

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

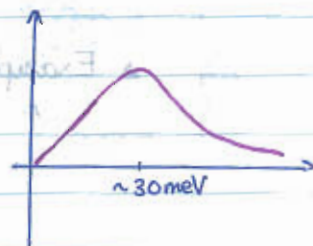
• Neutron with matter:

- (1) strong (nuclear) interaction $\left\{ \begin{array}{l} \text{elastic: lattice structure} \\ \text{inelastic: lattice dynamics} \end{array} \right.$
- (2) magnetic (dipole-dipole) interaction $\left\{ \begin{array}{l} \text{elastic: magnetic structure} \\ \text{inelastic: magnetic excitations.} \end{array} \right.$

• Neutron source: nuclear reactor



Alternative source can create higher energy neutrons.



• The basic quantity that concern us is differential cross-section $\frac{d\sigma}{d\Omega}$

▲ By Fermi's golden rule, $W = \frac{2\pi}{\hbar} |\langle \mathbf{k}_f | V | \mathbf{k}_i \rangle|^2 \rho_f(\epsilon)$

▲ Assume plane wave, incident flux = $\frac{\hbar \mathbf{k}_i}{m_n L^3}$

▲ For elastic scattering, $|\mathbf{k}_f| = |\mathbf{k}_i|$

▲ In Born approx, $\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar}\right)^2 \left| \int V(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d^3r \right|^2$ ← momentum transfer

▲ Example: short-ranged $V(\mathbf{r}) = \frac{2\pi\hbar^2}{m_n} b \delta(\mathbf{r} - \mathbf{R})$ ← scattering length

► For single nucleus, $\frac{d\sigma}{d\Omega} = |b|^2$

► For lattice of nuclei, $\frac{d\sigma}{d\Omega} = \frac{b^2 N (2\pi)^3}{V_0} \sum_{\mathbf{R}} \delta(\mathbf{Q} - \mathbf{R})$ ← reciprocal lattice vectors

► For non-bravais lattice, $\frac{d\sigma}{d\Omega} = \frac{N (2\pi)^3}{V_0} \sum_{\mathbf{R}} \delta(\mathbf{Q} - \mathbf{R}) |F_N(\mathbf{R})|^2$ ← form factor

▲ Example: elastic magnetic neutron scattering

$$\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar}\right)^2 |\langle \mathbf{k}_f m_f | \mathcal{H}_{\text{int}} | \mathbf{k}_i m_i \rangle|^2 \quad \mathcal{H}_{\text{int}} = -\vec{\mu}_n \cdot \vec{H}_e$$

$$= 4\pi \hat{\mathbf{Q}} \times (\hat{\mathbf{S}}_e \times \hat{\mathbf{Q}})$$

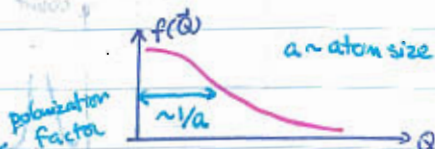
Collecting, $\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 |\langle m_f | \hat{\sigma} \cdot \hat{\mathbf{S}}_e | m_i \rangle|^2$

► For atom, just add form factor:

$$\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 [1 - (\hat{\eta} \cdot \hat{\mathbf{Q}})^2] |f(\mathbf{Q})|^2$$

$$f(\mathbf{Q}) = \frac{1}{\mu_B} \int \mathcal{M}(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d^3r \quad \text{where } \vec{M}(\mathbf{r}) = M(\mathbf{r}) \hat{\eta}$$

► Can similarly extend to lattice.



Example: ferromagnet on linear chain

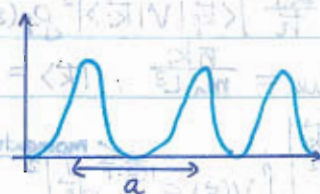


$$\Rightarrow \frac{d\sigma}{d\Omega} \sim |b|^2 + |\hat{n}|^2 + b\hat{n}$$

Example: antiferromagnet on linear chain



Example: vortex lattice is type II superconductor



$$a \sim \sqrt{\frac{\Phi_0}{H}} \quad \Phi_0 = \frac{h}{2e}$$

$$\sim 500 \text{ \AA} \text{ for } H = 1 \text{ T}$$

Inelastic neutron scattering

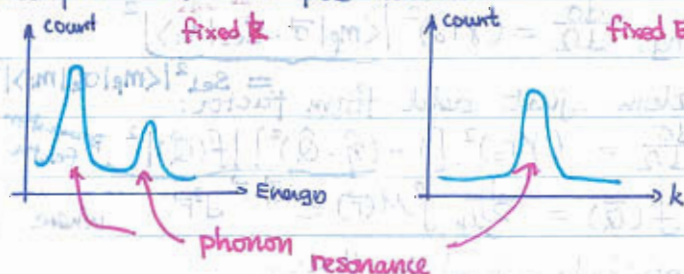
Now we need $\frac{d^2\sigma}{dE d\Omega}$

$$\frac{d^2\sigma}{dE d\Omega} = \frac{k_f}{k_i} \frac{1}{2\pi\hbar} \sum_{j,j'} b_j^* b_{j'} \int_{-\infty}^{\infty} \sum_i P_i \langle \lambda_i | e^{-i\vec{Q} \cdot \vec{R}_j(0)} e^{i\vec{Q} \cdot \vec{R}_{j'}(t)} | \lambda_i \rangle e^{-i\omega t} dt$$

← state of sample →

$$= \frac{\sigma_{coh}}{4\pi} \frac{k_f}{k_i} \frac{(2\pi)^3}{V_0} \frac{1}{2M} e^{-2W} \sum_{s,j} \frac{(\vec{Q} \cdot \vec{e}_s)^2}{\omega_s} \{ \langle n_s+1 \rangle \delta(\omega-\omega_s) \delta(\vec{Q}-\vec{q}-\vec{k}) + \langle n_s \rangle \delta(\omega+\omega_s) \delta(\vec{Q}+\vec{q}-\vec{k}) \}$$

Example: C₆₀ in fcc lattice

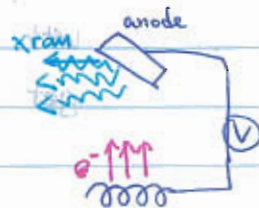
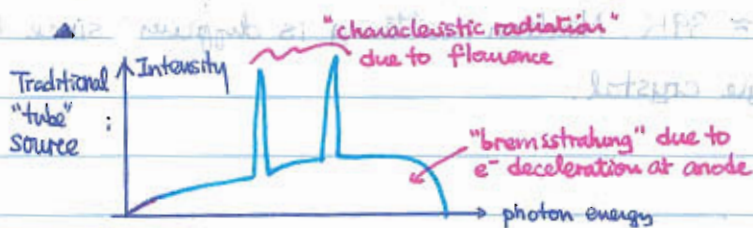


▲ For magnetic inelastic scattering:

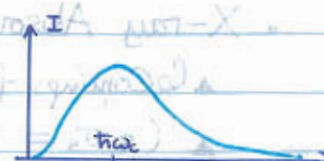
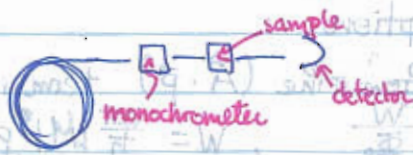
$$\frac{d^2\sigma}{dE d\Omega} = (\gamma r_0)^2 \frac{k_f}{k_i} N |F(\vec{Q})|^2 e^{-2W} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) S^{\alpha\beta}(\vec{Q}, \omega)$$

$$S^{\alpha\beta}(\vec{Q}, \omega) = \frac{1}{2\pi\hbar} \int \sum_i e^{i\vec{Q} \cdot \vec{r}_i} \langle S_i^\alpha(0) S_i^\beta(t) \rangle e^{-i\omega t} dt$$

• Next consider X-ray spectroscopy



▲ Synchrotron



▲ Major X-ray interaction with matter

► elastic scattering



► inelastic (Compton) scattering



► Photoelectric absorption



► Pair creation (very high energy)



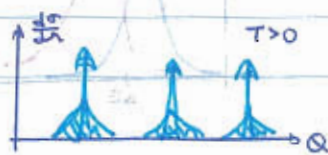
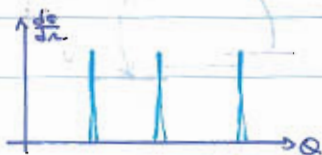
▲ For one electron, elastic scattering, $\frac{d\sigma}{d\Omega} = \frac{|E_{\text{ind}}|^2 R}{|E_{\text{in}}|^2} = r_0^2 \cos^2 \theta$

$$\frac{d\sigma}{d\Omega} = \left| r_0 \int \rho(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} d^3r \right|^2 \quad \text{for non-delta } \rho(\vec{r})$$

form factor

For lattice (Bravais),

$$\frac{d\sigma}{d\Omega} =$$



• Inelastic X-ray scattering

- ▲ photon energy $\sim 10 \text{ KeV}$, phonon energy $\sim 10 \text{ meV}$

$\Rightarrow$ very high resolution

- ▲ Scattering mostly come from core e^- , so again probe mostly lattice structure/dynamics.

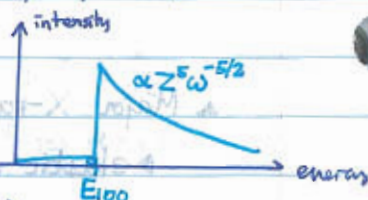
- ▲ Example: MgB_2 has B vibration that drives superconductivity, with $T_c \approx 39 \text{ K}$. Neutron scattering is difficult since hard to get single crystal.

• X-ray Absorption

- ▲ Coming dominantly from the $(\vec{A} \cdot \vec{p})$ term in interaction Hamiltonian

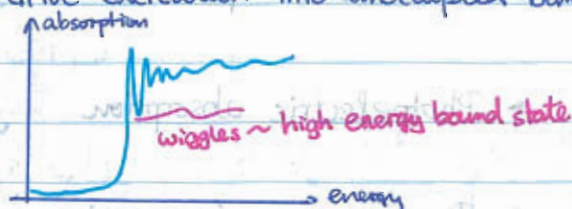
- ▲ $\sigma_a = \frac{W}{\Phi_0}$, $W = \frac{2\pi}{\hbar} |\mathcal{M}|^2 \rho(\epsilon_f)$, $\mathcal{M}_{fi} = \langle f | \mathcal{H}_{int} | i \rangle$

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



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

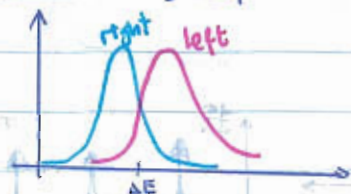
- ▲ X-ray can also drive excitation into unoccupied bands:



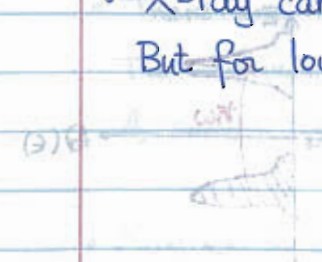
- ▲ Magnetic Circular Dichroism

- ▲ by selection rule, $m_j = \begin{cases} +1 \rightarrow 0 \\ -1 \rightarrow 0 \end{cases}$ transition driven by $\begin{cases} \text{right} \\ \text{left} \end{cases}$ 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.



$$E_{\text{in}} = E_{\text{out}} = E$$

primary or -- no scattering

secondary or -- scattered and not to be counted

scattered or -- most primary as well

• intensity resolved $\rightarrow$ a dependence of elastic structure
• a function of surface is measured

• light can go through 1000 Å in one second $\rightarrow$ it is a few Å from the surface $\Rightarrow$ Rel. surface



• intensity of $I(Q) \propto A^2(Q) \propto F(Q)^2$
• intensity is higher (with normal) as maximum appears

• surface wave

• "three step model" for the transition of "phonon state"

(1) photoexcitation of a "phonon state" (2) "phonon state" is generated

(3) "phonon state" is generated (4) "phonon state" is generated

(5) "phonon state" is generated (6) "phonon state" is generated

• "phonon state" is generated (7) "phonon state" is generated

• "phonon state" is generated (8) "phonon state" is generated

• Momentum conservation is up to reciprocal lattice vector

• "phonon state" is generated (9) "phonon state" is generated

$$\frac{1}{N} \sum_{\mathbf{r}} \left(\frac{1}{2} \left(\frac{\partial \phi}{\partial \mathbf{r}} \right)^2 + \frac{1}{2} \left(\frac{\partial \phi}{\partial \mathbf{r}} \right)^2 \right) = \frac{1}{2} \left(\frac{\partial \phi}{\partial \mathbf{r}} \right)^2$$

• "phonon state" is generated (10) "phonon state" is generated

• "phonon state" is generated (11) "phonon state" is generated

• "phonon state" is generated (12) "phonon state" is generated