Neutron and X-ray Spectroscopy (I) [Keimer]

- Neutron with matter:
  1. Strong (nuclear) interaction \{ elastic: lattice structure, inelastic: lattice dynamics

- Neutron source: nuclear reactor
  e.g. $^{235}U + n \rightarrow A + B + 2.3n$
  Alternative source can create higher energy neutrons.

- The basic quantity that concern us is differential cross-section $d\sigma/d\Omega$
  - By Fermi's golden rule, $W = \frac{2\pi}{\hbar} |\langle f|\hat{V}|i\rangle|^2 \delta(E_f - E_i)$
  - Assume plane wave, incident flux $= \frac{\nu_k}{m_n l_s}$
  - For elastic scattering, $|k_i| = |k_f|$
  - In Born approx., $\frac{d\sigma}{d\Omega} = \frac{(m_n a)^2}{(2\pi\hbar)^2} \int |V(r)|^2 \delta^{(3)}(\mathbf{p}_i - \mathbf{p}_f) d\mathbf{p}_f$
  - Example: short-ranged $V(r) = \frac{2m_n a}{m_n} \delta^{(3)}(\mathbf{r} - \mathbf{R})$
    - For single nucleus, $\frac{d\sigma}{d\Omega} = |b|^2$
    - For lattice of nuclei, $\frac{d\sigma}{d\Omega} = \frac{a^2 N (2m)^2}{V_0} \sum|\delta^{(3)}(\mathbf{Q} - \mathbf{R})|^2$
    - For non-braun's lattice, $\frac{d\sigma}{d\Omega} = \frac{a^2 N (2m)^2}{V_0} \sum|\delta^{(3)}(\mathbf{Q} - \mathbf{R})| \frac{f_n(R)}{f_n(R)}|^2$
  - Example: elastic magnetic neutron scattering
    $\frac{d\sigma}{d\Omega} = \frac{(m_n a)^2}{(2\pi\hbar)^2} \left|\langle f|m|H_{\text{int}}|i|n\rangle\right|^2$
    $H_{\text{int}} = -\mathbf{\mu}_n \cdot \mathbf{H}$
    Collecting, $\frac{d\sigma}{d\Omega} = \left(\gamma r_0\right)^2 \left|\langle f|m|\mathbf{S}_{\text{el}}|i\rangle\right|^2$

- For atom, just add form factor:
  $\frac{d\sigma}{d\Omega} = \left(\gamma r_0\right)^2 \left[1 - (\hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}}^*)\right] |f(\mathbf{Q})|^2$
  $f(\mathbf{Q}) = \frac{1}{2\mu_0} \int M(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r}$
  where $\overline{M}(\mathbf{r}) = M(\mathbf{r}) \hat{\mathbf{Q}}$

- Can similarly extend to lattice.
Example: ferromagnet on linear chain

\[ \frac{d\phi}{dt} \sim 1b_{l}^{2} + \sum_{n} \phi \frac{2}{5} \]

Example: antiferromagnet on linear chain

Example: vortex lattice in type II superconductor

\[ \alpha \sqrt{\frac{k_{B}}{H}} \beta = \frac{h}{2\pi} \]

\[ \sim 500 \text{ Å for } H = 17 \]

Inelastic neutron scattering:

\[ \frac{\partial \sigma}{\partial E_{F}} = \frac{k_{F}}{2\pi n} \sum_{j} b_{j}^{k} b_{j}^{\dagger} \sum_{\omega} \sum_{\nu} \langle \nu | e^{-iE_{\omega}(t - \tau)} e^{iE_{\nu}(t + \tau)} | \nu \rangle e^{-i\omega t} dt \]

Example: Cu in fcc lattice:
For magnetic inelastic scattering:
\[
\frac{dE}{d\Omega} = \frac{(\gamma_\epsilon \omega)^2}{k_f} N \sum_{n} e^{2i\epsilon_{\epsilon} - \epsilon_{\epsilon} \sigma_{\epsilon}} \int \frac{d^2\kappa}{2\pi^2} \left| \sum_{p} e^{i\kappa \cdot \rho_p} \langle S_p(\theta) e^{i\epsilon_p} \rangle e^{-i\omega t} \right|^2
\]

Next consider X-ray spectroscopy.

- Characteristic radiation due to fluorescence
- Bremsstrahlung due to electron deceleration or anode
- Photon energy

Synchrotron

- Major X-ray interaction with matter
- Elastic scattering
- Inelastic (Compton) scattering
- Photoelectric absorption
- Pair creation (very high energy)

For one electron, elastic scattering
\[
\frac{d\sigma}{d\Omega} = \frac{|E_m^2 R_{E_m}|^2}{|E_e^2|} = r_0^2 \cos^2 \theta
\]

For lattice (Bravais):
\[
\frac{d\sigma}{d\Omega} = \sum_{\mathbf{G}} \frac{1}{|G|^2} \frac{1}{\pi^2} \int \frac{d \mathbf{p}}{2\pi^2} e^{i\mathbf{p} \cdot \mathbf{G}} e^{-i\mathbf{G} \cdot \mathbf{R}}
\]

\[ \mathbf{G} \] for Bravais lattices...
Inelastic X-ray scattering

- photon energy \( \approx 10 \text{ keV} \), phonon energy \( \approx 10 \text{ meV} \)
  \( \implies \) very high resolution

- Scattering mostly come from core e\(^{-}\), so again probe mostly lattice structure/dynamics.

- Example: MgB\(_2\) has B vibration that drive superconductivity with \( T_c \approx 39 \text{ K} \). Neutron scattering is difficult since hard to get single crystal.

X-ray Absorption

- Coming dominantly from the \( (\mathbf{A} \cdot \mathbf{p}) \) term in interaction Hamiltonian
  \[ \sigma_a = \frac{W}{\mathcal{E}_0}, \quad W = \frac{\hbar}{2\pi} |\mathbf{M}|^2 \rho(\mathbf{E}_f), \quad \mathcal{E}_f = \langle \mathbf{f} | H_{\text{int}} | \mathbf{f} \rangle \]

- For transition from hydrogenic (100) state to continuum.

- The technique is useful for chemical analysis (element content, valence state, etc.).

- X-ray can also drive excitation into unoccupied bands:

Magnetic Circular Dichroism

- By selection rule, \( m_f = \pm 1 \to 0 \) transition driven by right circularly polarized light.

- Thus, with (e.g.) spin-orbit coupling, spectrum shifts.
X-ray can be focused easily and so works for small sample. But for low-energy phonon modes, neutrons have higher resolution.