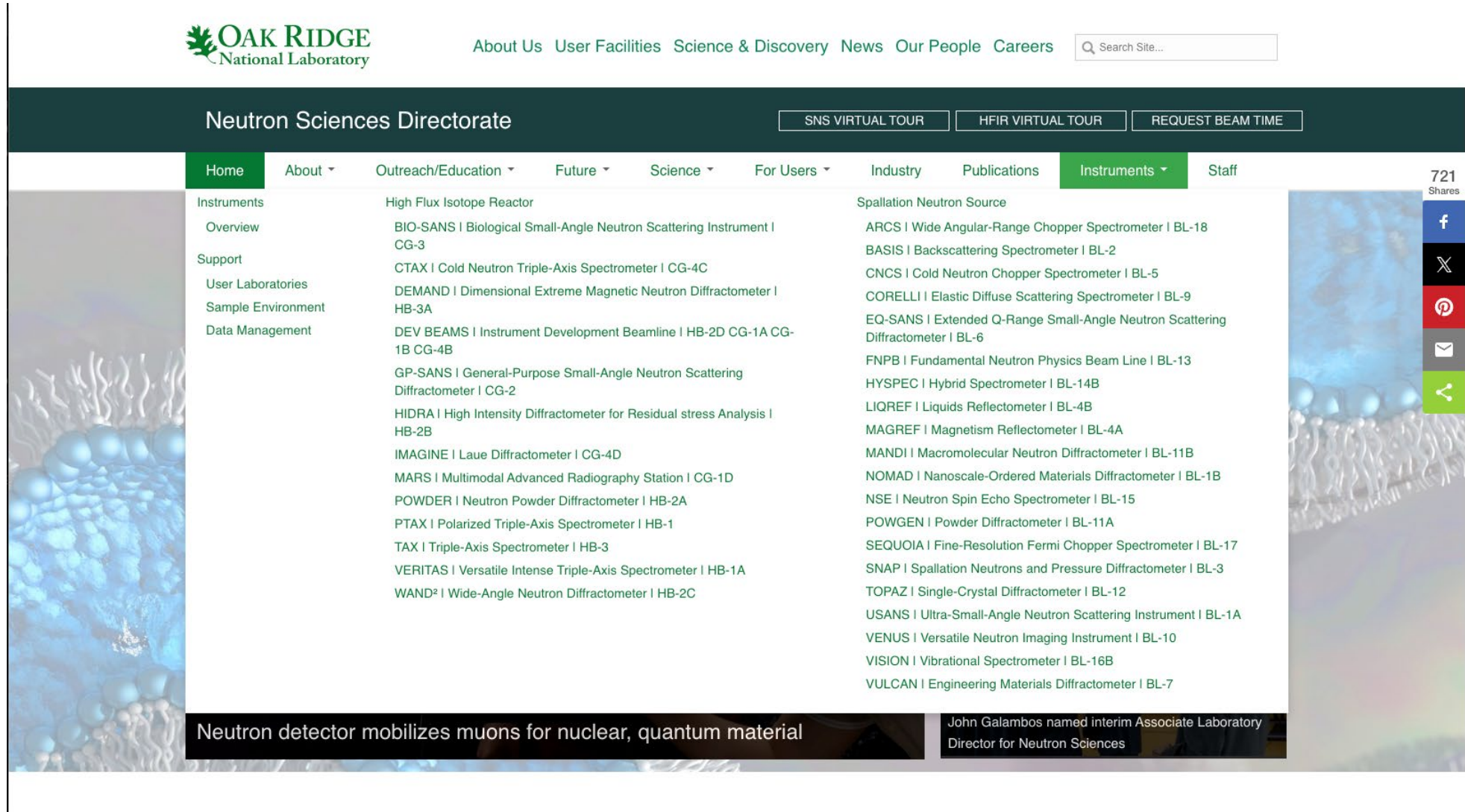


# Resolution

- Finest resolution instruments are at spallation source
- Finest resolution is often not the best configuration
  - It comes with longer counting times or reduced  $Q, \omega$  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



**OAK RIDGE National Laboratory**

About Us User Facilities Science & Discovery News Our People Careers

Search Site...

## Neutron Sciences Directorate

SNS VIRTUAL TOUR HFIR VIRTUAL TOUR REQUEST BEAM TIME

Home About Outreach/Education Future Science For Users Industry Publications Instruments Staff

**Instruments**

- Overview
- Support
- User Laboratories
- Sample Environment
- Data Management

**High Flux Isotope Reactor**

- BIO-SANS | Biological Small-Angle Neutron Scattering Instrument | CG-3
- CTAX | Cold Neutron Triple-Axis Spectrometer | CG-4C
- DEMAND | Dimensional Extreme Magnetic Neutron Diffractometer | HB-3A
- DEV BEAMS | Instrument Development Beamline | HB-2D CG-1A CG-1B CG-4B
- GP-SANS | General-Purpose Small-Angle Neutron Scattering Diffractometer | CG-2
- HIDRA | High Intensity Diffractometer for Residual stress Analysis | HB-2B
- IMAGINE | Laue Diffractometer | CG-4D
- MARS | Multimodal Advanced Radiography Station | CG-1D
- POWDER | Neutron Powder Diffractometer | HB-2A
- PTAX | Polarized Triple-Axis Spectrometer | HB-1
- TAX | Triple-Axis Spectrometer | HB-3
- VERITAS | Versatile Intense Triple-Axis Spectrometer | HB-1A
- WAND<sup>2</sup> | Wide-Angle Neutron Diffractometer | HB-2C

**Spallation Neutron Source**

- ARCS | Wide Angular-Range Chopper Spectrometer | BL-18
- BASIS | Backscattering Spectrometer | BL-2
- CNCS | Cold Neutron Chopper Spectrometer | BL-5
- CORELLI | Elastic Diffuse Scattering Spectrometer | BL-9
- EQ-SANS | Extended Q-Range Small-Angle Neutron Scattering Diffractometer | BL-6
- FNPB | Fundamental Neutron Physics Beam Line | BL-13
- HYSPEC | Hybrid Spectrometer | BL-14B
- LIQREF | Liquids Reflectometer | BL-4B
- MAGREF | Magnetism Reflectometer | BL-4A
- MANDI | Macromolecular Neutron Diffractometer | BL-11B
- NOMAD | Nanoscale-Ordered Materials Diffractometer | BL-1B
- NSE | Neutron Spin Echo Spectrometer | BL-15
- POWGEN | Powder Diffractometer | BL-11A
- SEQUOIA | Fine-Resolution Fermi Chopper Spectrometer | BL-17
- SNAP | Spallation Neutrons and Pressure Diffractometer | BL-3
- TOPAZ | Single-Crystal Diffractometer | BL-12
- USANS | Ultra-Small-Angle Neutron Scattering Instrument | BL-1A
- VENUS | Versatile Neutron Imaging Instrument | BL-10
- VISION | Vibrational Spectrometer | BL-16B
- VULCAN | Engineering Materials Diffractometer | BL-7

721 Shares

Neutron detector mobilizes muons for nuclear, quantum material

John Galambos named interim Associate Laboratory Director for Neutron Sciences

# 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



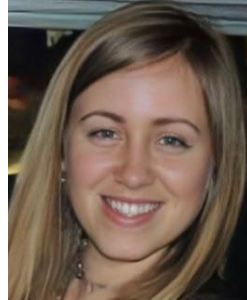
Ovi  
Garlea

# Triple Axis Spectroscopy

HB3



Songxue  
Chi



Ellie  
Clements

HB1A

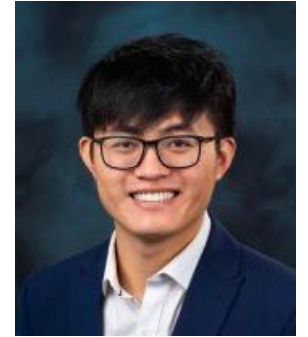


Wei  
Tian



Adam  
Aczel

Wollaston Prisms



Fankang  
Li

CTAX



Tao  
Hong



Hodaka  
Kikuchi

HB1

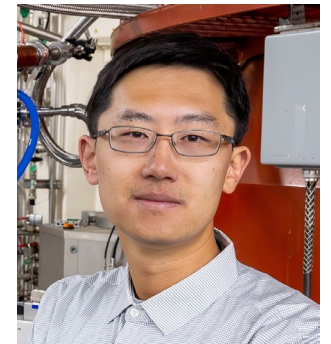


Masa  
Matsuda



Avishek  
Maity

Software



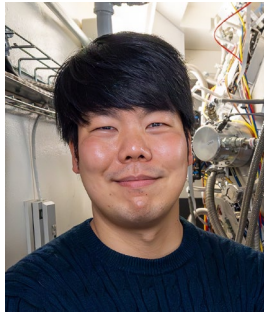
Kyle  
Ma

# Indirect Spectroscopy and NSE

## Vision



Murillo  
Martins



Hyun June  
Moon

## BASIS



Niina  
Jalarvo



Naresh  
Osti

## NSE



Laura  
Stingaciu

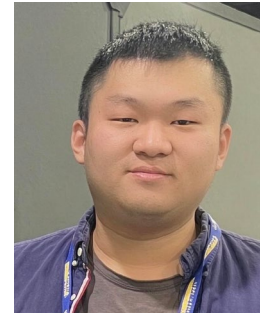


Piotr  
Zolnierczuk

## Software



Yongqiang (YQ)  
Chen



Bowen  
Han

**(Green:  
Supports  
Polarization  
Analysis )**

Cold Moderator  
/  
 $2 \text{ meV} < E_i < 100 \text{ meV}$

Thermal  
Moderator /  
 $5 \text{ meV} < E_i < 2000 \text{ meV}$

1-3% elastic E  
resolution /  
less flux

CNCS

SEQUOIA

3-5% elastic E  
resolution /  
high flux

**HYSPEC**

ARCS

Direct  
Geometry  
Spectrometers

Highest time-  
averaged flux,  
localized &  
finite Q,  $\omega$

CTAX

HB1A, **HB1**, HB3

Triple-  
Axis  
Spectrometers

Fine energy  
resolution with  
flat dispersion /  
high throughput

BASIS, NSE

VISION

Indirect  
Geometry  
Spectrometers

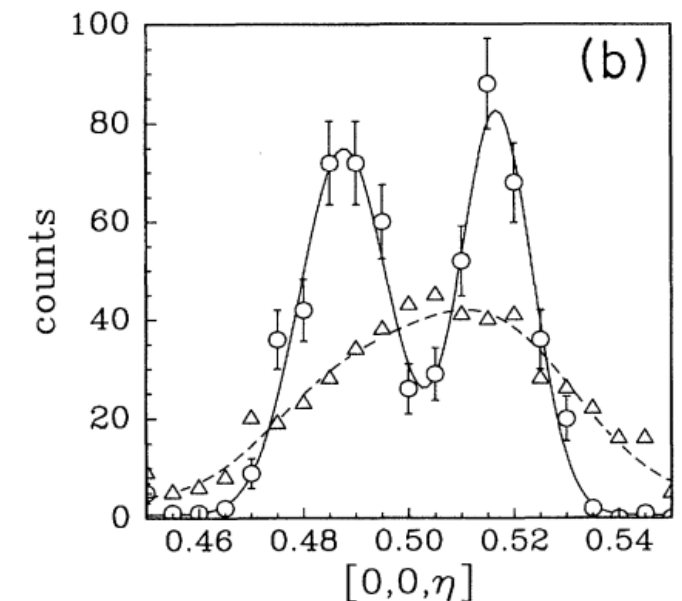
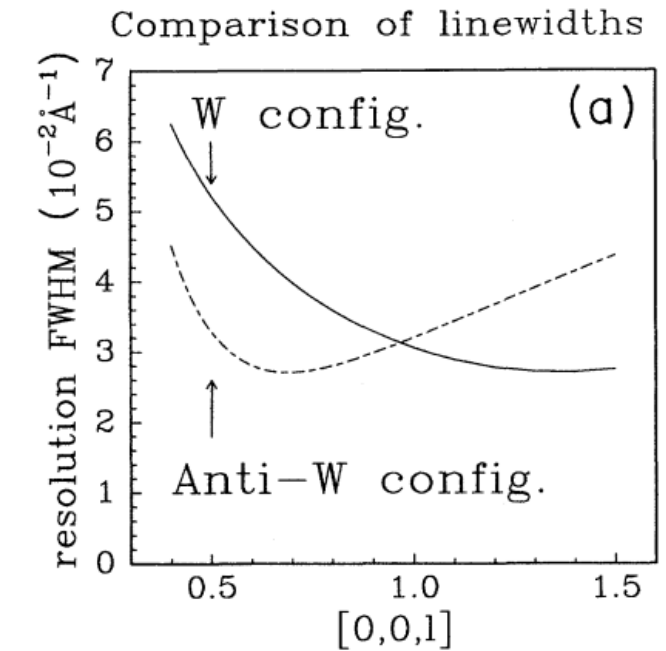
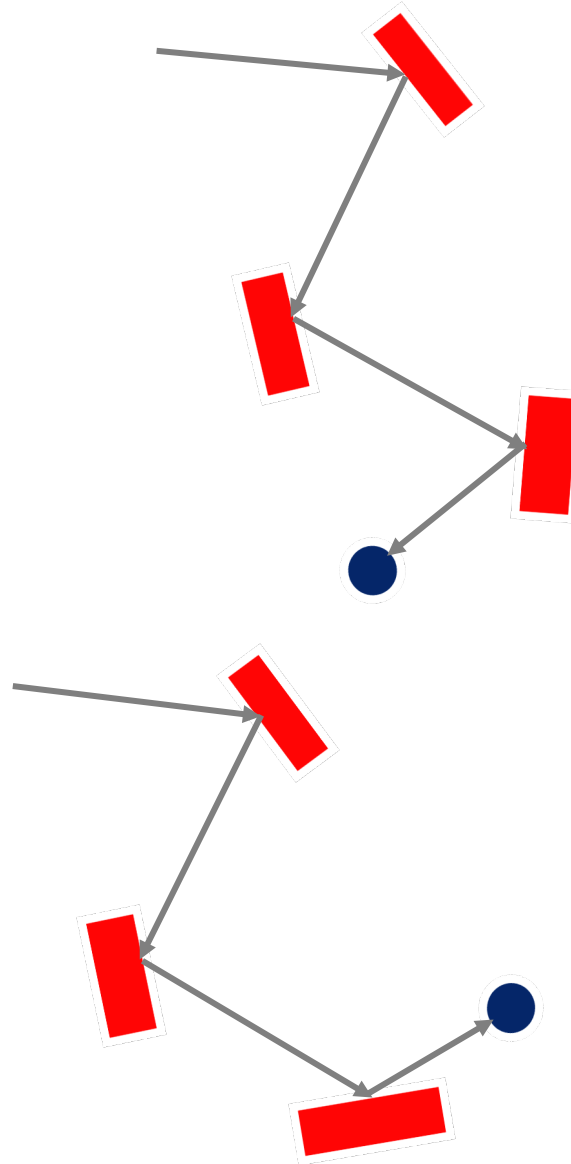
# Summary

- 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



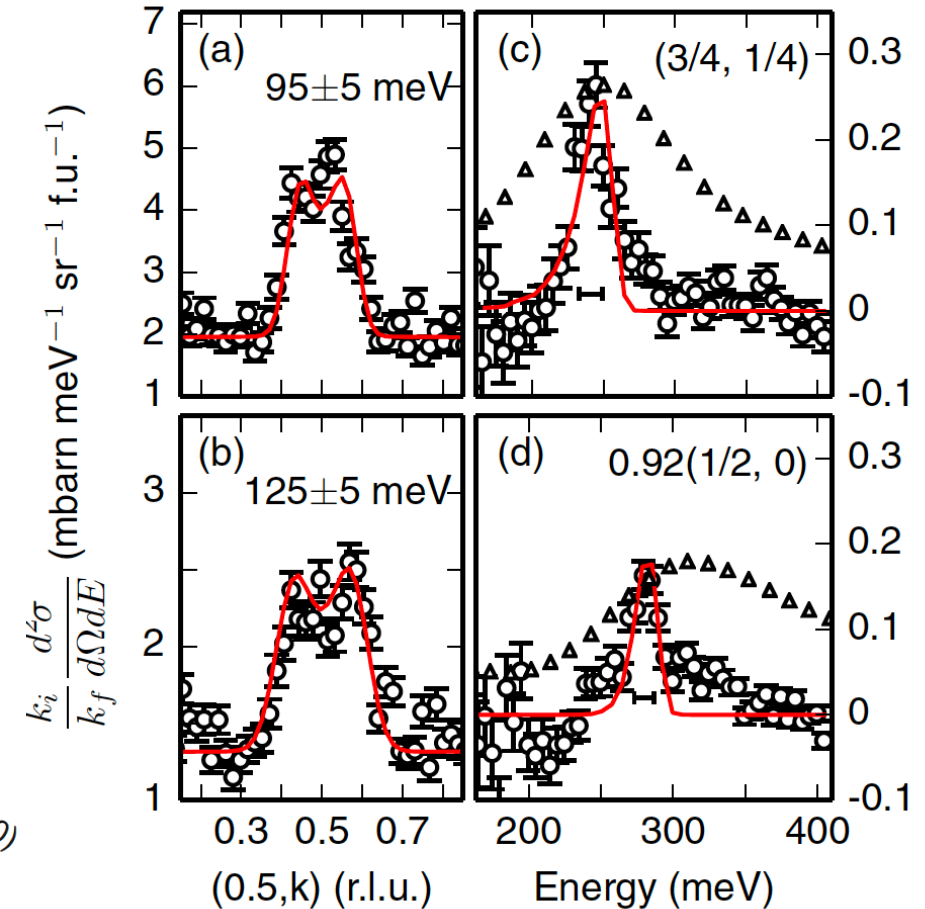
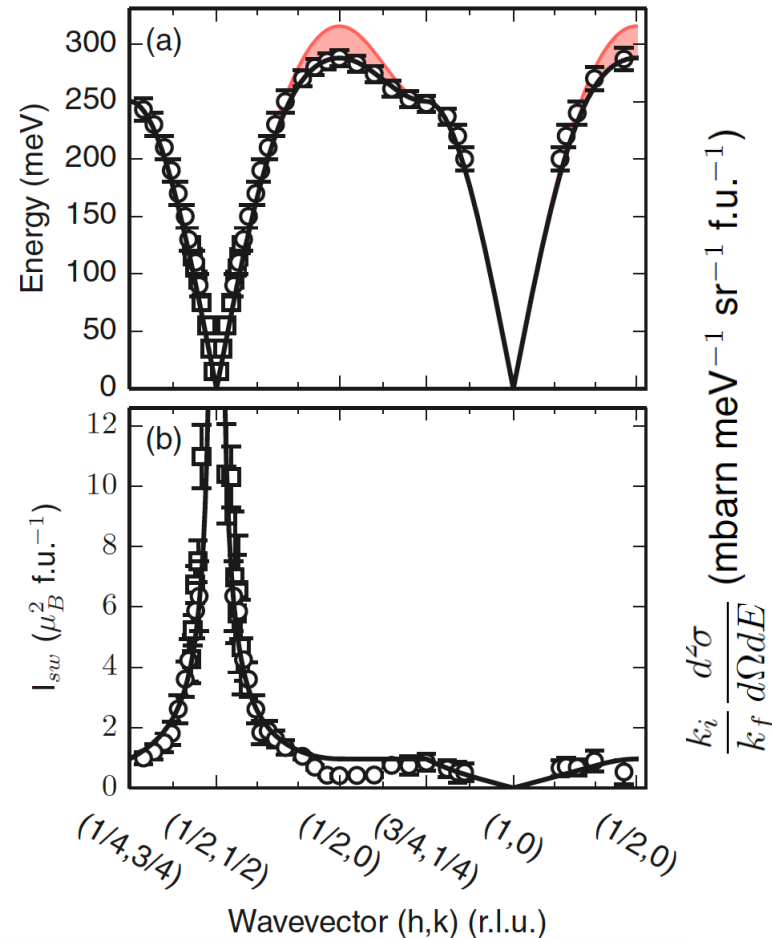
# TAS Resolution Example

- Chain coupling in  $\text{KCuF}_3$
- At small  $l$ 
  - Anti- W configuration cuts the excitation in a focusing condition
  - W configuration does not
- Performed on TAS at HFBR



# DGS Resolution example

- Zone Boundary Modes in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$
- 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)

