Introduction to Triple Axis Neutron Spectroscopy

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- The triple axis spectrometer
- Constant-Q and constant E
- Practical concerns
- Resolution and Spurions

Brockhouse Institute
for Materials Research
Neutron interactions with matter

• **Properties of the neutron**
  - Mass \( m_n = 1.675 \times 10^{-27}\) kg
  - Charge 0
  - Spin-1/2, magnetic moment \( \mu_n = -1.913 \mu_N \)

• **Neutrons interact with...**
  - Nucleus
  - Crystal structure/excitations (eg. Phonons)
  - Unpaired electrons via dipole scattering
  - Magnetic structure and excitations

![Nuclear scattering](attachment:image1.png)

![Magnetic dipole scattering](attachment:image2.png)
Brockhouse and Shull Share 1994 Nobel Prize in Physics
Most recent Nobel Prize awarded to a scientist working in Canada

When the neutrons collide with atoms in the sample material, they change direction (are scattered) = elastic scattering.

Detectors record the directions of the neutrons and a diffraction pattern is obtained. The pattern shows the positions of the atoms relative to one another.

Crystal that sorts and forwards neutrons of a certain wavelength (energy) = monochromatized neutrons

Changes in the energy of the neutrons are first analysed in an analyser crystal...

...and the neutrons then counted in a detector.

B

Retna N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, received one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

Clifford C. Shull, MIT, Cambridge, Massachusetts, USA, received one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.
The Basic Experiment:

Incident Beam:
- monochromatic
- “white”
- “pink”

Scattered Beam:
- Resolve its energy
- Don’t resolve its energy
- Filter its energy
Brockhouse’s Triple Axis Spectrometer

\[ | \mathbf{k}_i | = \frac{2 \pi}{\lambda_i} \]

\[ | \mathbf{k}_f | = \frac{2 \pi}{\lambda_f} \]
Momentum Transfer:

\[ Q = k_i - k_f \]

Energy Transfer:

\[ \delta E = \frac{h^2}{2m} (k_i^2 - k_f^2) \]
Mapping Momentum – Energy (Q-E) space

Origin of reciprocal space;
Remains fixed for any sample rotation
Bragg diffraction:

Constructive Interference

\[ Q = \text{Reciprocal Lattice Vector} \]

Elastic scattering: \[ |k_i| = |k_f| \]
Bragg diffraction:

Constructive Interference

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Elastic scattering: \( |k_i| = |k_f| \)
Elementary Excitations in Solids

- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)

Energy vs Momentum

- Forces which bind atoms together in solids
Bragg’s Law: $n\lambda = 2d \sin(\theta)$
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Two Axis Spectrometer:

- 3-axis with analyser removed
- Powder diffractometer
- Small angle diffractometer
- Reflectometers

Diffractometers often employ working assumption that all scattering is *elastic*. 
Soller Slits: Collimators

Define beam direction to +/- 0.5, 0.75 etc. degrees
Filters:
Remove $\lambda/n$ from incident or scattered beam, or both
Single crystal monochromators:

Bragg reflection and harmonic contamination

\[ n\lambda = 2d \sin(\theta) \]

Get: \( \lambda, \lambda/2, \lambda/3, \text{ etc.} \)
Pyrolitic graphite filter:

- $E = 14.7$ meV
- $\lambda = 2.37$ Å
- $v = 1.6$ km/s
- $2 \times v = 3.2$ km/s
- $3 \times v = 4.8$ km/s
Two different ways of performing constant-Q scans
Mapping Momentum – Energy (Q-E) space

Origin of reciprocal space;
Remains fixed for any sample rotation

\[ \frac{2\pi}{a} \]
Spurions

- **Bragg – incoherent – Bragg**
  - Eg. \( k_i - 2k_f \)
    - \( \hbar \omega = 41.1 \text{ meV} \)
    - \( E_f = 13.7 \text{ meV} \)
    - \( E_i = 54.8 \text{ meV} \)
    - \( 4E_f = 54.8 \text{ meV} \)
    - Incoherent elastic scattering visible from analyzer \( \lambda/2 \)

- **incoherent – Bragg – Bragg**
  - Sample \( 2\theta \) in Bragg condition for \( k_f - k_f \)
  - Even for inelastic config, weak incoherent from mono
Elementary Excitations in Solids

- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)

Energy vs Momentum

- Forces which bind atoms together in solids
Constant Q, Constant E
3-axis technique allow us to
Put Q-Energy space on a grid,
And scan through as we wish

Map out elementary excitations
In Q-energy space (dispersion Surface)
Phonons

- Normal modes in periodic crystal $\rightarrow$ wavevector

$$u(l, t) = \frac{1}{\sqrt{NM}} \sum_{j} \varepsilon_j(q) \exp(iq \cdot l) \hat{B}(q_j, t)$$

- Energy of phonon depends on $q$ and polarization

FCC structure


FCC Brillouin zone
Phonon intensities

\[
S_{1+}(Q, \omega) = \frac{1}{2NM} e^{-Q^2\langle u^2 \rangle} \sum_{j \mathbf{q}} |Q \cdot \varepsilon_j(\mathbf{q})|^2 \left(1 + n(\omega)\right)\delta(Q - \mathbf{q} - \tau)\delta(\omega - \omega_j(\mathbf{q}))
\]
More complicated structures


La$_2$CuO$_4$
Detectors

- **Gas Detectors**
- $n + ^3\text{He} \rightarrow ^3\text{H} + p + 0.764 \text{ MeV}$
- Ionization of gas
- $e^-$ drift to high voltage anode
- High efficiency

- **Beam monitors**
- Low efficiency detectors for measuring beam flux
Resolution

- **Resolution ellipsoid**
  - Beam divergences
  - Collimations/distances
  - Crystal mosaics/sizes/angles

- **Resolution convolutions**

\[
I(Q_0, \omega_0) = \int S(Q_0, \omega_0)R(Q - Q_0, \omega - \omega_0)dQd\omega
\]
Resolution focusing

- Optimizing peak intensity
- Match slope of resolution to dispersion
References

**General neutron scattering**

**Polarized neutron scattering**

**Triple-axis techniques**

**Time-of-flight techniques**
Constant $k_f$:

- $k_f, \theta_A$ do not change; therefore analyser “efficiency” is constant

- $k_i, \theta_M$ do change, but monitor detector normalizes to incident neutron flux

- Monitor detector (low) efficiency goes like $\sim 1/\nu \sim 1/k_i$
Monochromators

- Selects the incident wavevector

\[ Q(hkl) = \frac{2\pi}{d(hkl)} = 2k_1 \sin \theta \]

- Reflectivity
- focusing
- high-order contamination eg. \( \lambda/2 \) PG(004)

<table>
<thead>
<tr>
<th>Mono</th>
<th>d(hkl)</th>
<th>uses</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG(002)</td>
<td>3.353</td>
<td>General</td>
</tr>
<tr>
<td>Be(002)</td>
<td>1.790</td>
<td>High ( k_i )</td>
</tr>
<tr>
<td>Si(111)</td>
<td>3.135</td>
<td>No ( \lambda/2 )</td>
</tr>
</tbody>
</table>
Guides

• Transport beam over long distances
• Background reduction
• Total external reflection
  – Ni coated glass
  – Ni/Ti multilayers (supermirror)
Samples

- **Samples need to be BIG**
  - ~ gram or cc
  - Counting times are long (mins/pt)

- Sample rotation
- Sample tilt

Co-aligned CaFe$_2$As$_2$ crystals