Choosing the Right Spectrometer

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Interaction of radiation with materials

From Roger Pynn
– Neutron Primer
Neutron Source: Moderation

Maxwellian Distribution

\[ \Phi \sim \nu^3 e^{-m\nu^2/2k_B T} \]

Liquid Hydrogen

Heavy Water (D\textsubscript{2}O)

Hot Graphite

“Fast” neutrons: \( \nu = 20,000 \text{ km/sec} \)

Fuel

Moderation

The core is immersed in D\textsubscript{2}O, which acts as
• The primary coolant
• The moderator
• The reflector to inject
neutrons back in the
core, essential for the
reactor to go critical
Neutrons show where the atoms are…. **Cliff Shull**

...and what the atoms do.

**Bertram Brockhouse**
A single isolated nucleus will scatter neutrons with an intensity (isotropic)

- \( I = I_0 \sigma = I_0[4\pi b^2] \)
  - where \( I_0 \) = incident neutron intensity,
  - \( b \) = scattering amplitude for nucleus

What happens when we put nucleus (atom) in lattice?

- Scattering from \( N \) nuclei can add up because they are on a lattice (constructive interference)
- Adding is controlled by phase relationship between waves scattered from different lattice planes
- Intensity is no longer isotropic
  - Bragg law gives directional dependence
    - \( \lambda = 2d \sin \theta \)
  - Wave vector \( |k| = 2\pi/\lambda \)

- Intensity \( I(Q, \text{ or } \theta) \) is given by a scattering cross-section

Path difference for neutrons (waves) scattered from two adjacent atomic planes

\[ = 2d \sin \theta = m \lambda \] for constructive interference to occur
How do we find the wavelength to make the Bragg law work?

- **Reactor**
  - Fission of U$^{235}$ produces neutrons
  - Fission spectrum moderated (slowed down) by either D$_2$O or H$_2$O (less effective moderator) and neutrons are extracted through beam tubes for spectrometers – fixed wavelength used

- **Spallation source**
  - High E protons (e.g., 800 MeV) impinge on target (W, Hg or U)
  - Nucleus of target is “exploded” by proton impact and emits 15 – 25 neutrons per proton with average E = 55 MeV (+ γs, nucleons and neutrinos)
  - Neutrons moderated by liquid H, H$_2$O or methane
  - Spallation sources generally operate in pulse mode – 60 Hz at SNS

Time of flight is used to sort out wavelengths

Monochromator crystal is used to saw-out a discrete wavelength
Methods of Specifying and Measuring $\vec{k}_i$ and $\vec{k}_f$

1. Bragg Diffraction
   
   BT7, MACS, HFBS

2. Time-of-Flight (TOF)
   
   DCS, HFBS

3. Larmor Precession
   
   NSE

Larmor precession angle of neutron mag moment acts as a clock – if $\Delta E \neq 0$ precession angles before and after sample are different.
It’s all about Conservation of Momentum
\( p = \hbar k \) and Energy \( (E = \hbar \omega = \frac{p^2}{2m}) \)

\[
Q = k_i - k_f \quad \text{Wave vector transfer to excitation}
\]

\[
\Delta E = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 k_f^2}{2m} \quad \text{Energy transfer to/from excitation}
\]

\[
\mathbf{Q}_C = \mathbf{\tau} + \mathbf{q}
\]

Reciprocal lattice vector
Wave vector of excitation

\[ (000) \quad (000) \quad q \]
Energy, wave vector, and wavelength relations for various probes

\[ E_{\text{neutron}}(\text{meV}) = 2.0719k^2 = 81.7968 / \lambda^2 \]

\[ E_{\text{photon}}(\text{keV}) = 2.0k = 12.4 / \lambda \]

\[ E_{\text{electron}}(\text{eV}) = 3.8k^2 = 150 / \lambda^2 \]

1 meV = 11.6 K \quad (k_B T)
1 meV = 8.06 cm\(^{-1}\) \quad (E /hc)
1 meV = 0.2418 THz \quad (E /h)
1 meV / \mu_B = 17.3 T \quad (E / \mu_B)
Golden Rule of Neutron Scattering

- We don’t take pictures of atoms!

- Job security for neutron scatterers – we live in reciprocal space
(3) The scattered neutron flux $\Phi(Q, h\omega)$ is proportional to the space ($\vec{r}$) and time ($t$) Fourier transform of the probability $G(\vec{r}, t)$ of finding one or two atoms separated by a particular distance at a particular time.

$$\Phi \propto \frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \int \int e^{i(Q \cdot \vec{r} - \omega t)} G(\vec{r}, t) d^3 \vec{r} dt$$
The NCNR Menagerie of Instruments
Because neutron scattering is an intensity-limited technique. Thus detector coverage and resolution MUST be tailored to the science.

Uncertainties in the neutron wavelength and direction imply $Q$ and $\hbar \omega$ are only defined with a finite selectable precision.

The total signal in a scattering experiment is proportional to the resolution volume → better resolution leads to lower count rates! Choose carefully …
How do I Choose the Right Spectrometer?

Two basic considerations:

1. What are the time scales ($\hbar \omega$) of interest?
2. What are the length scales ($Q$) of interest?

(Some spectrometers overlap → the choice may boil down to one of resolution)

Two additional considerations:

1. What energy resolution ($\Delta \hbar \omega$) is required?
2. What momentum resolution ($\Delta Q$) is required?
Different Spectrometers Cover Different Regions of Phase Space

Do you see a pattern here?

Larger “objects” tend to exhibit slower motions.
Inelastic Spectrometers

Thermal triple-axis instruments (BT-7) (BT-4)  
Cold neutron triple-axis instrument (MACS) (SPINS)  
Disk chopper time-of-flight spectrometer (DCS) (FANS)  
High flux backscattering spectrometer (HFBS)  
Spin-echo spectrometer (NSE)

$S(Q, E)$  
$S(Q, t)$

Approx. Resol.

1 meV  
~250 $\mu$eV  
1 $\mu$eV  
$\delta t \to ~10$ neV

All these different spectrometers are designed differently to optimize intensity and resolution for different measurement requirements.
1. What are the energies ($\hbar \omega$), i.e. time scales ($\Delta t \sim 1/\omega$), of interest?

   $\hbar \omega \approx 1\text{-}100 \text{ meV}$ - use a thermal triple-axis spectrometer like BT7.

   $\hbar \omega \approx 20\text{-}30 \mu\text{eV}$ - use HFBS or NSE.

   In between - use MACS or DCS or a cold-neutron triple-axis spectrometer like SPINS.

2. Make sure that the length scales $L$ of the relevant motions lie within the range of the spectrometer. For example, consider the HFBS

   $Q_{\text{min}} = 0.25 \text{ Å}^{-1} \rightarrow L_{\text{max}} \sim 25 \text{ Å}$

   $Q_{\text{max}} \approx 1.75 \text{ Å}^{-1} \rightarrow L_{\text{min}} \sim 3.5 \text{ Å}$

   $Q = \frac{2\pi}{L}$

REMEMBER - $Q_{\text{min}}$ and $Q_{\text{max}}$ are inversely proportional to the incident neutron wavelength
More Rules of Thumb

Is your sample polycrystalline or amorphous?

Does ONLY the magnitude (not the direction) of \( Q \) matter?

Is the expected \( Q \)-dependence of the scattering weak?

This often means that you want to look at a large region of \( Q, \hbar \omega \) space, or that you can sum the data over a large region of \( Q, \hbar \omega \) space.

**YES?** Consider instruments with large analyzer areas.

**NO?** Consider using BT7, SPINS, or NSE.
Things to Consider When Choosing DCS

Quantities varied
- wavelength $\lambda$
- chopper slot widths $W$

Remember – Intensity $\downarrow$
Resolution $\uparrow$
Example: DCS versus BT7

**DCS**
Broad surveys in **Q-ω**

**BT7**
Limited regions in **Q-ω**

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**Rules of Thumb:** (think carefully before violating)

DCS, MACS – systems requiring resolution < 400 µeV

BT7 – single crystals – resolution > 100 µeV

depends on collimation and monochromator/anaizer
Things to Consider When Choosing BT7

Triple axis spectrometers are typically used when either -
(1) the *direction* of $\mathbf{Q}$ is important or
(2) the interesting region of $\mathbf{Q}$-$\omega$ space is of *limited extent*.

Remember – *Intensity* ↓
*Resolution* ↑

One data point at a time …
Things to Consider When Choosing HFBS

Do the features of interest lie within this $h\omega$-range?

$0.25 \text{ Å}^{-1} < Q < 1.75 \text{ Å}^{-1}$

Can you live with such coarse Q-resolution?

$\delta Q < 0.1 - 0.2 \text{ Å}^{-1}$

Do the length scales of interest lie within this Q-range?

Do you really require such good energy resolution $\delta E \sim 1 \text{ μeV}$?
General Sample “Design”

Know as much about your sample as possible!!
(Beamtime costs ~ $5000/day!!)

Other considerations:
What’s the structure (in a general sense)?
Are there any phase transitions (or a glass transition)?
What isotopes are present?
Supplementary data from other measurements …

Magnetization vs T  
Muon spin relaxation  
X-ray data  
Specific heat vs T  
Raman spectroscopy
General Sample “Design”

Try to avoid isotopes that are strongly absorbing.

\(^6\text{Li} \quad ^{10}\text{B} \quad ^{113}\text{Cd} \quad ^{157}\text{Gd}\)

For a complete listing go to

http://www.ncnr.nist.gov/resources/n-lengths
Single crystals yield the most information.

Increase the intensity by increasing the amount of sample.

If you have a powder, use a cylindrical container (rather than flat plate).

Annular may be the best sample geometry if your sample is absorbing.

Transmission of the beam should be \(~70\text{-}90\%\).

\[ \frac{I}{I_0} = \exp(-n\sigma_AT) \]

Almost all experiments of collective excitations involve coherent scattering

→ If sample contains H it should be deuterated (D).
Does the sample contain H?  
Remember: **Neutrons LOVE H!!**

Create a sample where -  
the “interesting” portions are **hydrogenated** and  
the “uninteresting” portions are **deuterated**.
Typical Distributions of Science by Instrument

- Magnetism: 39%
- Materials Science: 22%
- Small Molecules: 12%
- Polymers: 4%
- Complex Fluids: 2%
- Biology: 21%

- Magnetism: 23%
- Materials Science: 7%
- Small Molecules: 8%
- Polymers: 6%
- Complex Fluids: 16%
- Biology: 40%

DCS
NSE
Some Summer School Success Stories

2001

Jae-Ho Chung
University Prof.

2003

Vicky Garcia-Sakai
ISIS Staff Scientist

1999

William Ratcliff
NCNR Staff Physicist

1997

Rob Dimeo
NCNR Director
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Enjoy the Science With Neutrons!