

# Choosing the right spectrometer

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Neutron and Xray School 2024

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

# Overview

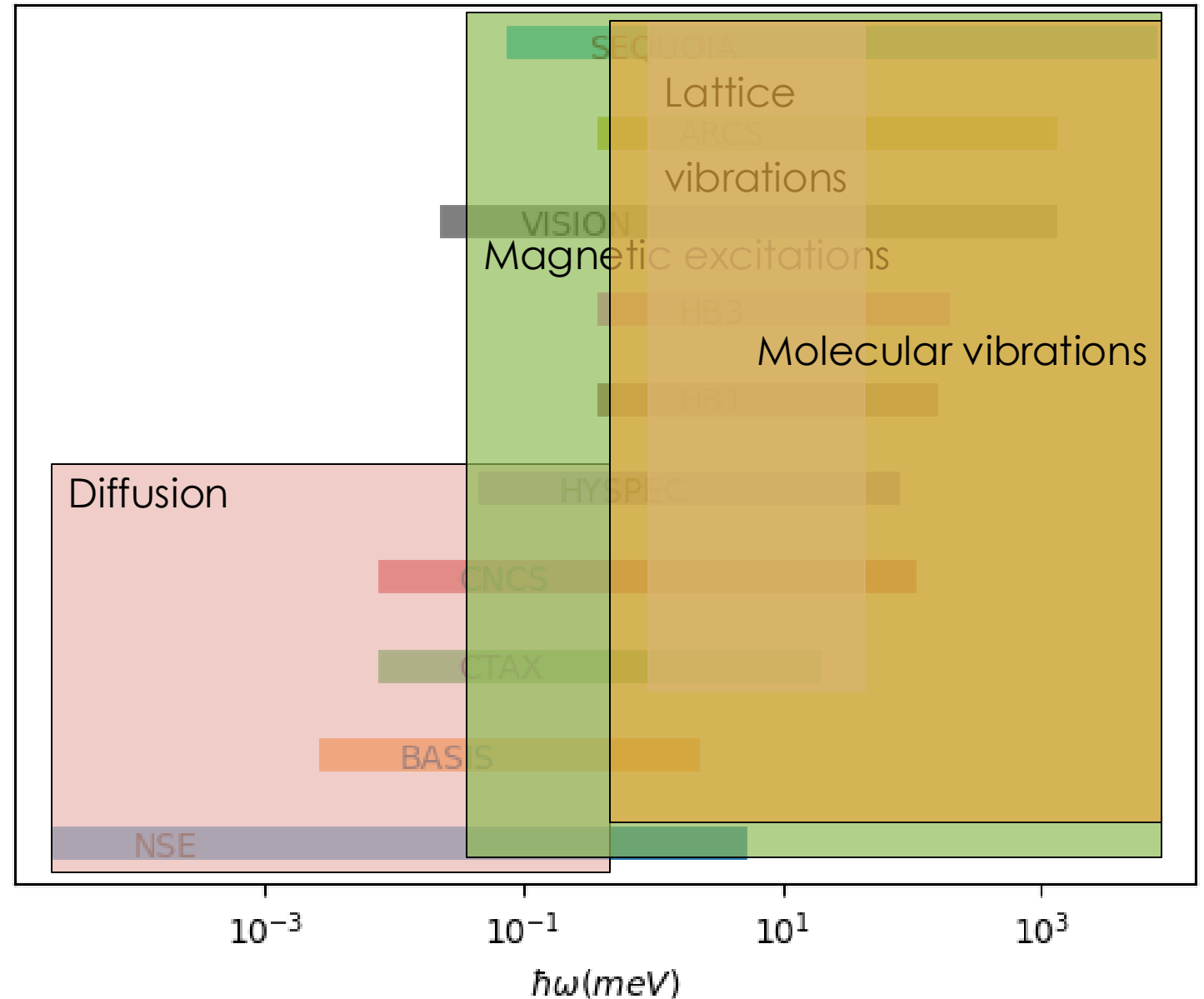
- Introduction
- Energy Range
- Q Dependence
- DGS vs. TAS Flux considerations
- Polarization Considerations
- Resolution considerations
- Background considerations
- Summary

# 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.

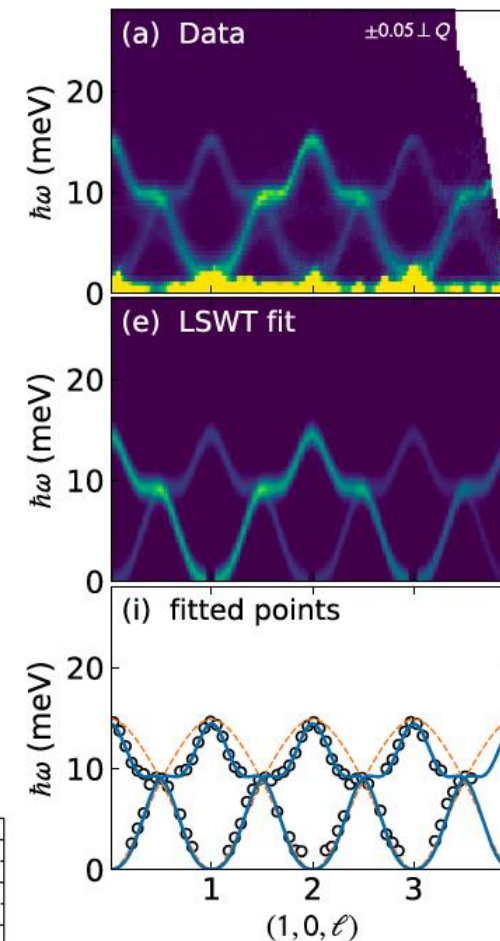
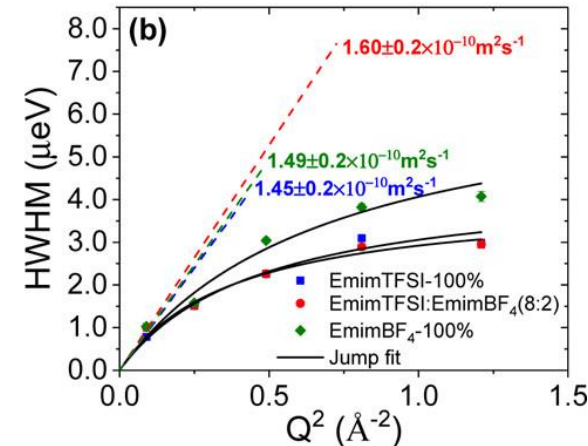
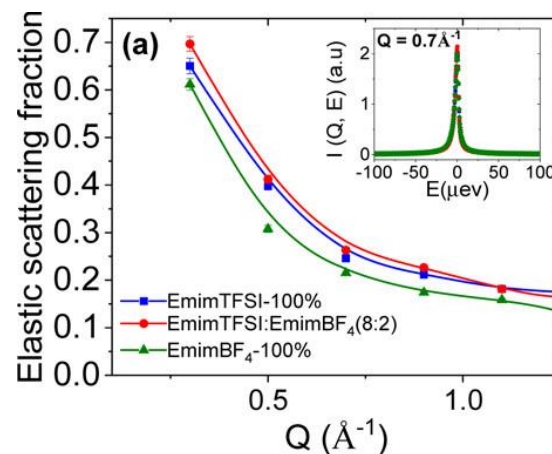
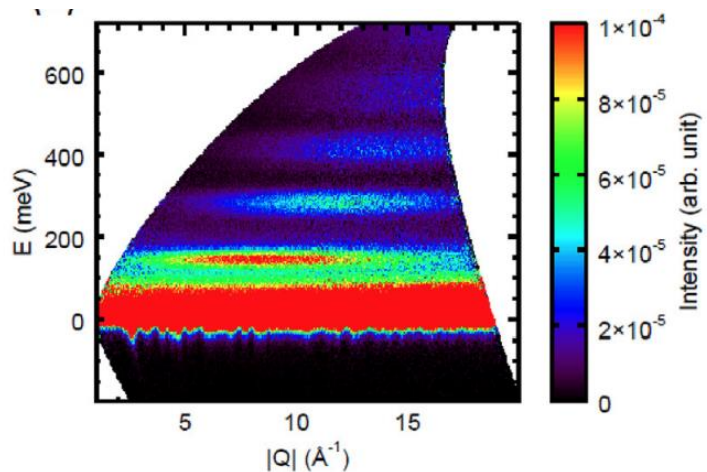
# What Energy scale?

- Coldest 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, etc.
- 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)

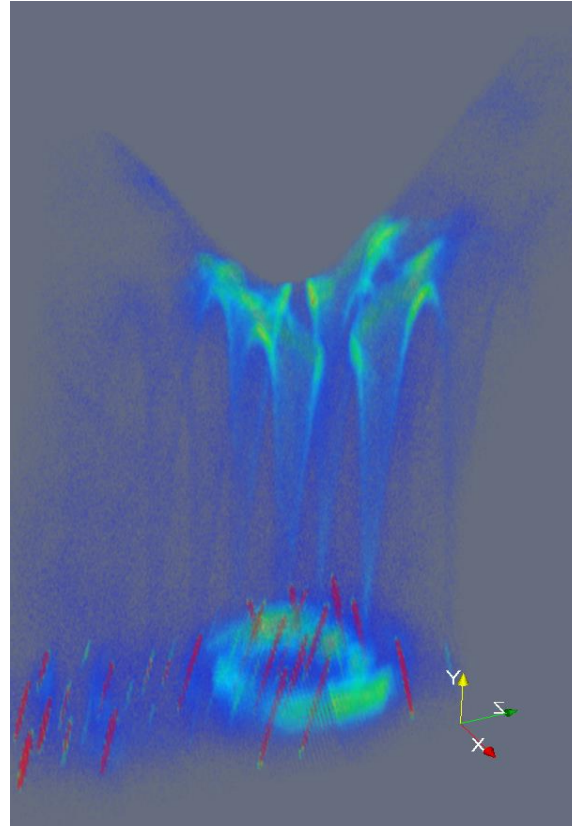
T.R. Prisk *et al.* *J. Alloys Comps.* **818** 152832 (2020)

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

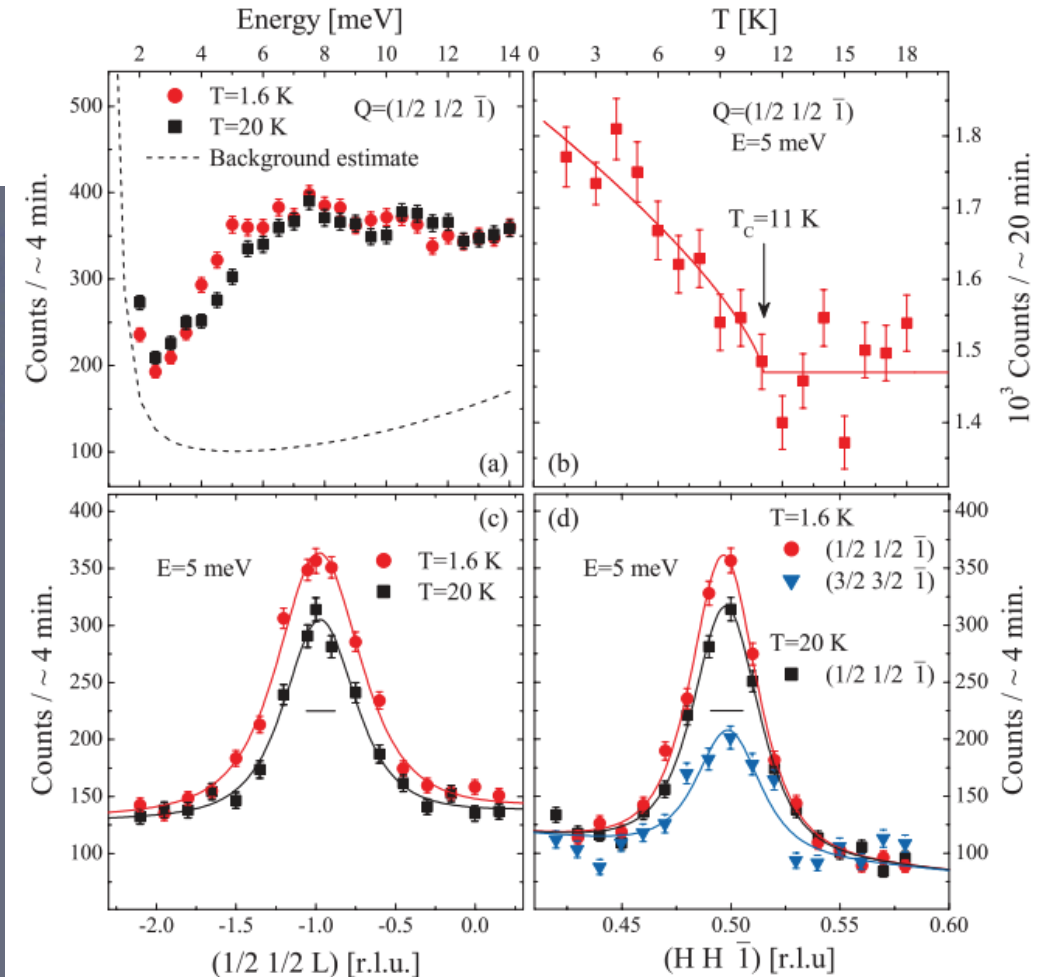


# Magnetic and Lattice excitations

- 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)



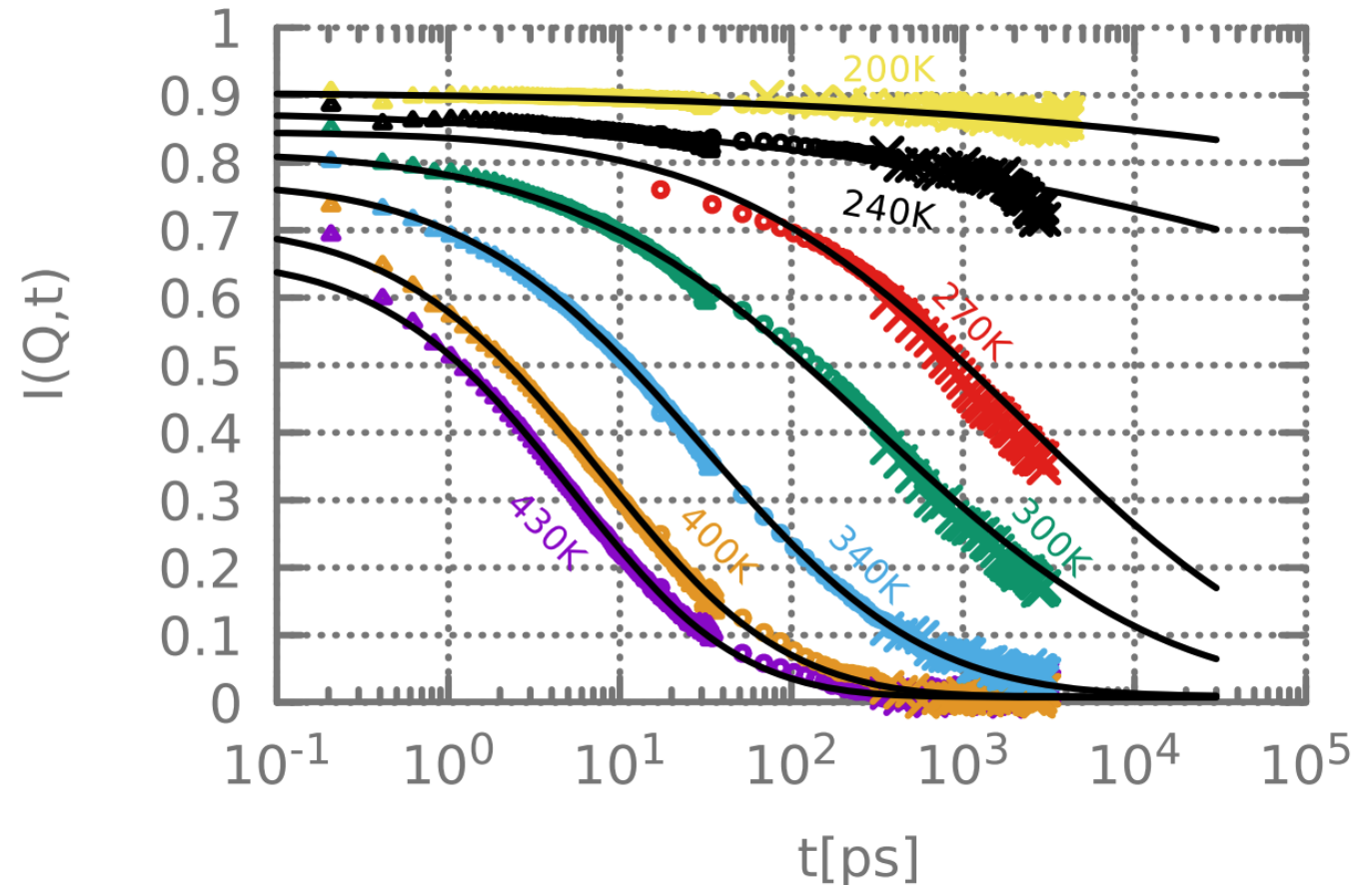
A. D. Christianson, *et al.*  
Phys. Rev. Lett. **103**, 087002 (2008)

# 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

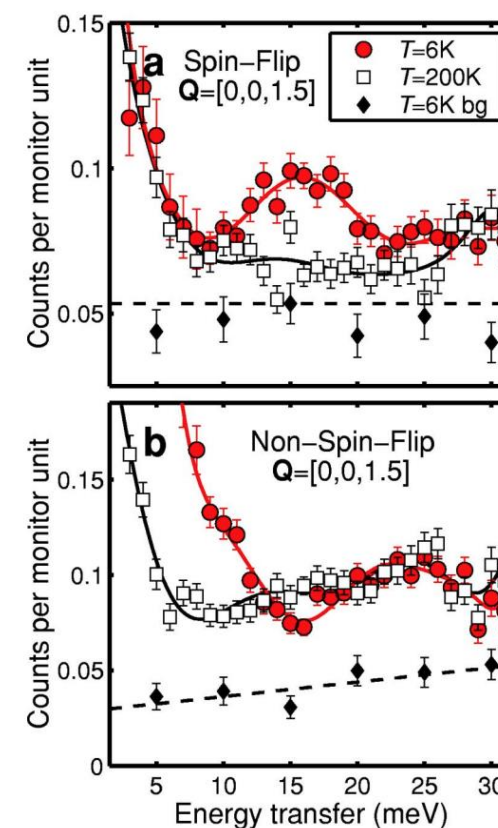
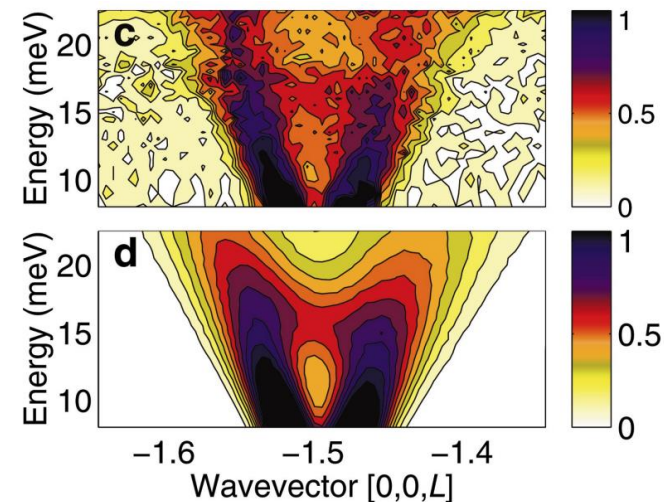


Hopfenmüller *et al.* J. Chem. Phys. **148**, 204906 (2018).



# Does the Beam Need to be polarized?

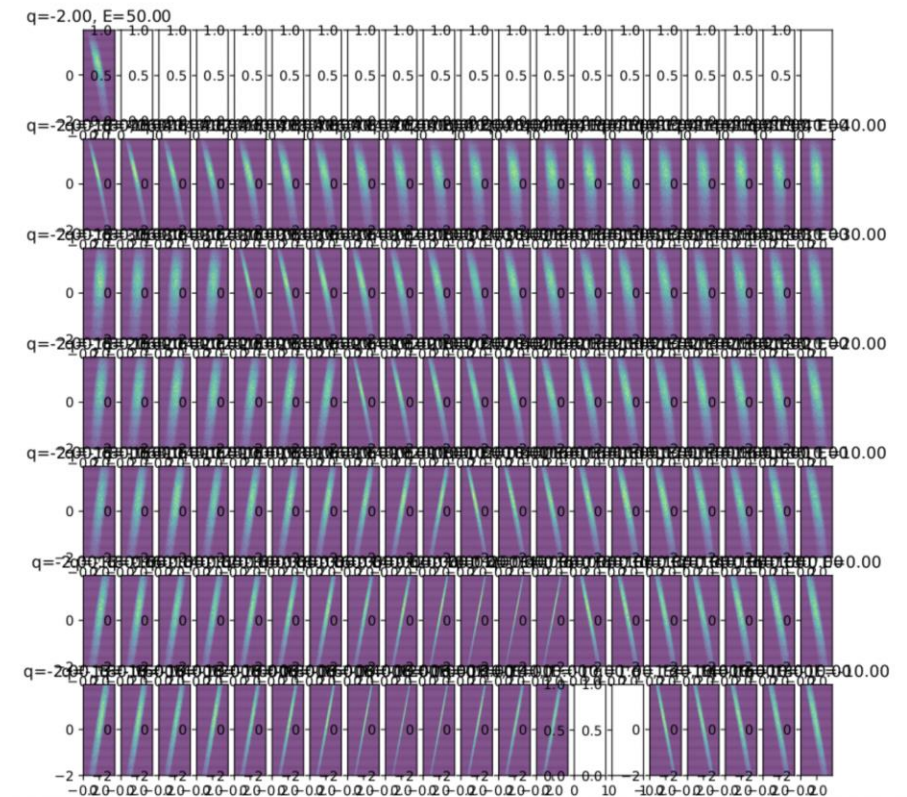
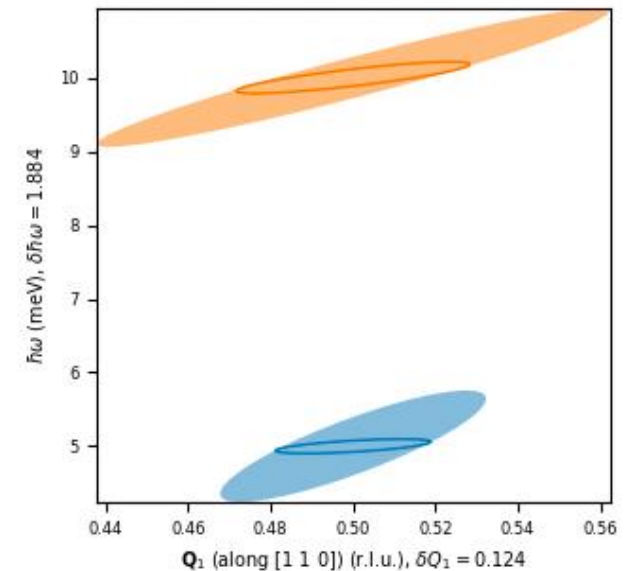
- Separating Magnetic and Lattice Modes
- Identifying type of spin excitation (Transverse vs. Longitudinal)
- Used for timing in Spin Echo
- Things to think about.
  - Flux on sample is < 50% of unpolarized flux
  - Polarized beams are limited to cold (HYSPEC and NSE) and Thermal (HB1 and HYSPEC beams)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

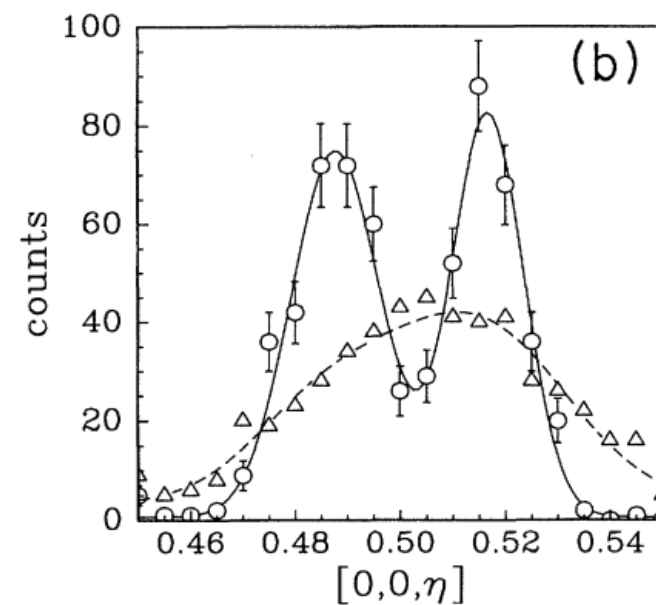
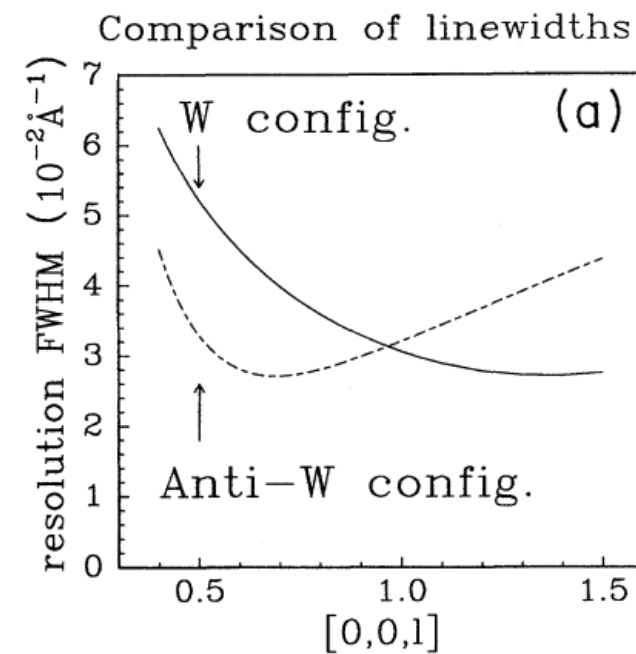
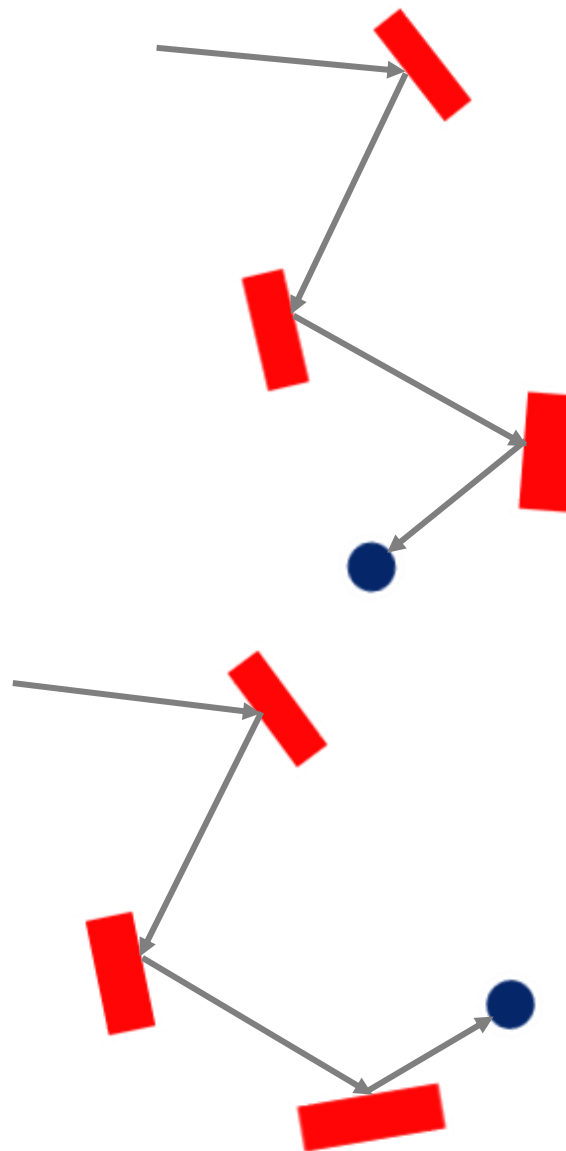
# Resolution

- 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)



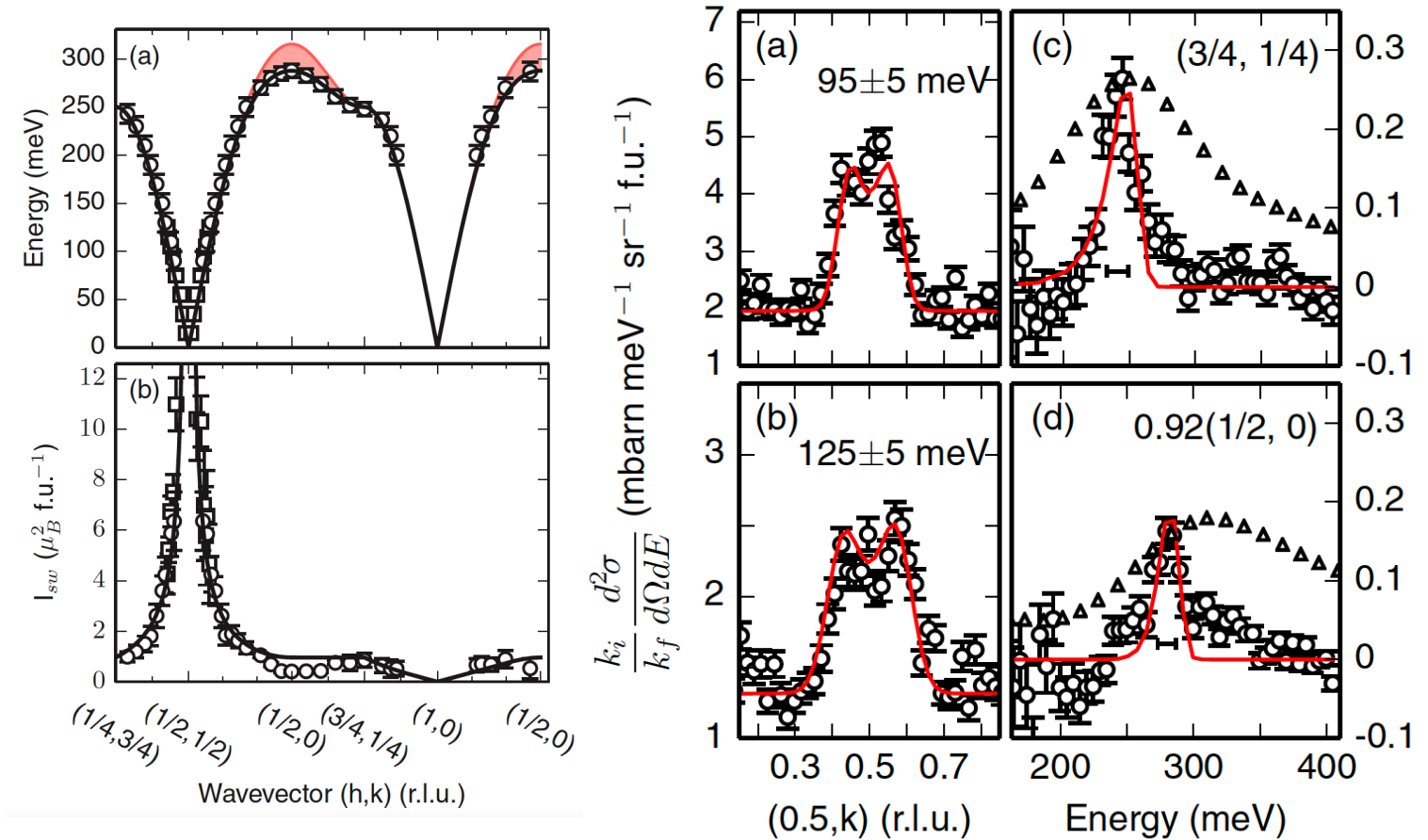
# TAS Resolution Example

- 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

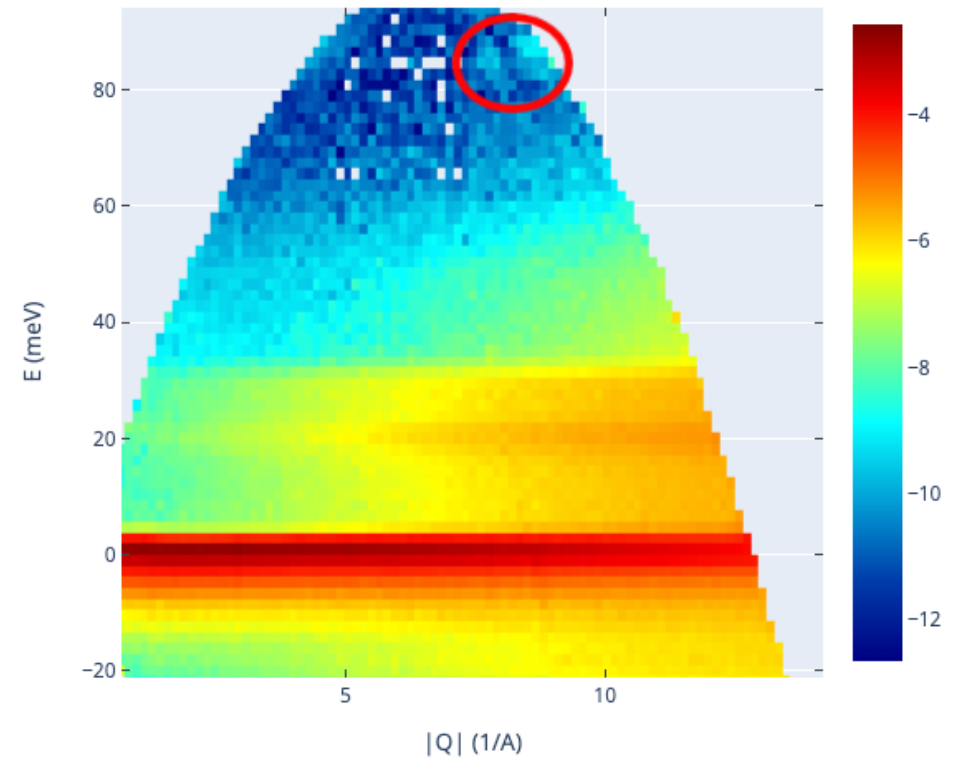
- Zone Boundary Modes in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$
- Resolution of SEQUOIA allowed fine measurement at zone boundary
- Energy Range and Flux Unique to SEQUOIA



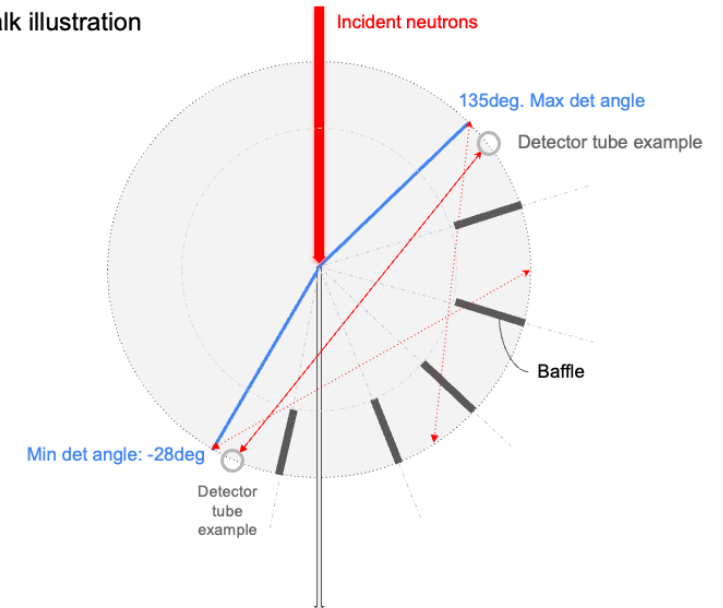
K. Plumb *et al.* Phys. Rev. B **89**, 180410(R) (2014)

# Background Considerations

- For triple axis spectrometers
  - Background tends to be flat , but larger than DGS instruments
  - Spurious 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





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

The screenshot shows the website's navigation menu with 'Instruments' selected. The main content area lists various neutron instruments under three categories: High Flux Isotope Reactor, Spallation Neutron Source, and a central column. The 'Instruments' menu is highlighted in green. On the right side, there are social media sharing icons for Facebook, Twitter, and LinkedIn, along with a '550 Shares' counter.

Category	Instrument Name
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
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	

## Neutrons for New Discoveries and Solutions

Breakthroughs in medicine, energy, technology, and industry follow advances in the understanding of materials. Oak Ridge National Laboratory (ORNL) is at the US epicenter for one of the most powerful techniques exploring the nature of materials and energy—neutron scattering.

ORNL hosts two of the world's most powerful sources of neutrons for research: the [High Flux Isotope Reactor \(HFIR\)](#) and the [Spallation Neutron Source \(SNS\)](#). Neutrons have no electrical charge, which allows them to easily and safely pass through a sample, revealing information about the material's structure and properties.

Neutron scattering is used in many industries—automotive, aerospace, steel, defense, industrial materials, energy storage, data storage, biomedicine, and others—to address the 21<sup>st</sup> century's major scientific challenges.

## Contact



Jens Dilling  
Associate Laboratory Director  
Neutron Sciences Directorate  
[dillingj@ornl.gov](mailto:dillingj@ornl.gov)

## Research Highlights

<https://neutrons.ornl.gov/instruments>



# Direct Geometry Spectroscopy

## ARCS



Doug Abernathy



Garrett Granroth



Christian Balz

## CNCS



Daniel Pajerowski



Andrey Podlesnyak

## Software



Andrei Savici

## SEQUOIA



Matt Stone



Sasha Kolesnikov



Colin Sarkis

## HYSPEC



Barry Winn



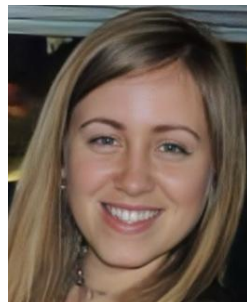
Ovi Garlea

# Triple Axis Spectroscopy

HB3



Songxue  
Chi



Ellie  
Clements

HB1A



Wei  
Tian



Adam  
Aczel

Wollaston Prisms



Fankang  
Li

CTAX



Tao  
Hong

HB1

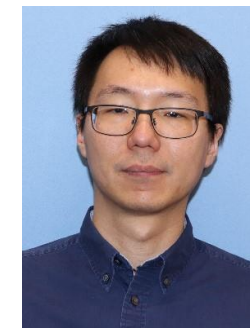


Masa  
Matsuda



Avishek  
Maity

Software



Bing  
Li

# Indirect Spectroscopy and NSE

## Vision



Luke  
Daemen



Murillo  
Martins

## BASIS

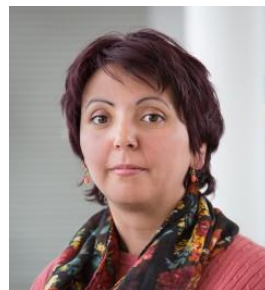


Niina  
Jalarvo

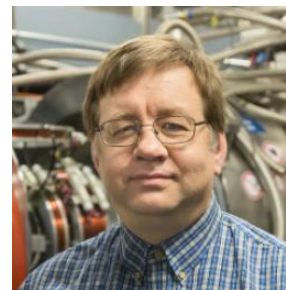


Naresh  
Osti

## NSE



Laura  
Stingaciu



Piotr  
Zolnierczuk

## Software



Yongqiang (YQ)  
Chen

(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

Direct  
Geometry  
Spectrometers

3-5% elastic E  
resolution /  
high flux

**HYSPEC**

ARCS

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
- Resolution, and background considerations are tricky
- **Ask Instrument staff for help**
- Comments on the presentation?



NXS Lecture - S. Calder & G. Granroth: "Diffraction and Spectroscopy at TOF vs.



