OAK RIDGE National Laboratory

Choosing the right spectrometer

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U.S. DEPARTMENT OF ENERGY

Overview

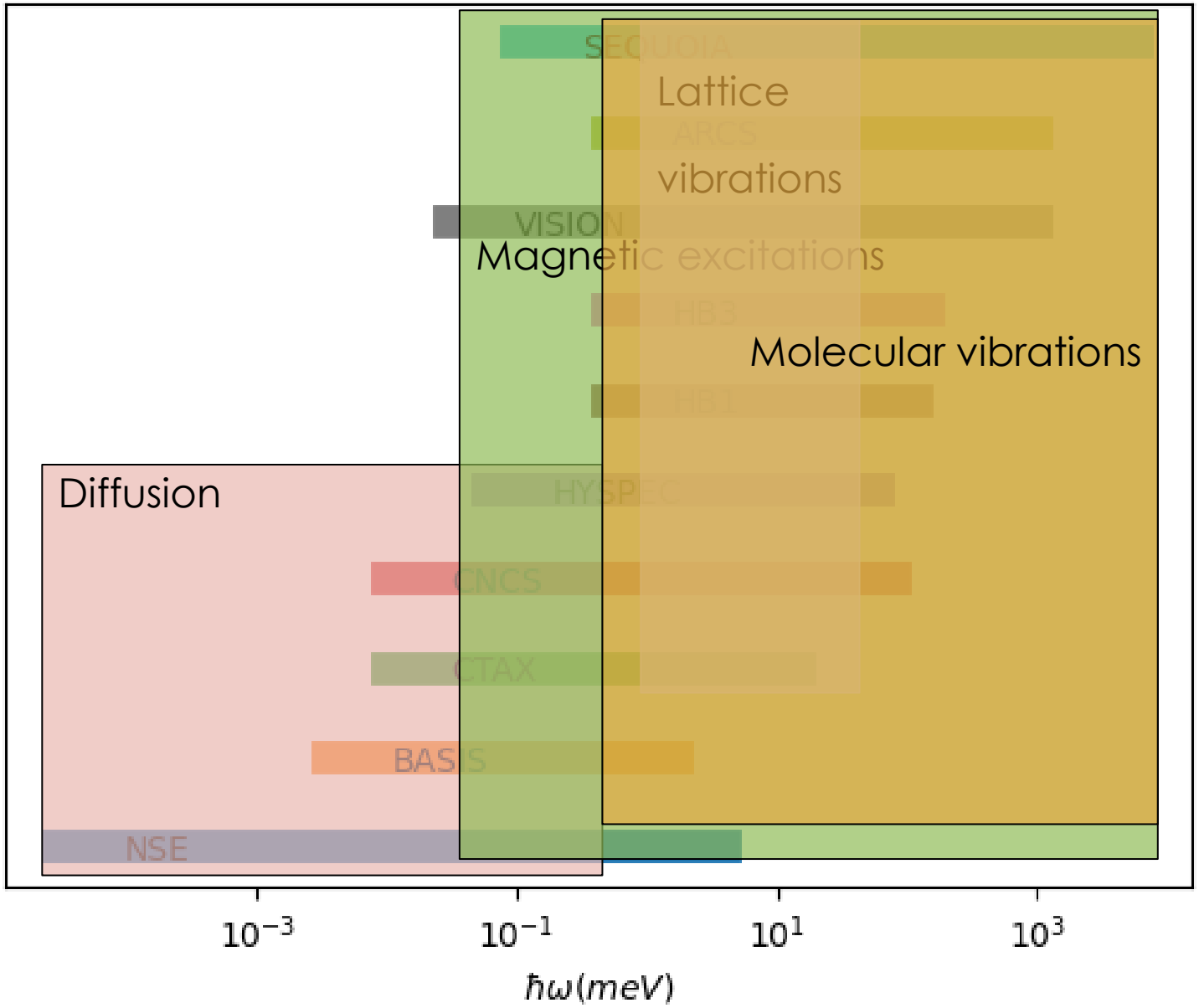
- Introduction
- Energy Range
- Q Dependence
- DGS vs. TAS Flux considerations
- Polarization Considerations
- Resolution considerations
- Background considerations
- Summary

Introduction

- Spectroscopy is checking if energy is a gained or lost during the neutron's interaction with the sample.
- Spectrometers at ORNL
  - PTAX- HB1, TAS-HB3, CTAX, 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.

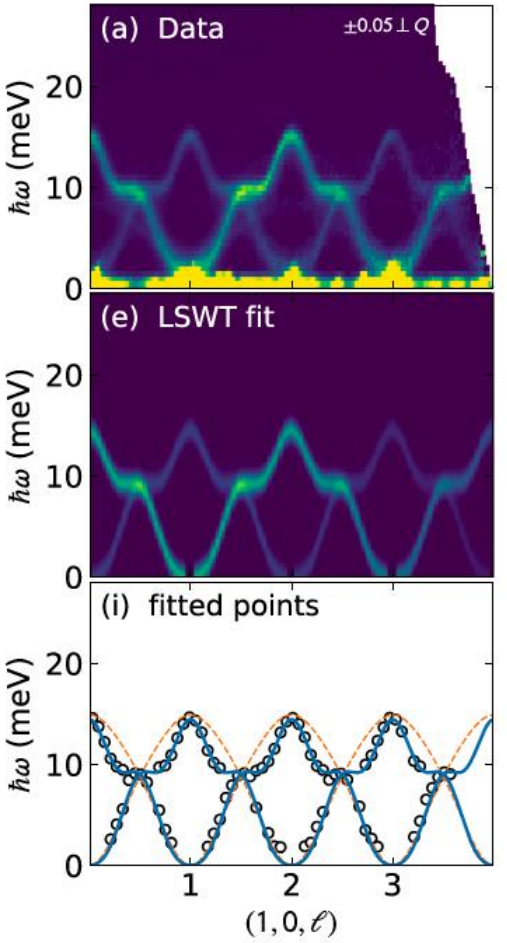
What Energy scale?

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

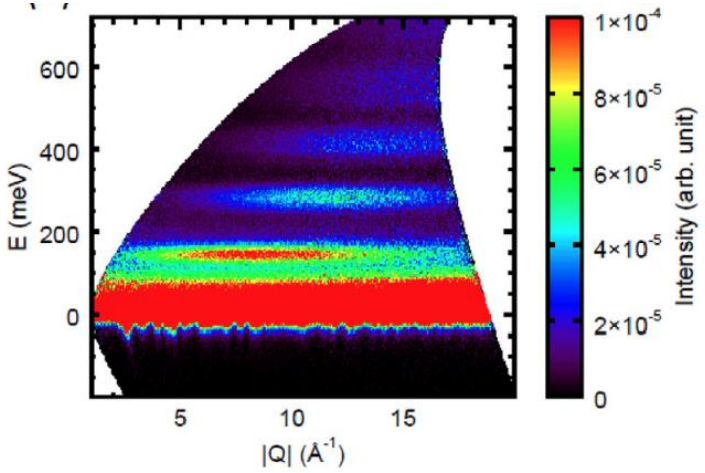


Will My data vary Quickly in Q?

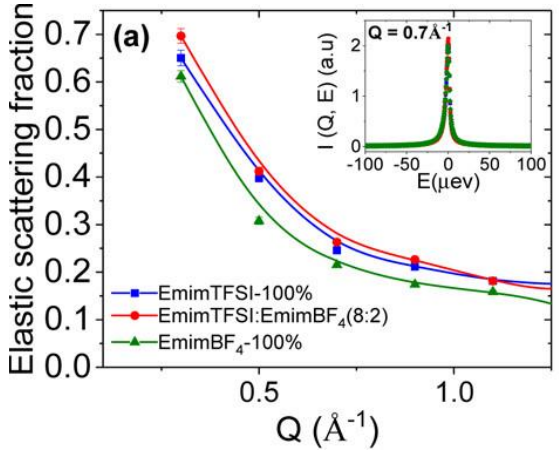
- Yes
  - Phonons, Magnons
  - ARCS, SEQUOIA, CNCS, HYSPEC, HB1,HB3,CTAX
- No
  - Molecular vibrations, diffusion
  - Vision, Basis, NSE

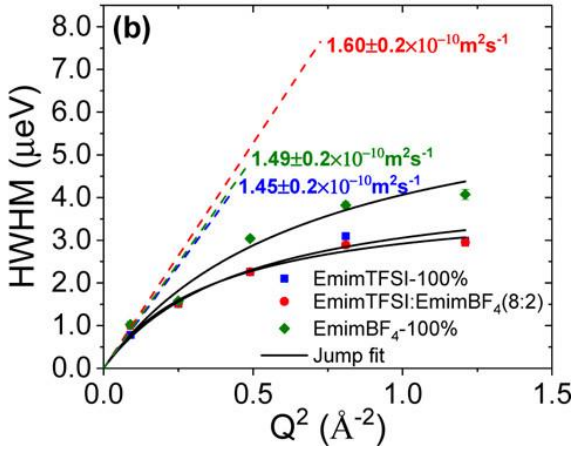


A. Sheie *et al. Phys. Rev. B* **105**, 104402 (2022)



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

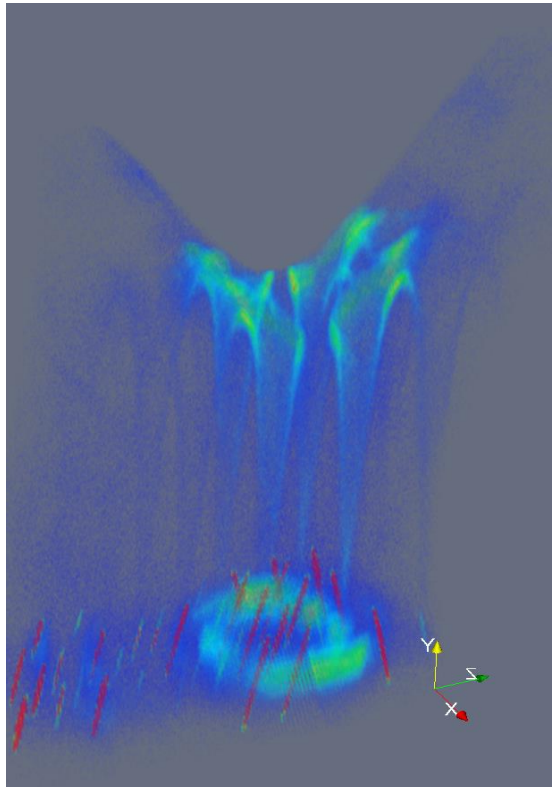




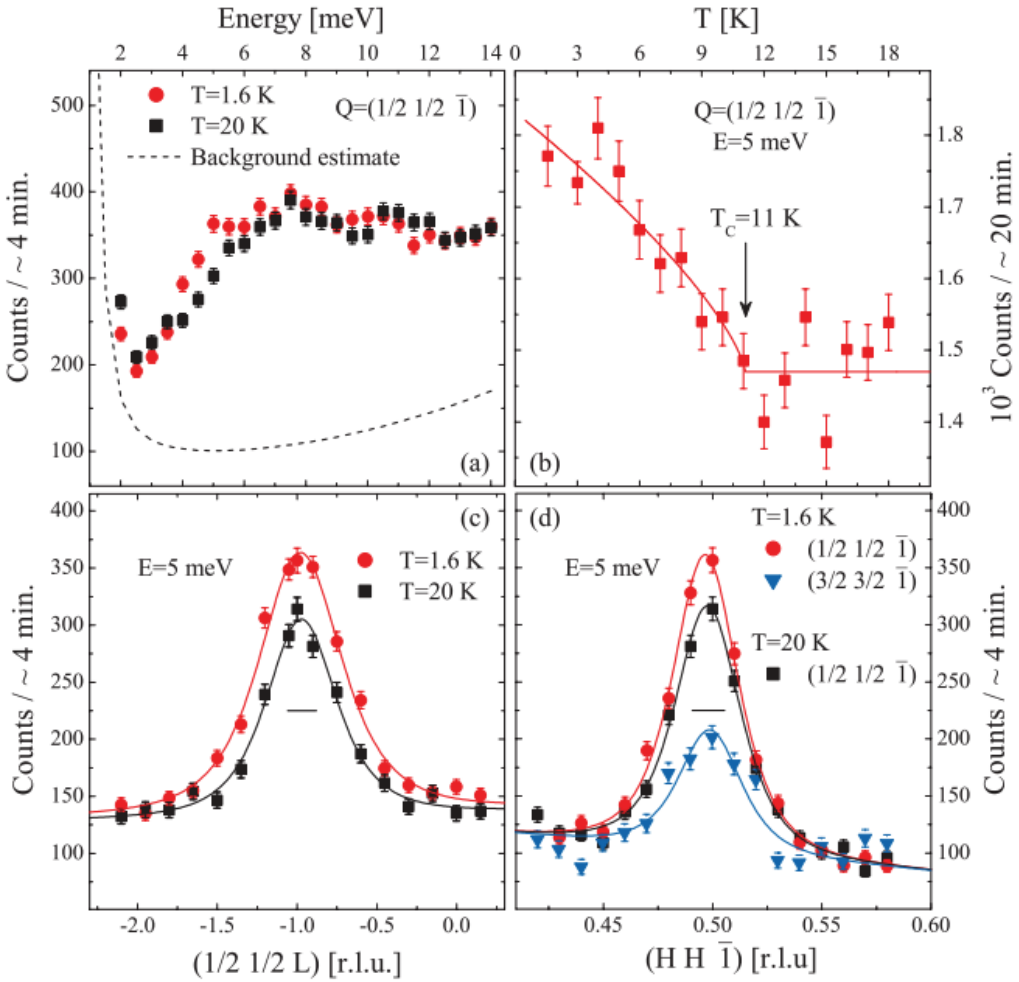
N. C. Osti et al. J. Phys. Chem. C, **122**, 10476 (2018)

Magnetic and Lattice excitations

- TAS instruments optimal to measure a small region in Q, ω space
  - HB1,HB3,CTAX
- DGS Instruments optimal to map Q, ω space
  - CNCS, HYSPEC, ARCS, SEQUOIA



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



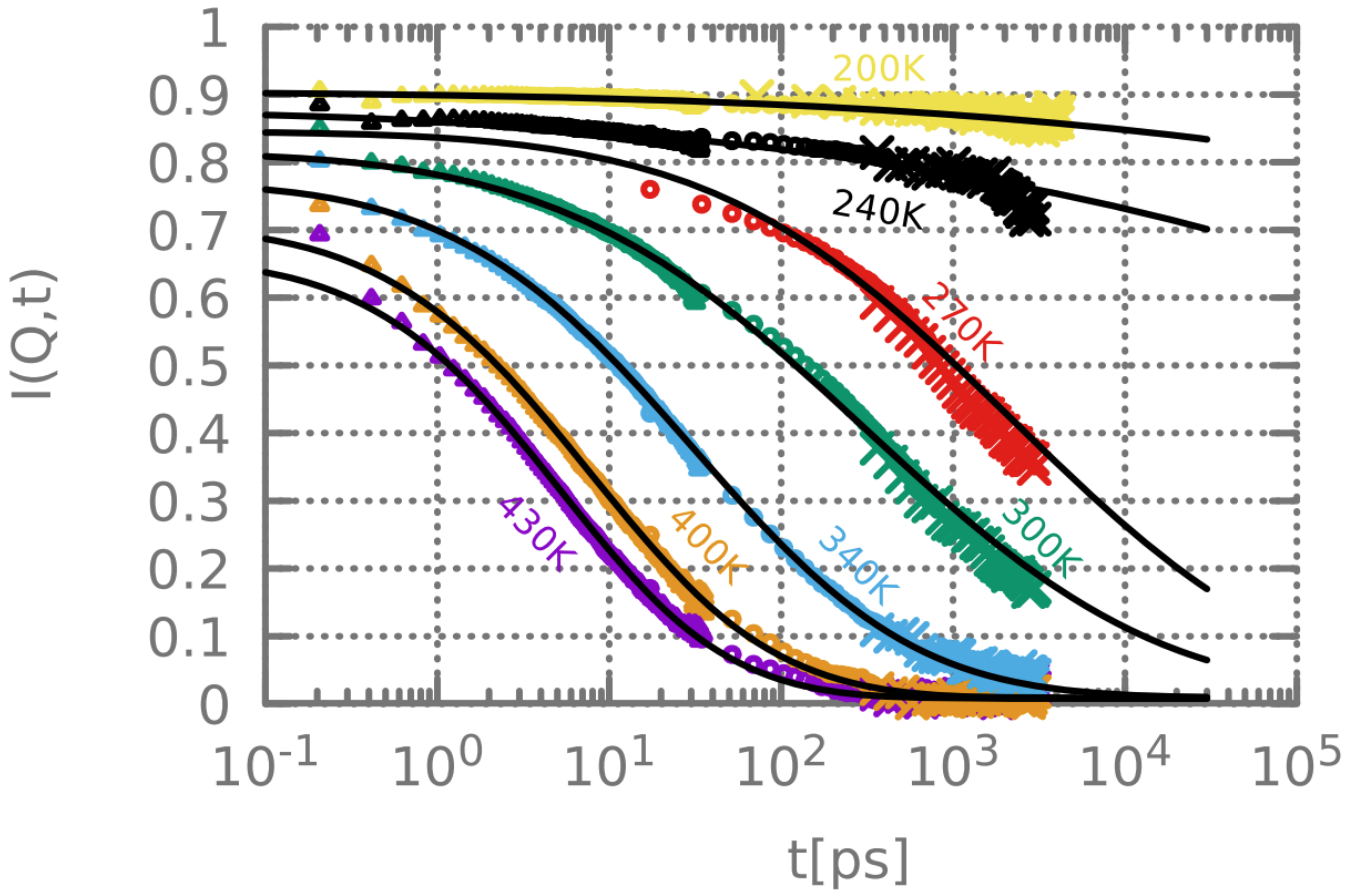
A. D. Christianson, *et al.*
Phys. Rev. Lett. **103**, 087002 (2008)

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

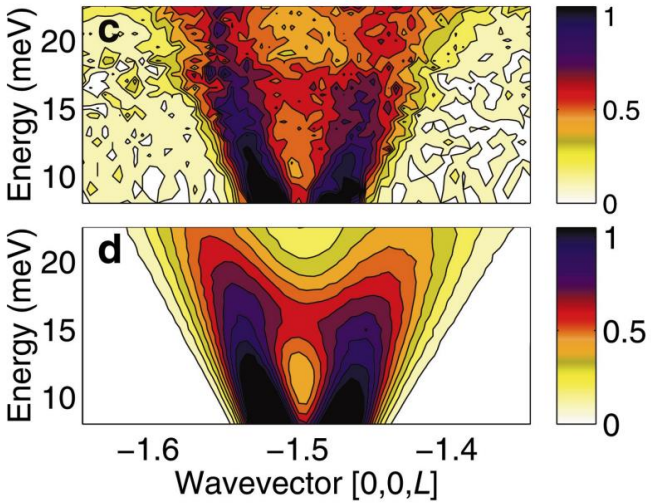
- Study of fractal diffusion in polymer fuel cell
- Many time scales
- Required 3 instruments
  - CNCS (△)
  - BASIS (O)
  - Spheres (×) (MLZ)
- Usually start with coarsest resolution

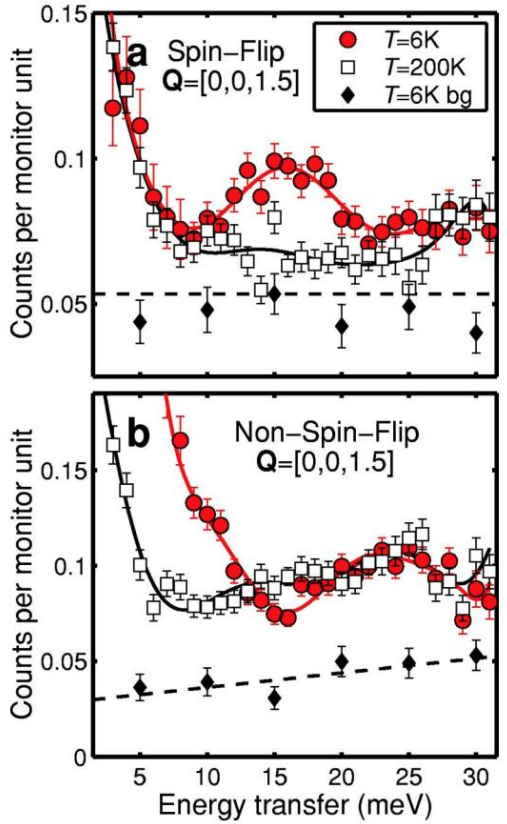


Hopfenmüller *et al.* J. Chem. Phys. **148**, 204906 (2018).

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





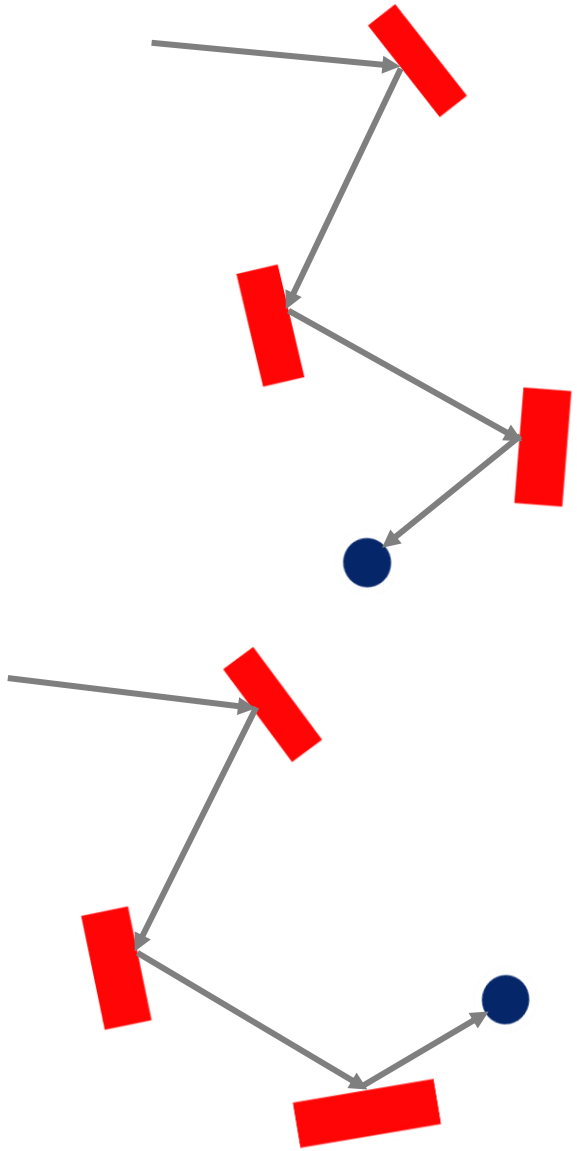
B. Lake, D. A. Tennant, S. E Nagler, Phys. Rev. B **71**, 134412 (2005)

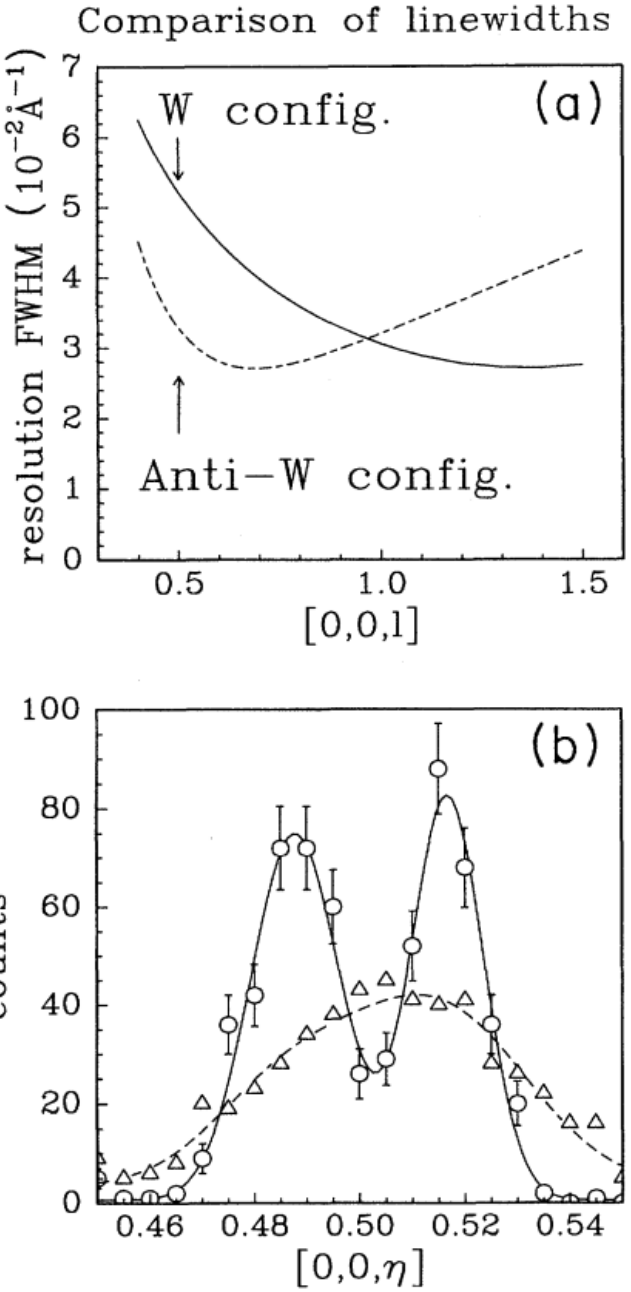
Resolution

- 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)

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

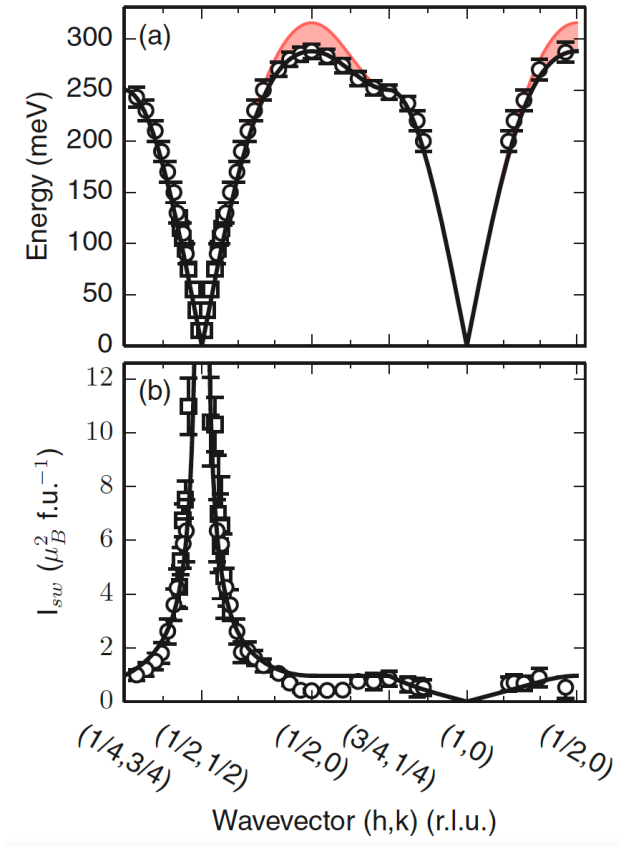


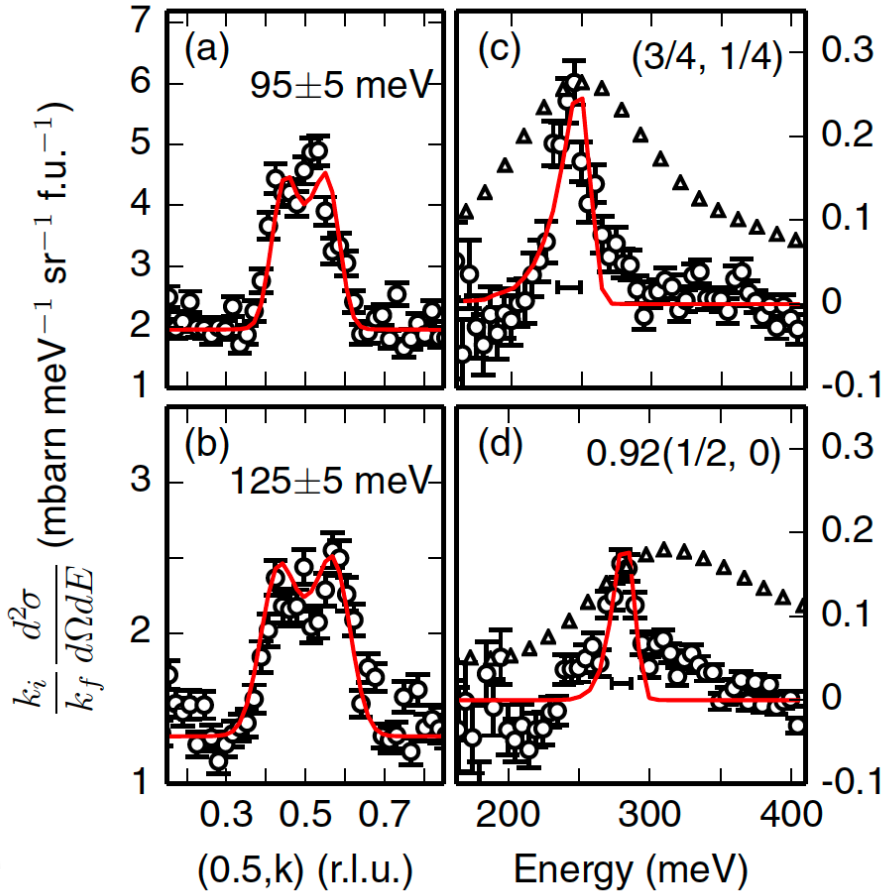


D. A. Tennant, *et al.* Phys. Rev. B **52**, 13381 (1995)

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





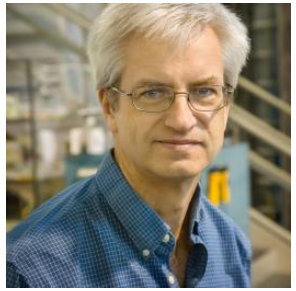
K. Plumb *et al.* Phys. Rev. B **89**, 180410(R) (2014)

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
  - Sometimes structured background is hard to distinguish from signal.

Direct Geometry Spectroscopy

ARCS



Doug Abernathy

Garrett Granroth

SEQUOIA

Matt Stone

Sasha Kolesnikov

Software

Andrei Savici

CNCS

Daniel Pajerowski

Andrey Podlesnyak

HYSPEC

Barry Winn

Ovi Garlea

Triple Axis Spectroscopy

HB3

Songxue Chi

Travis Williams

CTAX

Tao Hong

HB1A

Wei Tian

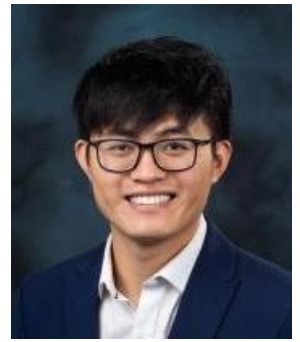
Adam Aczel

HB1

Masa Matsuda

Jaime Fernandez-Baca

Wollaston Prisms



Fankang Li

Indirect Spectroscopy and NSE

Vision

Luke Daemen

BASIS

Niina Jalarvo

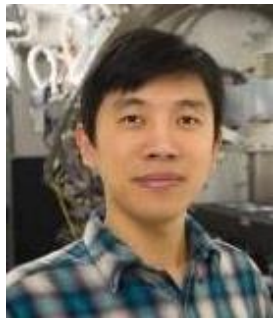
Naresh Osti

NSE

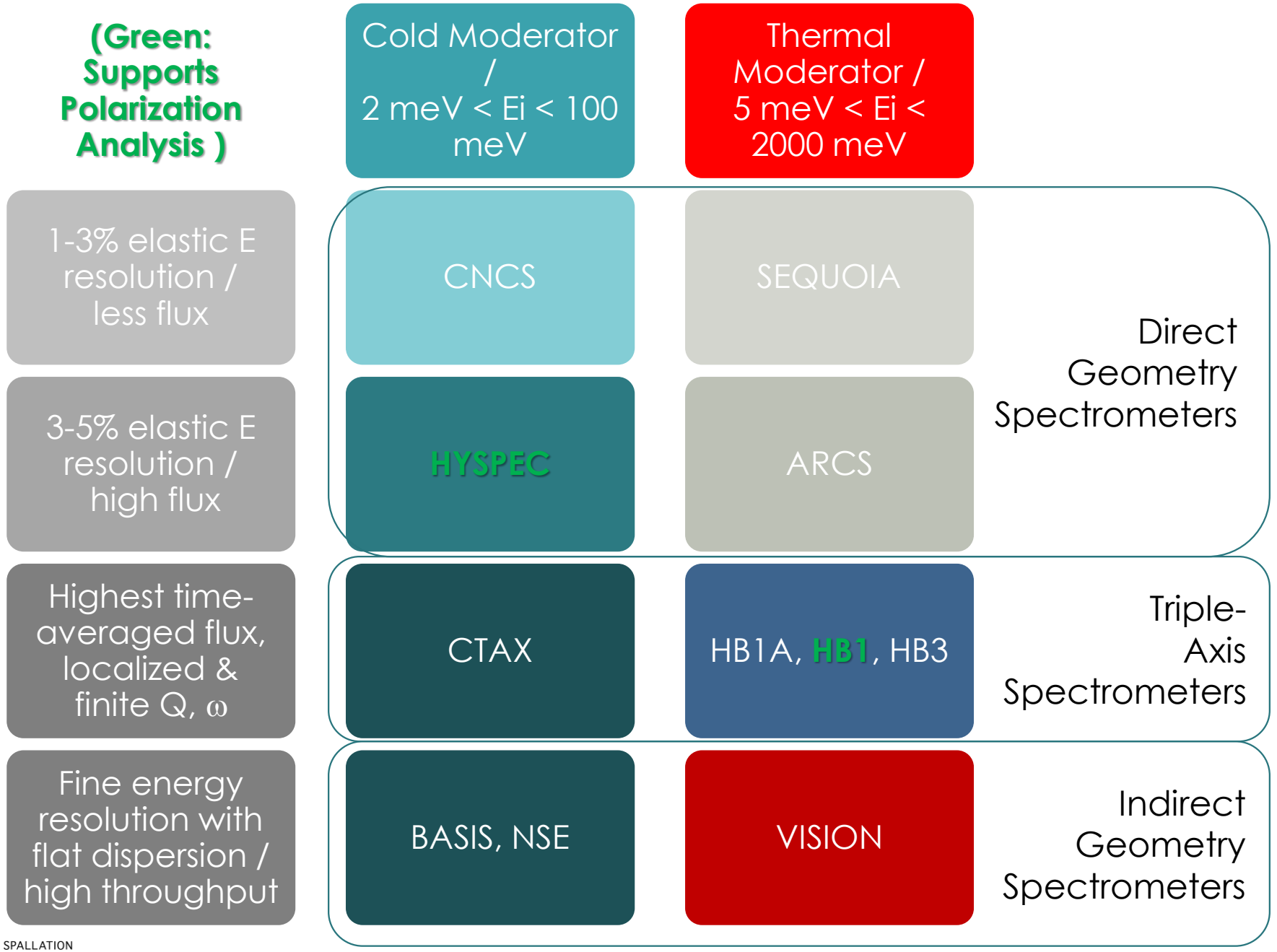
Laura Stingaciu

Piotr Zolnierczuk

Software



Yongqiang (YQ) Chen


(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
3-5% elastic E resolution / high flux
HYSPEC
ARCS
Direct Geometry Spectrometers
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, Resolution, and background considerations are tricky
- Ask Instrument staff for help
- Please provide your thoughts on this presentation at the survey accessed by the QR code.

https://forms.office.com/g/zydFTf6CTjU