Choosing the right spectrometer

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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, 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

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Magnetic and Lattice excitations

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

S. E. Hahn et al.

A. D. Christianson, et al.
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

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

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

DGS Resolution example

• Zone Boundary Modes in Sr$_2$CuO$_2$Cl$_2$

• Resolution of SEQUOIA allowed fine measurement at zone boundary

• Energy Range and Flux Unique to SEQUOIA

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

CNCS
Daniel Pajerowski
Andrey Podlesnyak

HYSPEC
Barry Winn
Ovi Garlea

Software
Andrei Savici
Triple Axis Spectroscopy

HB3
Songxue Chi

CTAX
Travis Williams

HB1A
Wei Tian

HB1
Masa Matsuda

Wollaston Prisms
Fankang Li

Tao Hong

Adam Aczel

Jaime Fernandez-Baca
Indirect Spectroscopy and NSE

BASIS

Niina Jalarvo

Naresh Osti

Vision

Luke Daemen

NSE

Laura Stingaciu

Piotr Zolnierczuk

Software

Yongqiang (YQ) Chen

Laura Stingaciu

Piotr Zolnierczuk
<table>
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<tr>
<th>Cold Moderator / 2 meV &lt; E&lt; 100 meV</th>
<th>Thermal Moderator / 5 meV &lt; E&lt; 2000 meV</th>
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<tr>
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<tr>
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<tr>
<td>BASIS, NSE</td>
<td>VISION</td>
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- **1-3% elastic E resolution / less flux**
- **3-5% elastic E resolution / high flux**
- **Highest time-averaged flux, localized & finite Q, ω**
- **Fine energy resolution with flat dispersion / high throughput**

- **Direct Geometry Spectrometers**
- **Triple-Axis Spectrometers**
- **Indirect Geometry Spectrometers**

*(Green: Supports Polarization Analysis)*
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/zydFt6CTjU