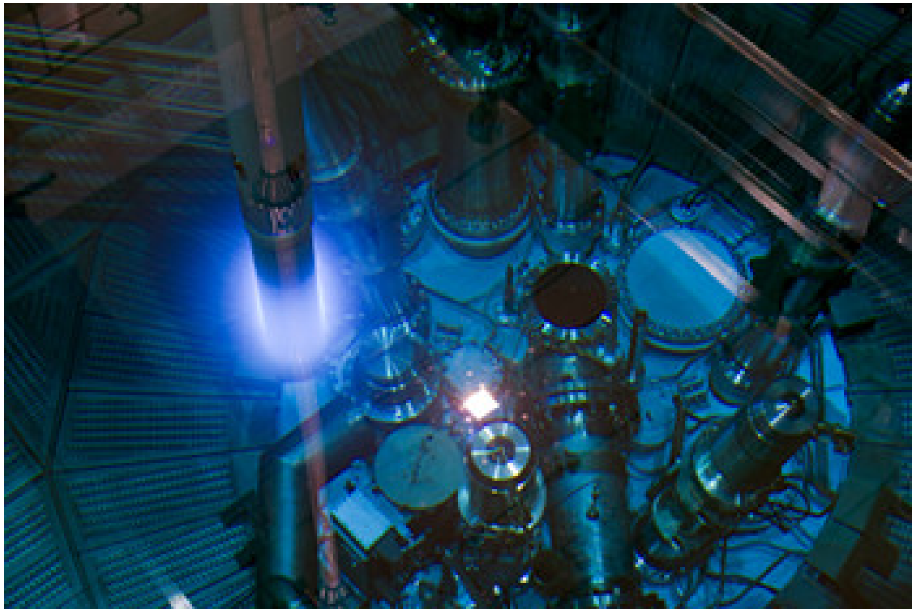
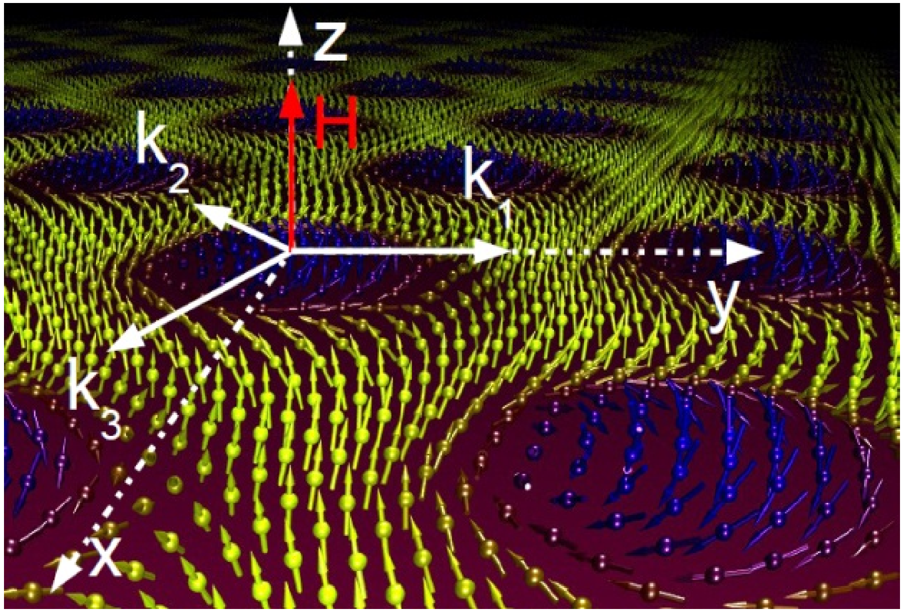
Physics with Neutrons I, WS 2015/2016



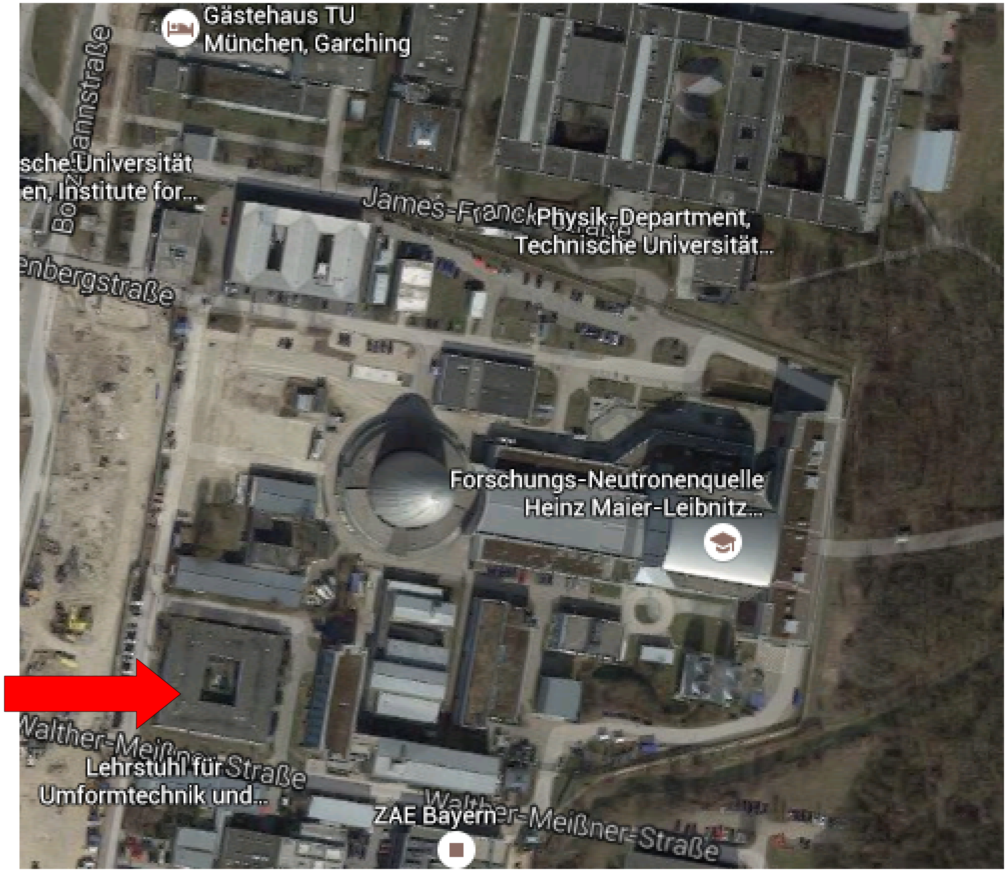


Lecture 11, 11.1.2016

Exam (after winter term)

- Registration: via TUM-Online between 16.11.2015 – 15.1.2015
- Email: sebastian.muehlbauer@frm2.tum.de for date arrangement

Room
E40a



Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

Fermis Golden Rule for scattering process: Born approximation

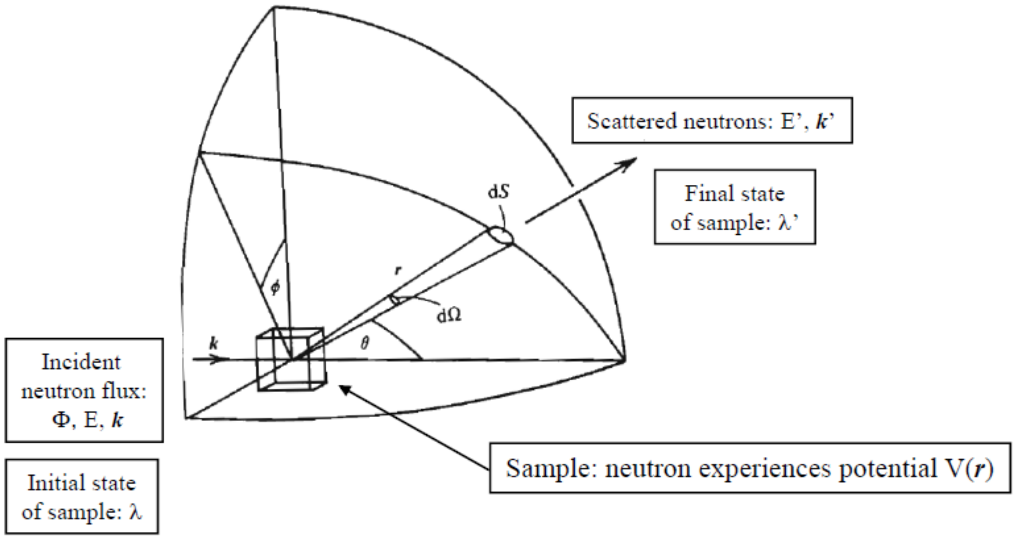
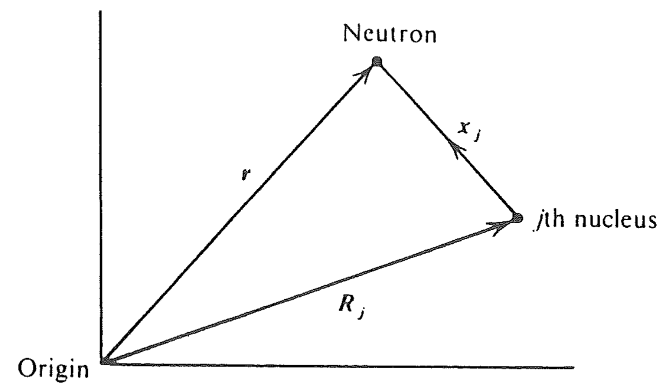


Fig. 2.1 Coordinates of nucleus and neutron.



$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi}\frac{1}{\Omega}\sum_{k'\ in\ \mathrm{d}\Omega} W_{k,\lambda\to k',\lambda'}$$

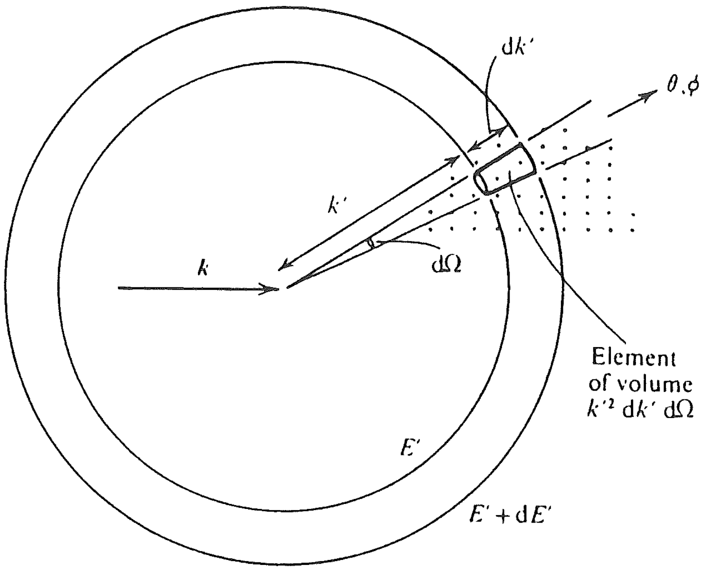
$$\sum_{k'\ in\ \mathrm{d}\Omega} W_{k,\lambda\to k',\lambda'} = \frac{2\pi}{\hbar}\varrho_k \left|\langle k'\lambda' \left|V\right| k\lambda\rangle\right|^2$$

$$\langle k'\lambda' \left|V\right| k\lambda\rangle = \int \Psi_{k'}^{*}\chi_{\lambda'}^{*} V \Psi_{k}^{*}\chi_{\lambda}^{*}\mathrm{drdR}$$

Challenge: Rewrite this mixed expression in terms of sample properties

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

1st step: Box Normalization to calculate ρ_k



$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \underline{\frac{k'}{k}\left(\frac{m}{2\pi\hbar}\right)^2} \left|\langle k'\lambda' \left|V\right| k\lambda\rangle\right|^2$$

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

2nd step: Energy conservation

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar}\right)^2 \left|\langle k'\lambda' \left|V\right| k\lambda\rangle\right|^2 \underline{\delta(E_\lambda - E_{\lambda'} + E - E')}$$

$$\int \delta(E_\lambda - E_{\lambda'} + E - E') = 1$$

3rd step: Integration with respect to neutron coordinate r

$$\langle k'\lambda' \left|V\right| k\lambda\rangle = \sum_j V_j(\kappa) \left\langle \lambda' \left| e^{i\kappa R_j} \right| \lambda \right\rangle \qquad \underline{V_j(\kappa) = \int V_j(x_j) e^{i\kappa x_j} \mathrm{d}x_j}$$

$$\kappa = k - k'$$

Interaction = Fourier transform of the potential function

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

4th step: Ansatz: Delta function potential for single nucleus

$$V(r) = a\delta(r)$$

Fermi pseudopotential: $V(r) = \frac{2\pi\hbar^2}{m} b\delta(r)$

- b can be bound or free scattering length!
- Fermi pseudopotential does NOT represent physical reality

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left|\sum_j b_j \left\langle k'\lambda' \left| e^{i\kappa R_j} \right| k\lambda \right\rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + E - E')$$

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

5th step: Integral representation of the delta function for energy.
Idea: Stick all the time dependence into the matrix element

$$\delta(E_\lambda - E_{\lambda'} + E - E') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{i(E_\lambda - E_{\lambda'})t/\hbar} e^{-i\omega t}\mathrm{dt}$$

H is the Hamiltonian of the scattering system with
Eigenfunctions λ and Eigenvalues E_λ

$$H|\lambda\rangle = E_\lambda|\lambda\rangle$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'}\int_{-\infty}^{\infty}\langle\lambda\,|e^{-i\kappa R_{j'}}|\,\lambda'\rangle\,\langle\lambda'\,|e^{iHt/\hbar}e^{i\kappa R_j}e^{-iHt/\hbar}|\,\lambda\rangle\, e^{-i\omega t}\mathrm{d}t$$

No terms of λ and λ' outside the matrix element anymore!

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

6th step: Sum over final states, average over initial states

- We use: $$\sum_{\lambda'} \langle \lambda | A | \lambda' \rangle \langle \lambda' | B | \lambda \rangle = \langle \lambda | AB | \lambda \rangle$$

$$p_\lambda = \frac{1}{Z} e^{\frac{-E_\lambda}{k_b T}}$$

$$\langle A \rangle = \sum_\lambda \langle \lambda | A | \lambda \rangle$$

- Stick the time evolution into the operator for the position R_j $$R_j(t) = e^{iHt/\hbar} R_j e^{-iHt/\hbar}$$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} = \frac{k'}{k} \frac{1}{2\pi\hbar} \sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \underline{\left\langle e^{-i\kappa R_{j'}(0)} e^{-i\kappa R_j(t)} \right\rangle} e^{-i\omega t} \mathrm{d}t$$

Correlation function

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

Assume a large sample with statistically variations of b_j

No correlations among *b*: $\overline{b_{j'}b_j} = (\bar{b})^2, j' \neq j$

$$\overline{b_{j'}b_j} = (\overline{b^2}), j' = j$$

Double differential crosssection spilts up into two terms:

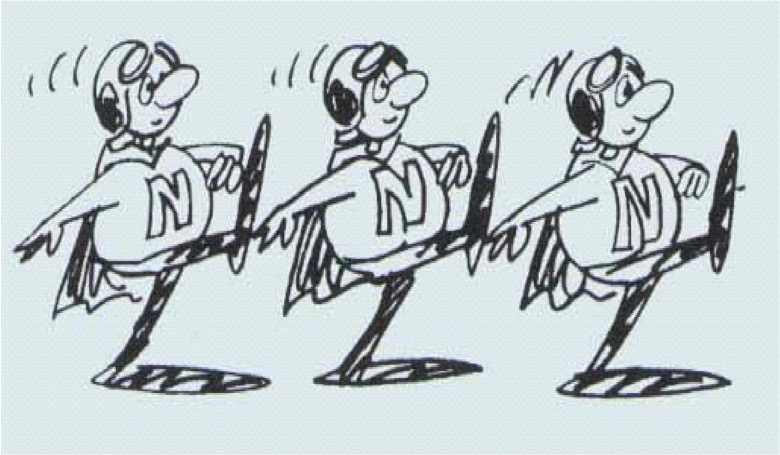
$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coherent} = \frac{\sigma_{coh.}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty}\underline{\left\langle e^{-i\kappa R_{j'}(0)}e^{-i\kappa R_j(t)}\right\rangle} e^{-i\omega t}dt$$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{incoherent} = \frac{\sigma_{inc.}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty}\underline{\left\langle e^{-i\kappa R_j(0)}e^{-i\kappa R_j(t)}\right\rangle} e^{-i\omega t}dt$$

$$\sigma_{coh.} = 4\pi\bar{b}^2 \qquad \sigma_{inc.} = 4\pi(\overline{b^2} - \bar{b}^2)$$

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

Coherent



Spatial and temporal correlations between different atoms

- Interference effects:
- Given by average of b
  Bragg scattering

Incoherent

Spatial and temporal correlations between the same atom

- Constant in *Q*
- Given by variations in b due to spin, disorder, random atomic motion....

Reminder: Elastic Scattering, Diffraction on Crystals

Starting point: Coherent elastic cross-section

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \left\langle e^{-i\kappa R_{j'}(0)} e^{-i\kappa R_j(t)} \right\rangle e^{-i\omega t} dt$$

Sample: Single X-tal in thermal equilibrium, consider static correlations!

$$\frac{d\sigma}{d\Omega} = \int_{\infty}^{\infty} \frac{d^2\sigma}{d\Omega dE'} d(\hbar\omega) = \sum_{j,j'} b_j b_{j'} \left\langle e^{-i\kappa R_{j'}} e^{-i\kappa R_j} \right\rangle$$

Drop the operator formalism for R_j as we look at static correlations

$$\frac{d\sigma}{d\Omega_{coh.el}} = \langle b\rangle^2 \sum_{j,j'} e^{-i\kappa(R_{j'}-R_j)}$$

⇨ Information on the position of the atoms

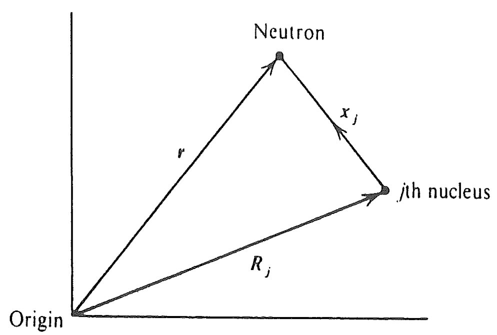
$$\frac{d\sigma}{d\Omega_{inc.}} = (\langle b^2\rangle - \langle b\rangle^2) \sum_{j=j'} e^{-i\kappa(R_{j'}-R_j} = N(\langle b^2\rangle - \langle b\rangle^2)$$

⇨ Isotropic, constant elastic background

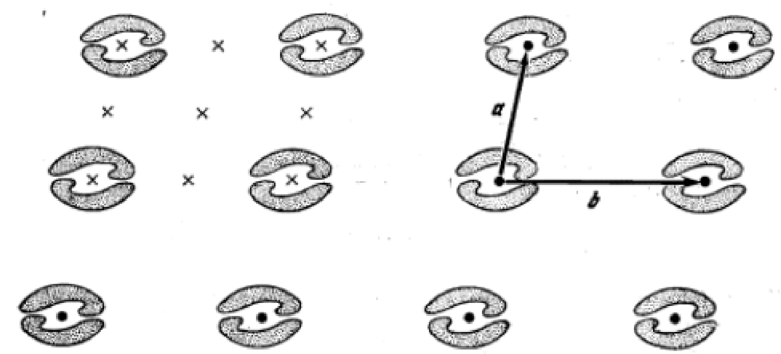
Reminder: Elastic Scattering, Diffraction on Crystals

What we used:

Fig. 2.1 Coordinates of nucleus and neutron.



Our sample is a periodic crystal!



Crystal= Basis+lattice

$$\frac{d\sigma}{d\Omega_{coh.el}} = \langle b \rangle^2 N_0 \sum_T e^{i\vec{\kappa}\vec{T}} \quad \text{with} \quad \vec{R}_{j'} - \vec{R}_j = \vec{T}$$

Lattice sum: $$\sum_{\vec{l}} e^{i\vec{\kappa}\vec{l}} = \frac{(2\pi)^3}{v_0} \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

Real space lattice

Reciprocal space lattice

Reminder: Elastic Scattering, Diffraction on Crystals

Lattice sum: $$\sum_{\vec{l}} e^{i\vec{\kappa}\vec{l}} = \frac{(2\pi)^3}{v_0} \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

Real space lattice

Reciprocal space lattice

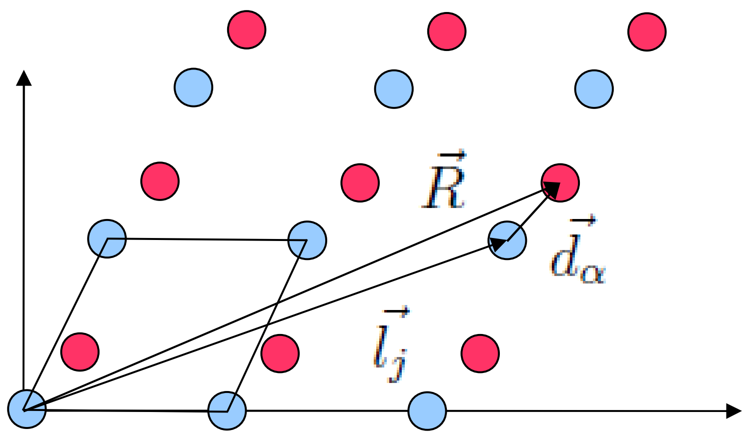
Braggs law: $$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} \langle b \rangle^2 \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

- Scattering occurs when κ meets a vector of the reciprocal lattice τ
- Reciprocal lattice vectors τ are perpendicular to a corresponding lattice plane indexed by the Miller index (h,k,l) and

$$d_{(h,k,l)} = \frac{2\pi}{|\vec{\tau}_{h,k,l}|}$$

Reminder: Elastic Scattering, Diffraction on Crystals, Structure Factor

More than one atom in the unit cell: $\vec{R} = \vec{l_j} + \vec{d_\alpha}$



$\vec{l_j}$ Position of the j-th unit cell

$\vec{d_\alpha}$ Position of the α-th atom in the unit cell

$$\frac{d\sigma}{d\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} \left| \sum_{\vec{d}} b_d e^{i\vec{\kappa}\vec{d}} \right|^2 \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

$$S_{\vec{\tau}} = \sum_{\vec{d}} b_d e^{i\vec{\kappa}\vec{d}}$$

Structure factor (sum over one unit cell)

Reminder: Master Formula for Neutron Diffraction

Going from operator to standard vector notation of R_j:

Neglect thermal vibration of atoms around their equilibrium position

$$2W(\vec{\kappa}) = \frac{1}{3}\kappa^2 \langle u^2 \rangle$$

Debye-Waller factor describes mean dispalcement $<u^2>$

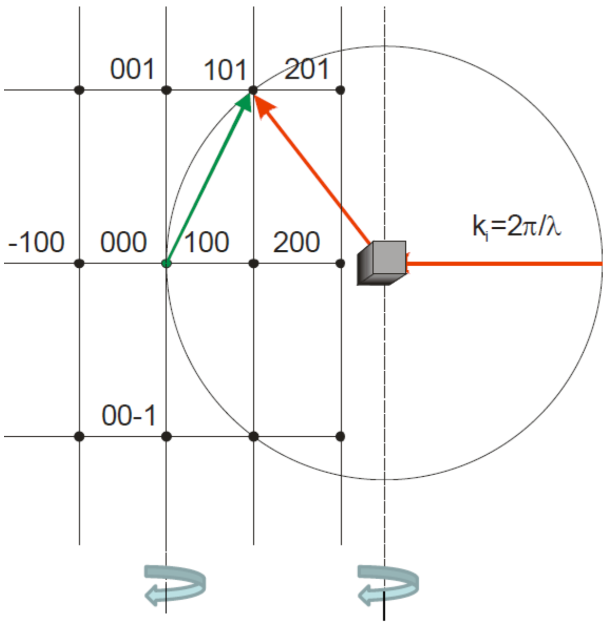
Final result for elastic coherent scattering on crystals

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} e^{-2W(\vec{\kappa})} \sum_{\vec{\tau}} |S_{\vec{\tau}}|^2 \, \delta(\vec{\kappa} - \vec{\tau})$$

Normalization Debye-Waller Structure factor Bragg positions

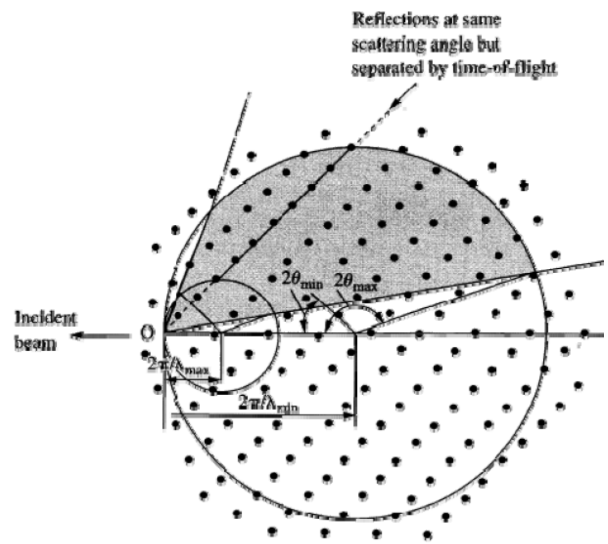
Reminder: Diffraction techniques

Monochromatic beam



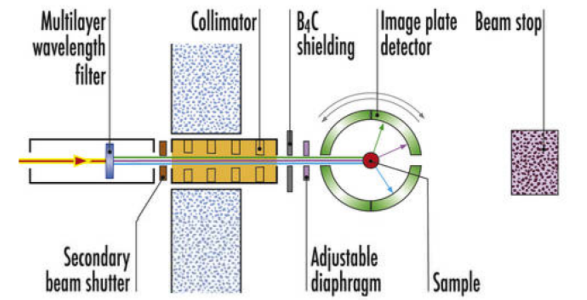
- Ewald construction
- Less intensity
- Rocking curve gives intensity of Bragg peak
- Clean data

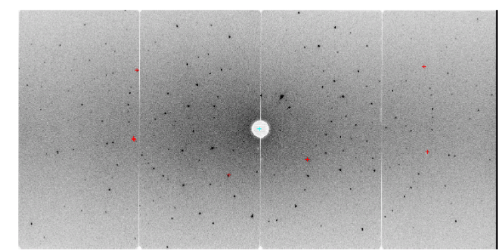
Time-of-flight (TOF)



- Ewald construction for each wavelength in the beam
- Rocking curve distributed in time and detector
- Waste less neutrons

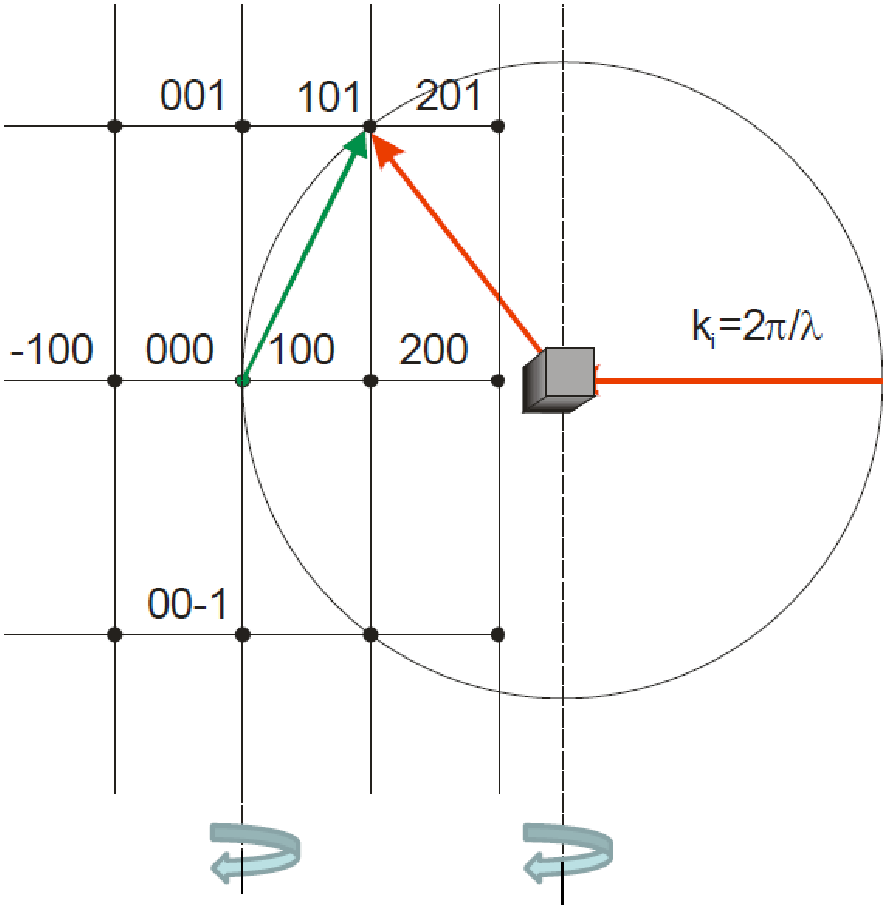
Laue (polychromatic beam)





- Essentially white beam
- More Bragg peaks (not stronger)
- Hard to get intensities
- Large background

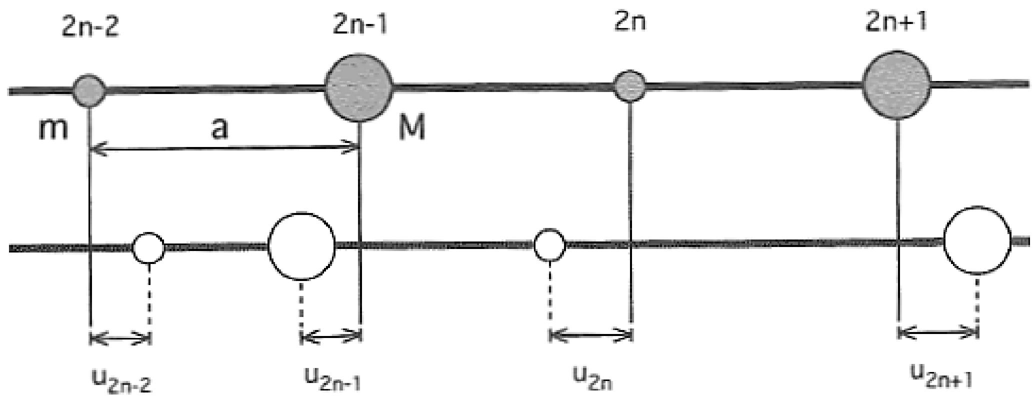
Reminder: Ewald construction for single crystal diffraction

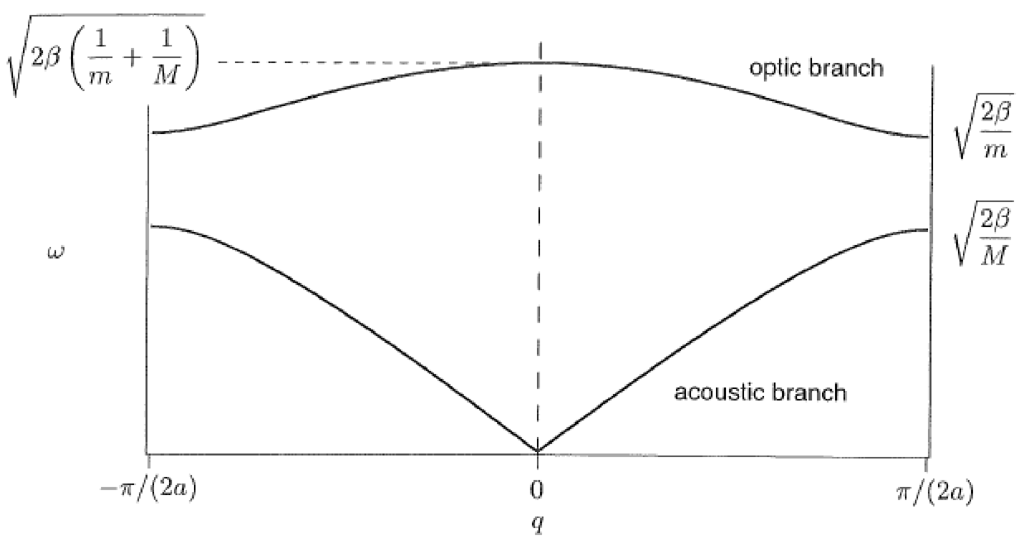


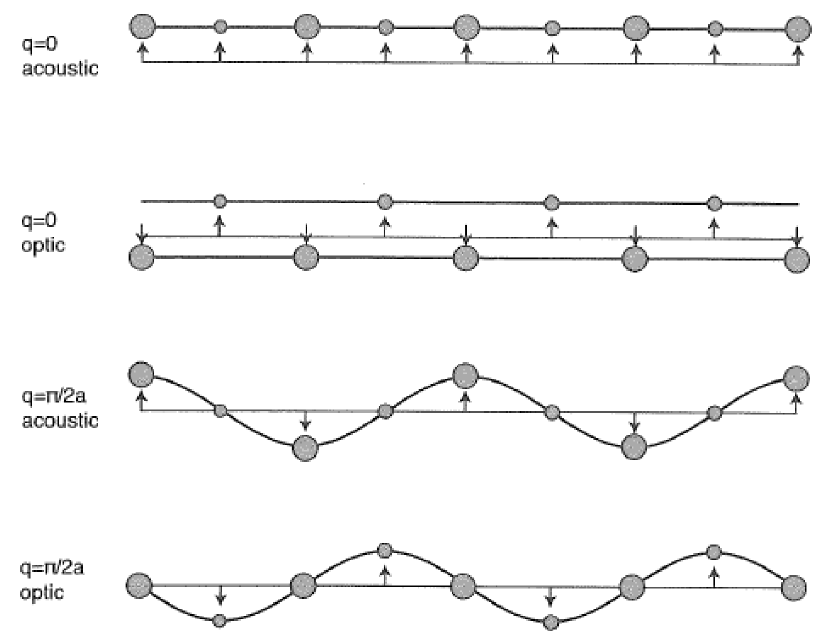
Ewald construction:

- Sphere around center of crystal (in real space)
- Origin of reciprocal space on transmitted beam at the edge of Ewald sphere
- Rotation of crystal (real space) corresponds to a rotation of reciprocal space

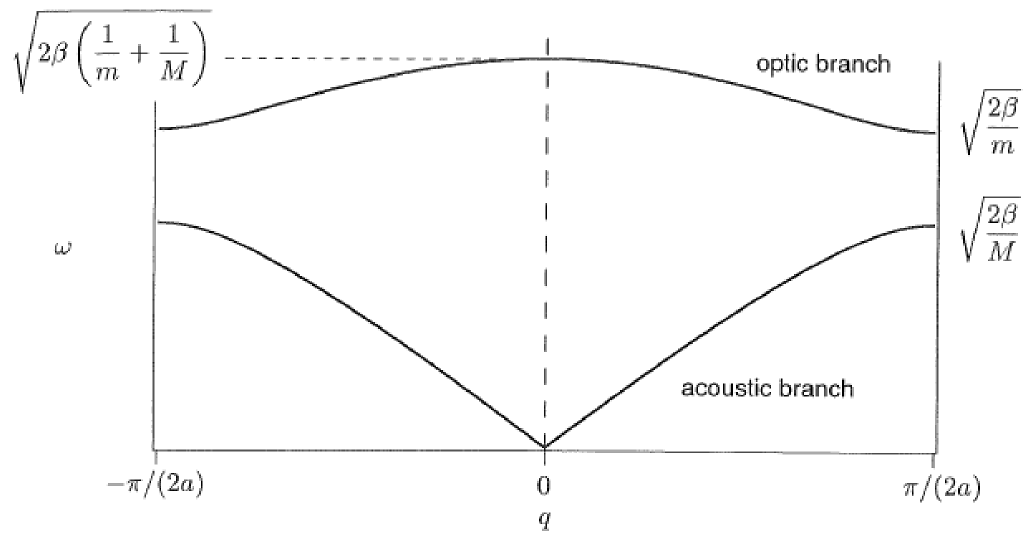
Basic idea: Phonons in a linear chain







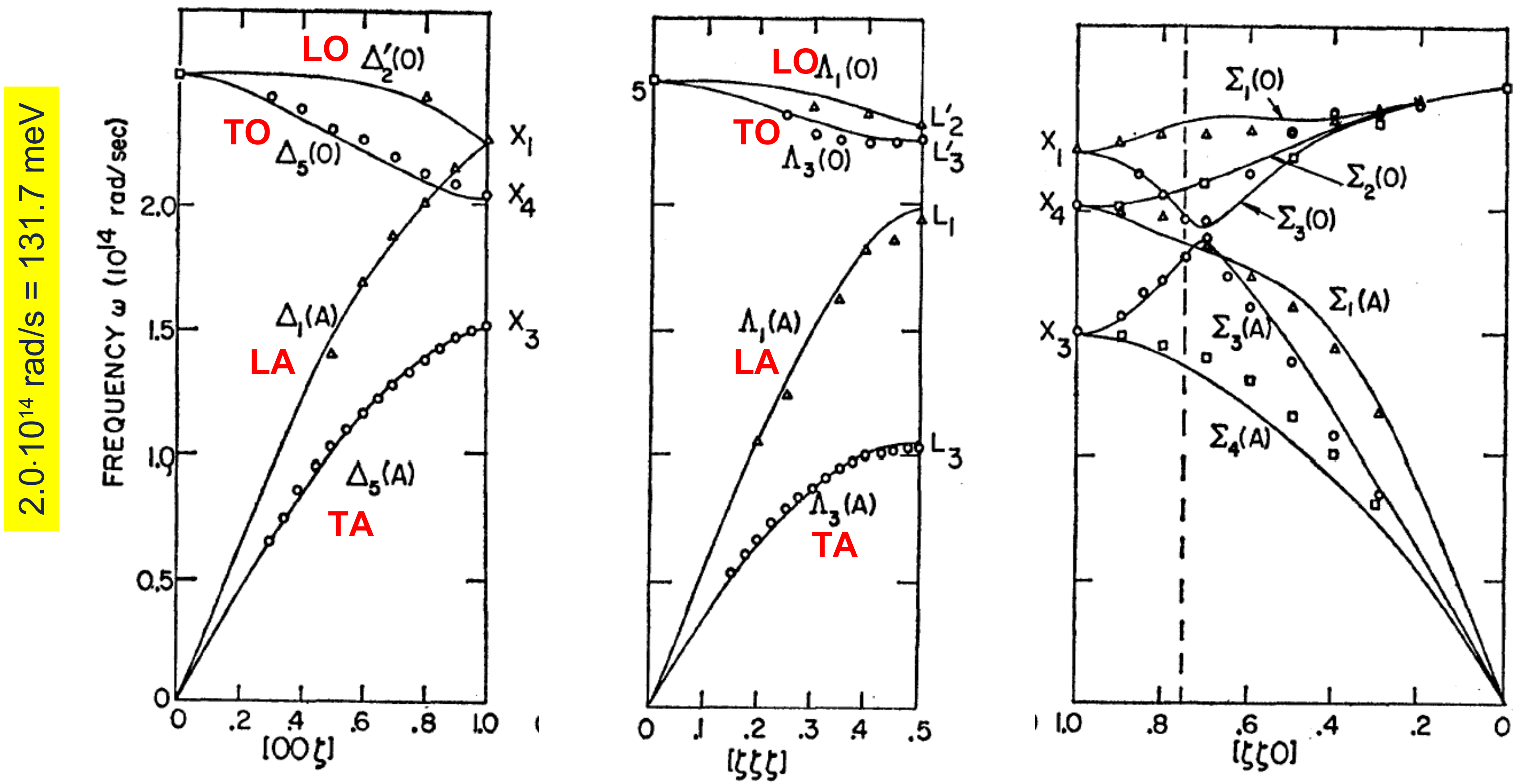
Properties of Phonons



- Collective excitation of atoms
- “Live” in the first Brillouin zone
- Description as dilute, non-interacting phonon gas”
- Quasiparticles (3N phonons for N atoms)
- Follow quasi-continuous dispersion relation
- Obey Bose-Einstein statistics (specific heat!)
- 3P phonon branches (3p-3 optical, 2 transverse acoustic, 1 longitudinal acoustic for P-atomic basis)
- QM picture (raising and lowering operator)

Inelastic scattering: Phonon dispersion

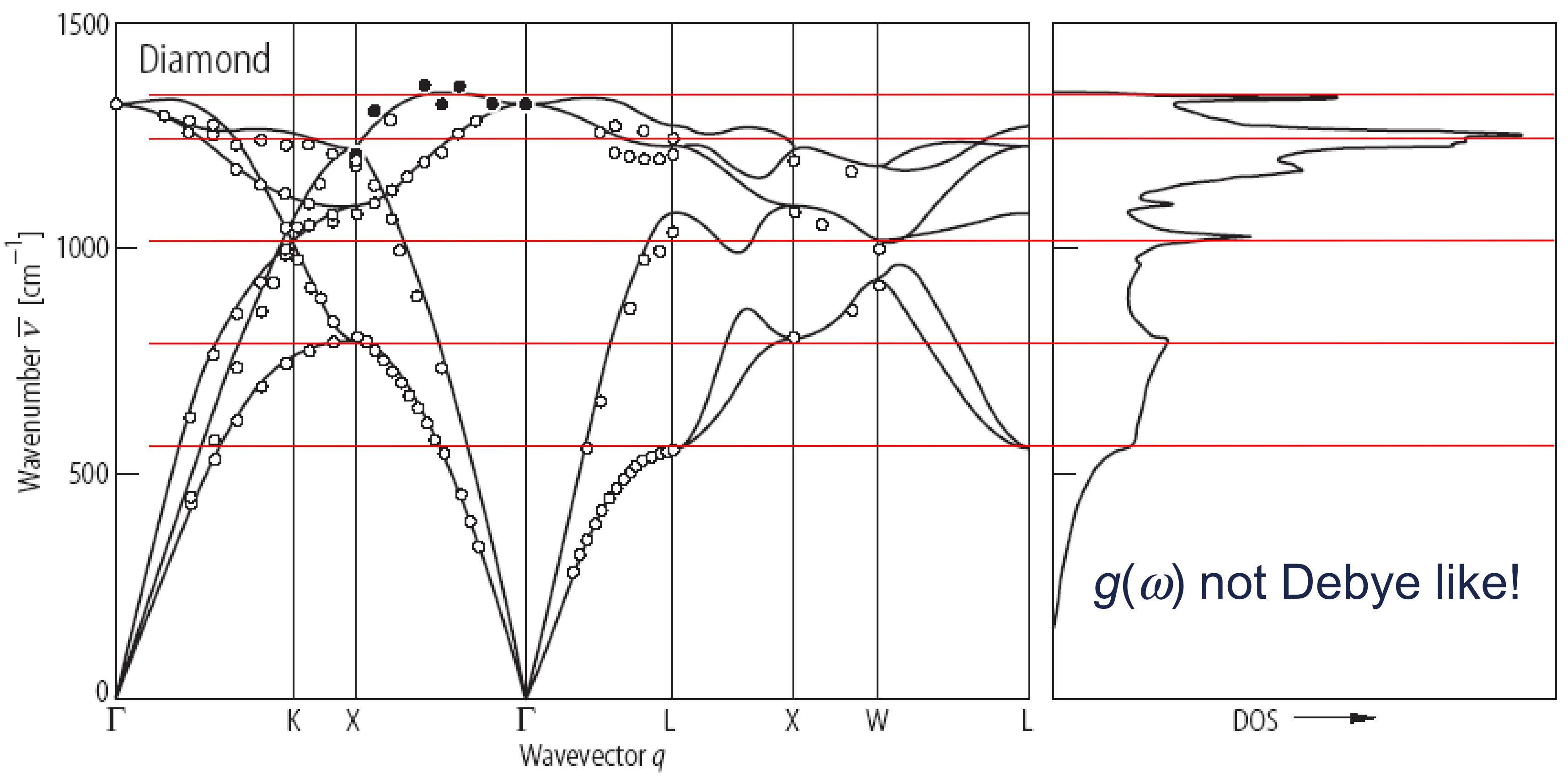
diamond: fcc, basis: (000), (¼ ¼ ¼) , *T* = 296 K, shell model fits



After: J. L. Warren et al., Phys. Rev. **158**, 805 (1967).

For X-ray data see: E. Burkel, Inelastic Scattering of X-Rays with Very High Energy Resolution, Springer Berlin (1991)

Reminder: Phonon DOS, specific specific heat, Debye approximation



Van Hove singularities are kinks or discontinuities in the density of states due to flat portions of the dispersion curves.

Inelastic scattering: Cross-section for phonon emission/absorption

Time dependendent position operator $\hat{\boldsymbol{R}}_j(t) = \boldsymbol{l}_j + \hat{\boldsymbol{u}}_j(t)$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} e^{\imath\boldsymbol{Q}\cdot(\boldsymbol{l}_j-\boldsymbol{l}_{j'})}\int_{-\infty}^{\infty}\langle e^{-\imath\boldsymbol{Q}\cdot\hat{\boldsymbol{u}}_{j'}(0)} e^{\imath\boldsymbol{Q}\cdot\hat{\boldsymbol{u}}_j(t)}\rangle e^{-\imath\omega t}\mathrm{d}t.$$

Displacement expressed in terms of normal mode (QM harmonic oscillator)

$$\hat{\boldsymbol{u}}_j(t) = \sqrt{\frac{\hbar}{2MN}}\sum_{s,\boldsymbol{q}}\frac{\boldsymbol{e}_s(\boldsymbol{q})}{\sqrt{\omega_s(\boldsymbol{q})}}\left(\hat{a}_s(\boldsymbol{q})e^{\imath[\boldsymbol{q}\cdot\boldsymbol{l}_j-\omega_s(\boldsymbol{q})t]} + \hat{a}_s^+(\boldsymbol{q})e^{-\imath[\boldsymbol{q}\cdot\boldsymbol{l}_j-\omega_s(\boldsymbol{q})t]}\right)$$

Ladder operators of QM oscillator

$$\hat{a}_s^+(\boldsymbol{q})|\lambda_n\rangle = \sqrt{n+1}|\lambda_{n+1}\rangle,$$

$$\hat{a}_s(\boldsymbol{q})|\lambda_n\rangle = \sqrt{n}|\lambda_{n-1}\rangle,$$

$$\langle\lambda_n|\hat{a}_s(\boldsymbol{q})\hat{a}_s^+(\boldsymbol{q})|\lambda_n\rangle = n_s(\boldsymbol{q}) + 1$$

$$\langle\lambda_n|\hat{a}_s^+(\boldsymbol{q})\hat{a}_s(\boldsymbol{q})|\lambda_n\rangle = n_s(\boldsymbol{q}),$$

Bose-Einstein statistics of phonons

$$n_s(\boldsymbol{q}) = \left(\exp\left(\frac{\hbar\omega_s(\boldsymbol{q})}{k_B T}\right) - 1\right)^{-1}$$

Inelastic scattering: Cross-section for phonon emission/absporption

Abbreviaton of the exponents

$$\hat{A} = -\imath \boldsymbol{Q} \cdot \hat{\boldsymbol{u}}_{j'}(0) = -\imath \sum_{s,\boldsymbol{q}} \left(\alpha_s(\boldsymbol{q}) \hat{a}_s(\boldsymbol{q}) + \alpha_s^*(\boldsymbol{q}) \hat{a}_s^+(\boldsymbol{q}) \right) \qquad \alpha_s(\boldsymbol{q}) = \sqrt{\frac{\hbar}{2MN}} \sum_{s,\boldsymbol{q}} \frac{\boldsymbol{Q} \cdot \boldsymbol{e}_s(\boldsymbol{q})}{\sqrt{\omega_s(\boldsymbol{q})}} e^{\imath \boldsymbol{q} \cdot \boldsymbol{l}_{j'}},$$

$$\hat{B} = \imath \boldsymbol{Q} \cdot \hat{\boldsymbol{u}}_j(t) = \imath \sum_{s,\boldsymbol{q}} \left(\beta_s(\boldsymbol{q}) \hat{a}_s(\boldsymbol{q}) + \beta_s^*(\boldsymbol{q}) \hat{a}_s^+(\boldsymbol{q}) \right), \qquad \beta_s(\boldsymbol{q}) = \sqrt{\frac{\hbar}{2MN}} \sum_{s,\boldsymbol{q}} \frac{\boldsymbol{Q} \cdot \boldsymbol{e}_s(\boldsymbol{q})}{\sqrt{\omega_s(\boldsymbol{q})}} e^{\imath [\boldsymbol{q} \cdot \boldsymbol{l}_j - \omega_s(\boldsymbol{q}) t]}$$

Taylor expansion of the time evolution

$$e^{\langle \hat{A}\hat{B} \rangle} = \underline{1} + \underline{\langle \hat{A}\hat{B} \rangle} + \frac{1}{2} \langle \hat{A}\hat{B} \rangle^2 + \cdots + \frac{1}{n!} \langle \hat{A}\hat{B} \rangle^n + \ldots$$

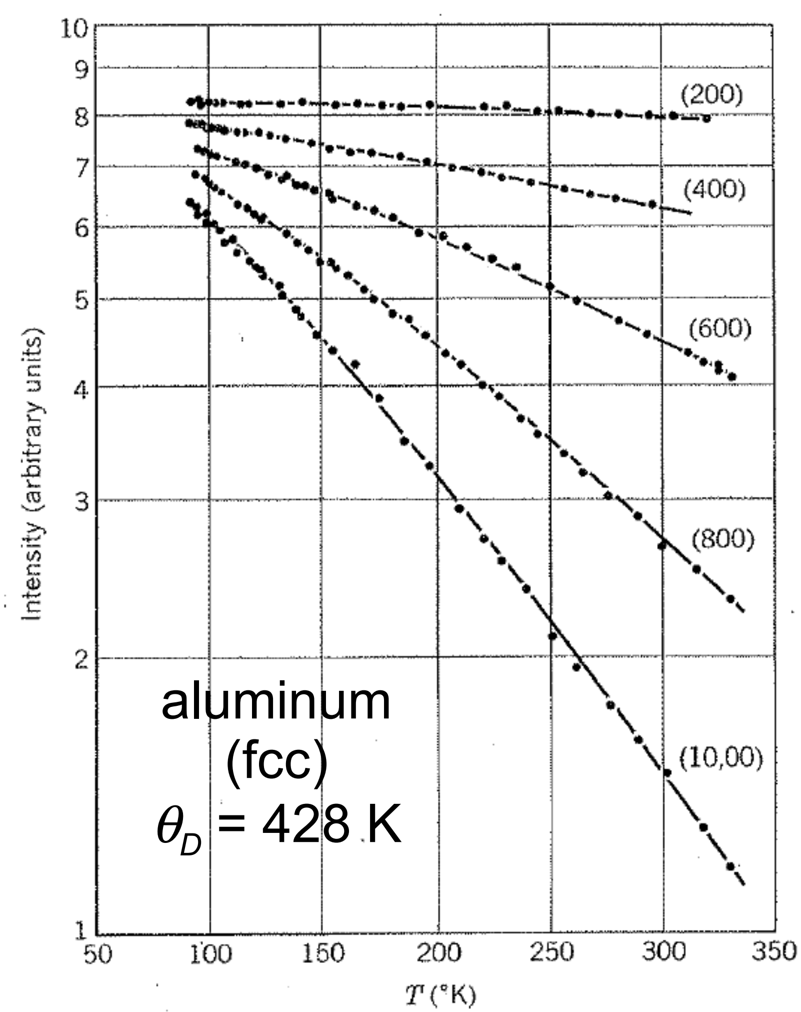
Elastic scattering (+ Debye Waller factor)

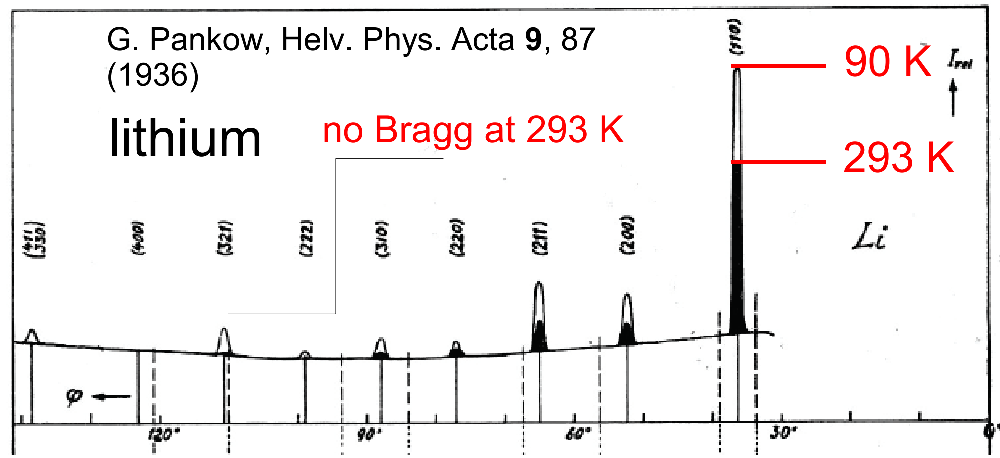
Single phonon processes

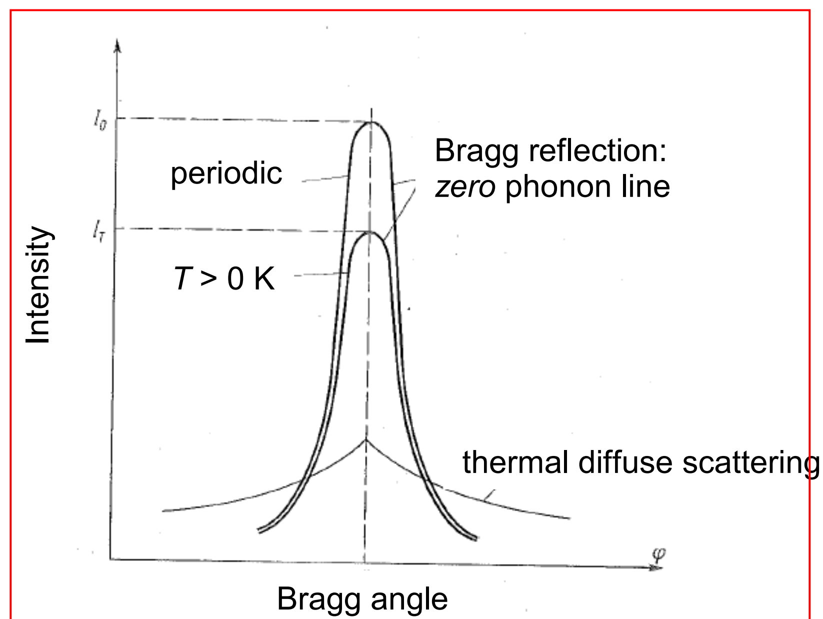
Write linear term in term of sample properties (QM harmonic oscillator!)

$$\langle \lambda_n | \hat{A}\hat{B} | \lambda_n \rangle = \langle \lambda_n | \sum_{s,\boldsymbol{q}} [\alpha_s(\boldsymbol{q}) \beta_s^*(\boldsymbol{q}) \hat{a}_s(\boldsymbol{q}) \hat{a}_s^+(\boldsymbol{q}) + \alpha_s^*(\boldsymbol{q}) \beta_s(\boldsymbol{q}) \hat{a}_s^+(\boldsymbol{q}) \hat{a}_s(\boldsymbol{q})] | \lambda_n \rangle$$

Inelastic scattering: Debye Waller factor: Aluminium/Lithium







Reminder: Inelastic scattering

Master formula for coherent inelastic scattering

Consider only coherent scattering (j≠j')

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{1}{4\pi M} \cdot \frac{k'}{k} \langle b \rangle^2 e^{-2W(\boldsymbol{Q})} \sum_{s,\boldsymbol{q}} \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s(\boldsymbol{q}))^2}{\omega_s(\boldsymbol{q})}$$

$$\times \left[(n_s(\boldsymbol{q})+1) \sum_{\boldsymbol{l}} e^{\imath(\boldsymbol{Q}-\boldsymbol{q})\cdot\boldsymbol{l}} \int_{-\infty}^{\infty} \mathrm{d}t e^{\imath(\omega_s(\boldsymbol{q})-\omega)t} \right.$$

$$\left. + n_s(\boldsymbol{q}) \sum_{\boldsymbol{l}} e^{\imath(\boldsymbol{Q}+\boldsymbol{q})\cdot\boldsymbol{l}} \int_{-\infty}^{\infty} \mathrm{d}t e^{-\imath(\omega_s(\boldsymbol{q})+\omega)t} \right] .$$

Convert integrals to delta functions using lattice sums (as for diffraction)

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{4\pi^3}{v_0 M} \cdot \frac{k'}{k} \langle b \rangle^2 e^{-2W(\boldsymbol{Q})} \sum_{s,\boldsymbol{q}} \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s(\boldsymbol{q}))^2}{\omega_s(\boldsymbol{q})}$$

$$\times \left[(n_s(\boldsymbol{q})+1)\delta(\omega-\omega_s(\boldsymbol{q})) \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{Q}-\boldsymbol{q}-\boldsymbol{\tau}) \right.$$

Phonon emission

$$\left. + n_s(\boldsymbol{q})\delta(\omega+\omega_s(\boldsymbol{q})) \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{Q}+\boldsymbol{q}-\boldsymbol{\tau}) \right] .$$

Phonon absorption

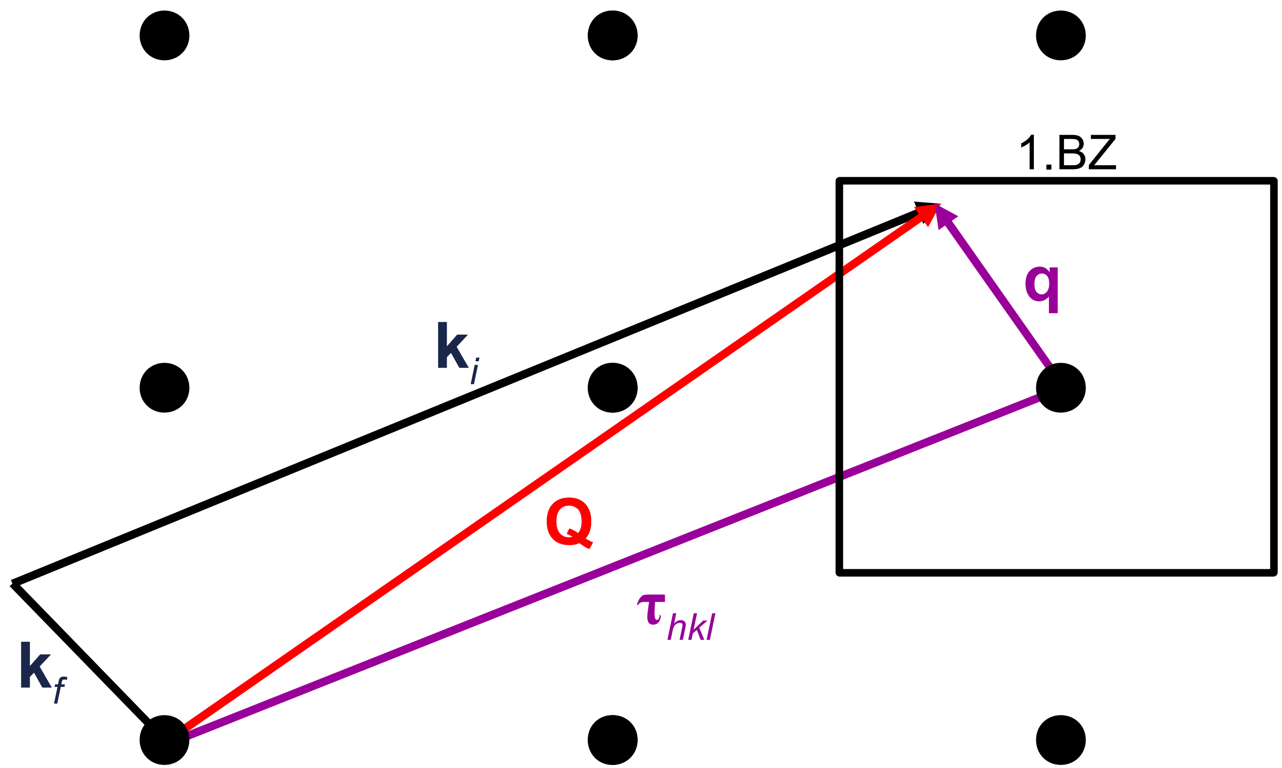
5 Inelastic scattering: Scattering „triangle“ for inelastic scattering

Example:

phonon creation

$$\omega = \omega_s(\mathbf{q})$$

$$\Rightarrow \; k_i^2 > k_f^2$$



Inelastic incoherent scattering: Phonon DOS

Now consider incoherent scattering (j=j')

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}e^{-2W(\boldsymbol{Q})}\sum_j b_j^2 \int_{-\infty}^{\infty} e^{\langle\hat{A}\hat{B}\rangle} e^{-\imath\omega t}\mathrm{d}t.$$

Similar to the coherent part, only consider the linear term in the Taylor expansion

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{1}{2M}\frac{k'}{k}\left(\langle b^2\rangle - \langle b\rangle^2\right)e^{-2W(\boldsymbol{Q})}\sum_{s,\boldsymbol{q}}\frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s(\boldsymbol{q}))^2}{\omega_s(\boldsymbol{q})}$$
$$\times\left[\underbrace{(n_s(\boldsymbol{q})+1)\delta\left(\omega-\omega_s(\boldsymbol{q})\right)}_{\text{Phonon emission}} + \underbrace{n_s(\boldsymbol{q})\delta\left(\omega+\omega_s(\boldsymbol{q})\right)}_{\text{Phonon absorption}}\right]$$

Phonon
emission

Phonon
absorption

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Compare to coherent part:

Energy conservation is fulfilled
No momentum conservation is fulfilled

All phonons with energy ω_s contribute!

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{4M}\frac{k'}{k}\left(\langle b^2\rangle - \langle b\rangle^2\right) e^{-W(\boldsymbol{Q})} \times \langle(\boldsymbol{Q}\cdot e_s(\boldsymbol{q}))^2\rangle \cdot \frac{g(\omega)}{\omega}\cdot\left[\coth\frac{\hbar\omega}{2k_BT} \pm 1\right]$$

With phonon DOS $g(\omega)$ $$\int_0^\infty g(\omega)d\omega = 3N$$

Inelastic incoherent scattering: Phonon DOS

For a (cubic) Bravais lattice only

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{1}{12M}\frac{k'}{k}\left(\langle b^2\rangle - \langle b\rangle^2\right)e^{-W(\boldsymbol{Q})}Q^2 \times \frac{g(\omega)}{\omega}\cdot\left[\coth\frac{\hbar\omega}{2k_BT}\pm 1\right].$$

➡ Inelastic incoherent scattering directly measures phonon DOS g(ω)