<u>Neutron and X-ray Spectroscopy (I)</u> [Keimer]

- Neutron with matter:

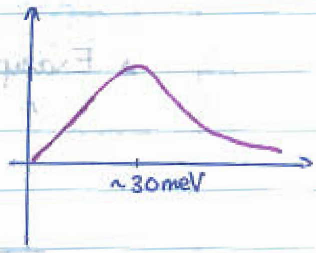
  (1) strong (nuclear) interaction $\begin{cases} \text{elastic: lattice structure} \\ \text{inelastic: lattice dynamics} \end{cases}$

  (2) magnetic (dipole-dipole) interaction $\begin{cases} \text{elastic: magnetic structure} \\ \text{inelastic: magnetic excitations.} \end{cases}$

- Neutron source: nuclear reactor

  e.g. $\quad {}^{235}U + n \longrightarrow A + B + 2.3n$

  Alternative source can create higher energy neutrons.



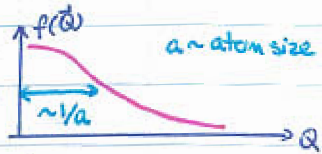
- The basic quantity that concern us is differential cross-section $\frac{d\sigma}{d\Omega}$
  - ▲ By Fermi's golden rule, $W = \frac{2\pi}{\hbar} |\langle \vec{k}_f | V | \vec{k}_i \rangle|^2 \rho_f(\varepsilon)$
  - ▲ Assume plane wave, incident flux $= \frac{\hbar k_i}{m_n L^3}$
  - ▲ For elastic scattering, $|\vec{k}_i| = |\vec{k}_f|$
  - ▲ In Born approx, $\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar}\right)^2 \left| \int V(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d^3\vec{r} \right|^2$ ← momentum transfer
  - ▲ Example: short-ranged $V(\vec{r}) = \frac{2\pi\hbar^2}{m_n} \underbrace{b}_{\text{scattering length}} \delta(\vec{r} - \vec{R})$
    - ▸ For single nuclear, $\frac{d\sigma}{d\Omega} = |b|^2$
    - ▸ For lattice of nuclei, $\frac{d\sigma}{d\Omega} = \frac{b^2 N (2\pi)^3}{v_0} \sum_{\vec{K}} \delta(\vec{Q} - \vec{K})$ ← reciprocal lattice vectors
    - ▸ For non-bravis lattice, $\frac{d\sigma}{d\Omega} = \frac{N(2\pi)^3}{v_0} \sum_{\vec{K}} \delta(\vec{Q} - \vec{K}) \underbrace{|F_N(\vec{K})|^2}_{\text{form factor}}$
  - ▲ Example: elastic magnetic neutron scattering

    $$\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar}\right)^2 \underbrace{|\langle \vec{k}_f m_f | \mathcal{H}_{int} | \vec{k}_i m_i \rangle|^2}_{= 4\pi \underbrace{\hat{Q} \times (\vec{S}_e \times \hat{Q})}_{= \vec{S}_{e\perp}}} \qquad \mathcal{H}_{int} = -\vec{\mu}_N \cdot \vec{H}_e$$

    Collecting, $\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 |\langle m_f | \vec{\sigma} \cdot \vec{S}_{e\perp} | m_i \rangle|^2$

    - ▸ For atom, just add form factor:

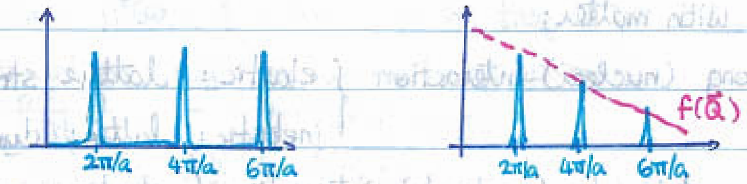
      $$\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 \underbrace{[1 - (\hat{\eta} \cdot \hat{Q})^2]}_{\text{polarization factor}} |f(\vec{Q})|^2$$

      $$f(\vec{Q}) = \frac{1}{2\mu_B} \int M(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d^3\vec{r} \qquad \text{where } \vec{M}(\vec{r}) = M(\vec{r}) \hat{\eta}$$

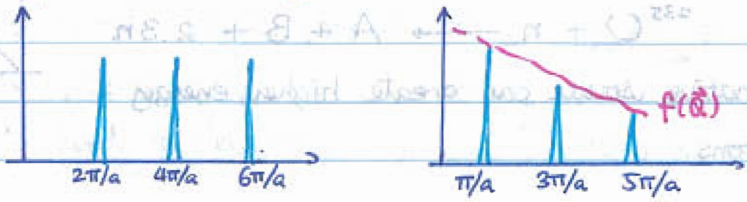
    - ▸ Can similarly extend to lattice.

▲ Example: ferromagnet on linear chain



$$\Longrightarrow \frac{d\sigma}{d\Omega} \sim |b|^2 + |\hat{\eta}|^2 + b\hat{\eta}$$

▲ Example: antiferromagnet on linear chain



▲ Example: vortex lattice is type II superconductor

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

~ 500 Å for $H = 1T$

• Inelastic neutron scattering :

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

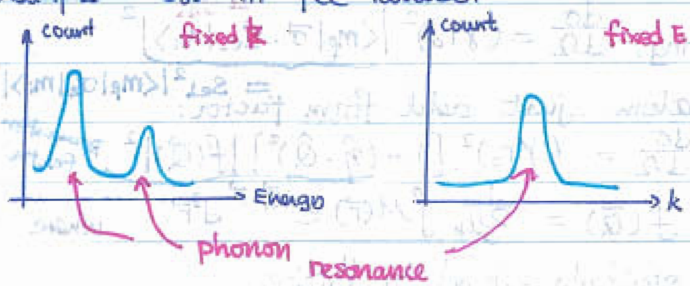
$\hbar\omega = E_i - E_f$

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

state of sample

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

▲ Example: C_{60} in fcc lattice:



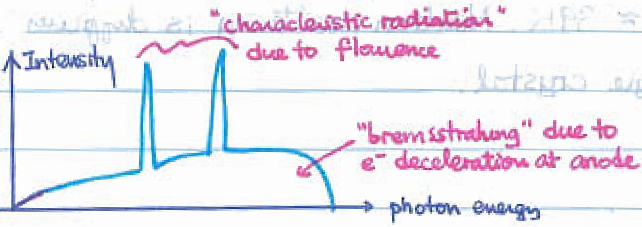
▲ For magnetic inelastic scattering:

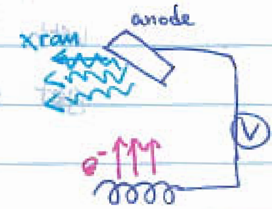
$$\frac{d^2\sigma}{dE\,d\Omega} = (\gamma r_0)^2 \frac{k_f}{k_i} N |F(\vec{Q})|^2 e^{-2W} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta)\, S^{\alpha\beta}(\vec{Q},\omega)$$

$$S^{\alpha\beta}(\vec{Q},\omega) = \frac{1}{2\pi\hbar} \int \sum_\ell e^{i\vec{Q}\cdot\vec{r}_\ell} \langle S_0^\alpha(0)\, S_\ell^\beta(t) \rangle e^{-i\omega t}\, dt$$

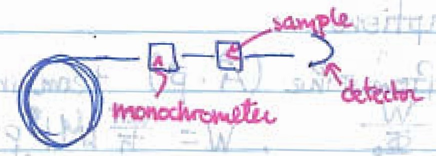
• Next consider X-ray spectroscopy

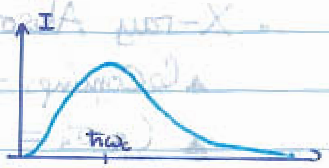
▲ Traditional "tube" source :





▲ Synchrotron





$\omega_c \sim 20$ KeV

▲ Major X-ray interaction with matter

▸ elastic scattering 

▸ inelastic (Compton) scattering 

▸ Photoelectric absorption 

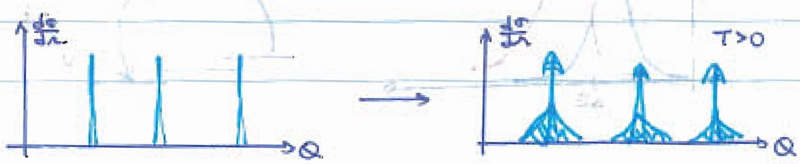
▸ Pair creation (very high energy) 

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

$$\frac{d\sigma}{d\Omega} = \Big| r_0 \underbrace{\int \rho(\vec{r})\, e^{i\vec{Q}\cdot\vec{r}}\, d^3 r}_{\text{form factor}} \Big|^2 \quad \text{for non-delta } \rho(\vec{r})$$

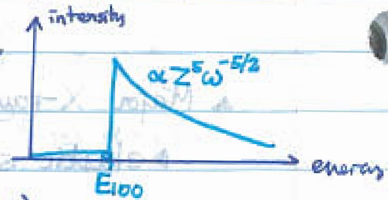
For lattice (Bravais),

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

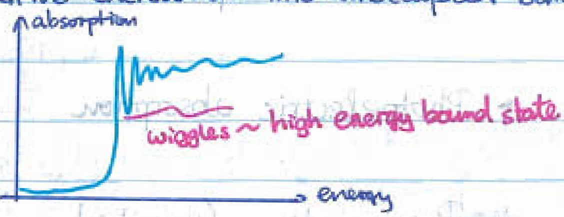


- Inelastic X-ray scattering
  - ▲ photon energy ~10 keV, phonon energy ~10 meV
    $\Longrightarrow$ very high resolution
  - ▲ Scattering mostly come from core e^-, so again probe mostly lattice structure / dynamics.
  - ▲ Example: MgB_2 has B vibration that drives superconductivity with $T_c \approx 39K$. Neutron scattering is difficult since hard to get single crystal.

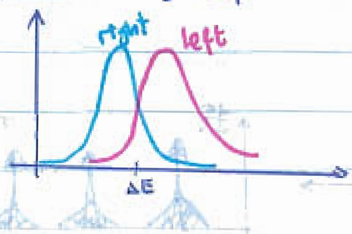
- X-ray Absorption
  - ▲ Coming dominantly from the $(\vec{A}\cdot\vec{p})$ term in interaction Hamiltonian
  - ▲ $\sigma_a = \frac{W}{\Phi_0}$, $W = \frac{2\pi}{\hbar}|M|^2\rho(\varepsilon_f)$, $M_{fi} = \langle f|\mathcal{H}_{int}|i\rangle$
  - ▲ For transition from hydrogenic (100) state to continuum.

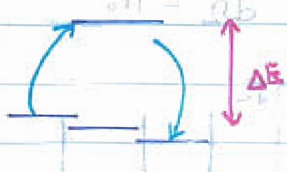


  - ▲ The technique is useful for chemical analysis (element content, valence state, etc.)
  - ▲ X-ray can also drive excitation into unoccupied bands:



  - ▲ Magnetic Circular Dichroism
    - ▶ by selection rule, $m_J = \begin{cases} +1\to 0 \\ -1\to 0 \end{cases}$ 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.