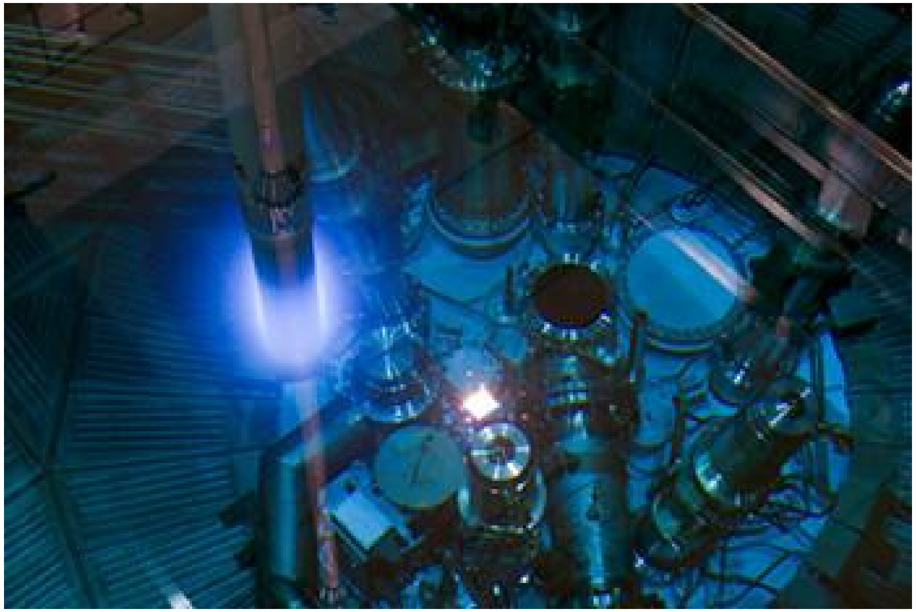
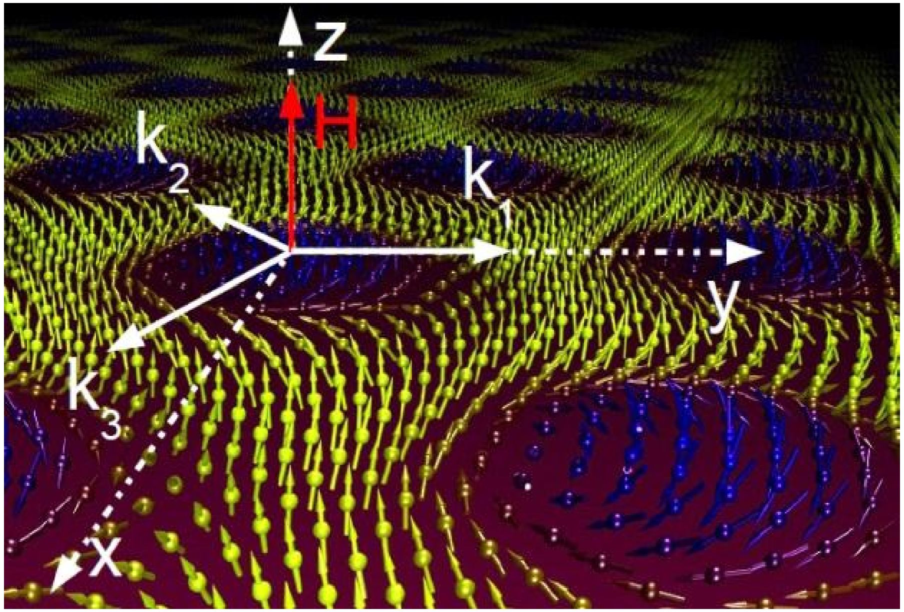
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons I, WS 2015/2016





Lecture 10, 21.12.2015

MLZ is a cooperation between:

JÜLICH
FORSCHUNGSZENTRUM

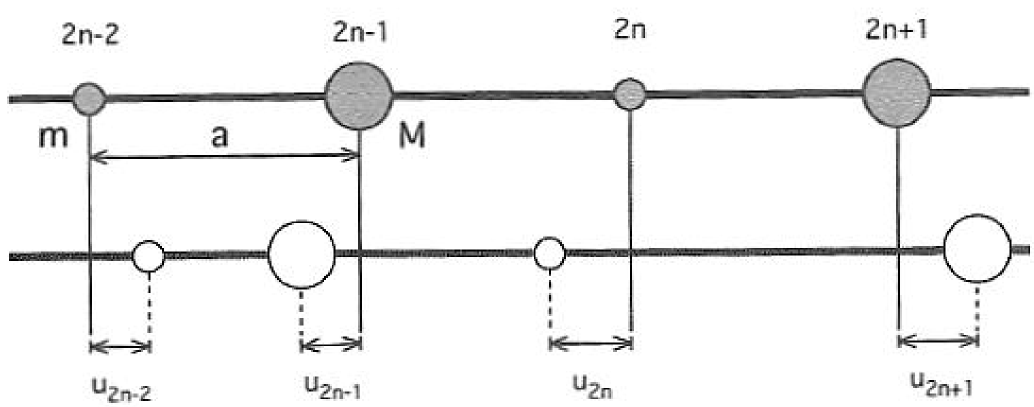
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

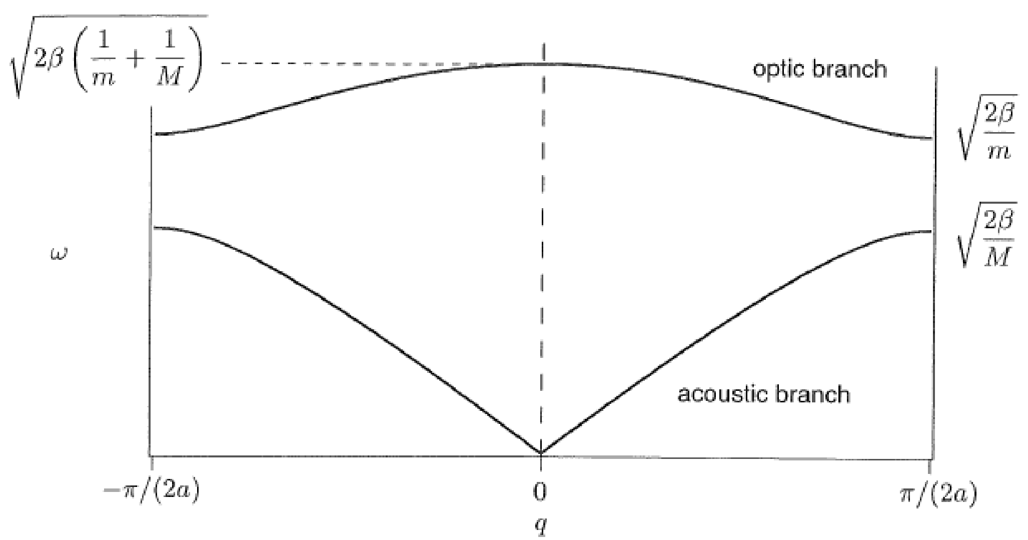
TUM
Technische Universität München

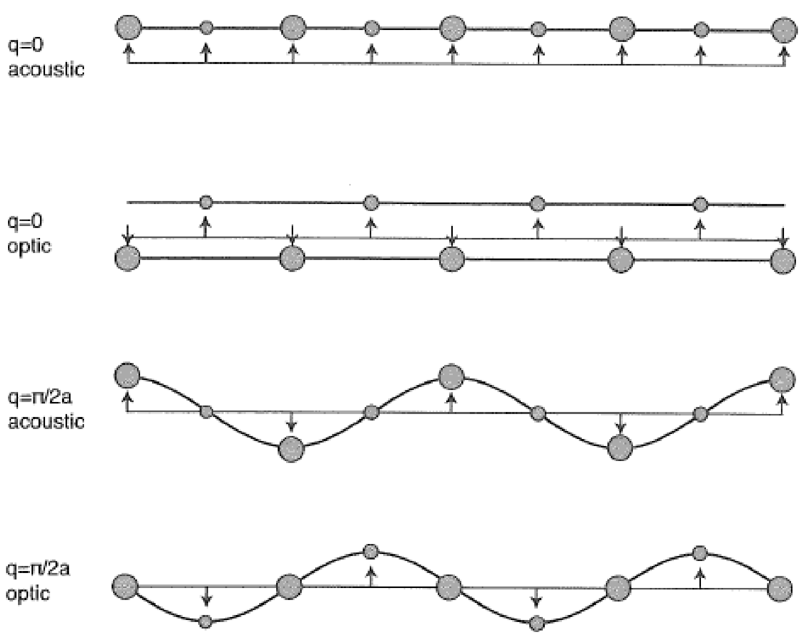
Exam (after winter term)

- Registration: via TUM-Online between 16.11.2015 – 15.1.2015
- Email: sebastian.muehlbauer@frm2.tum.de for date arrangement
- 30min oral exam

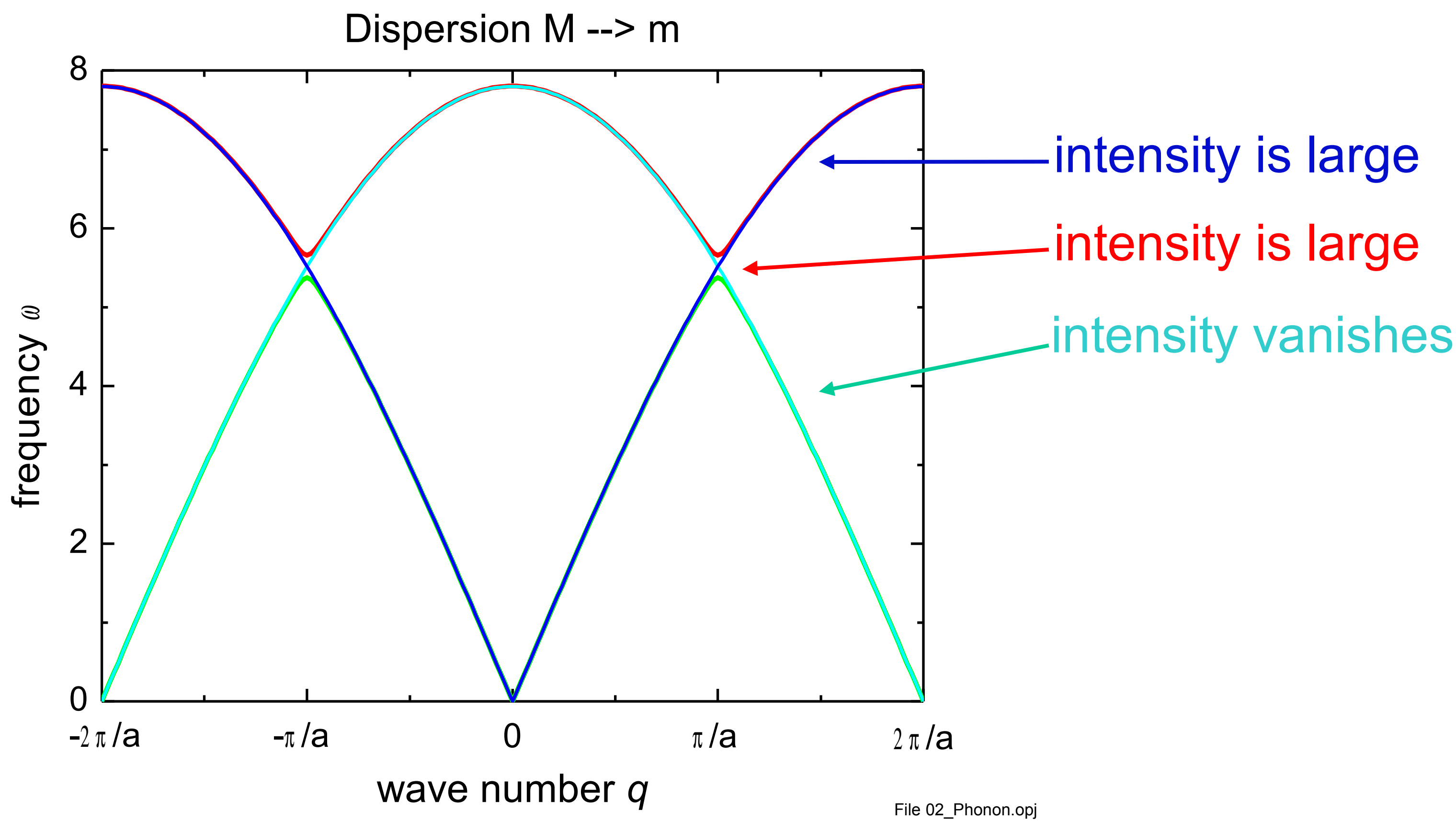
5 Reminder: Phonons, linear chain





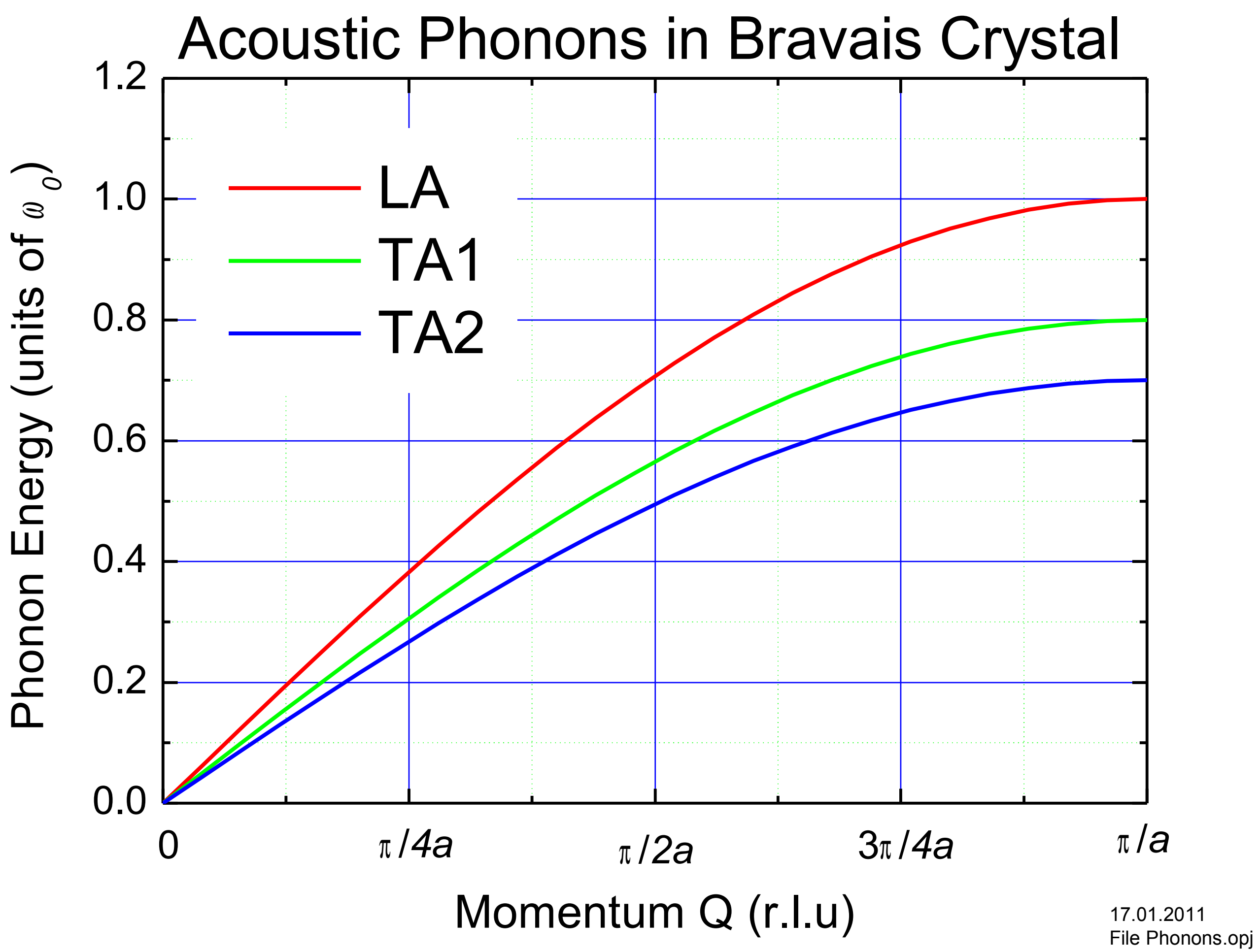


5 Reminder: Phonon dispersion for m->M



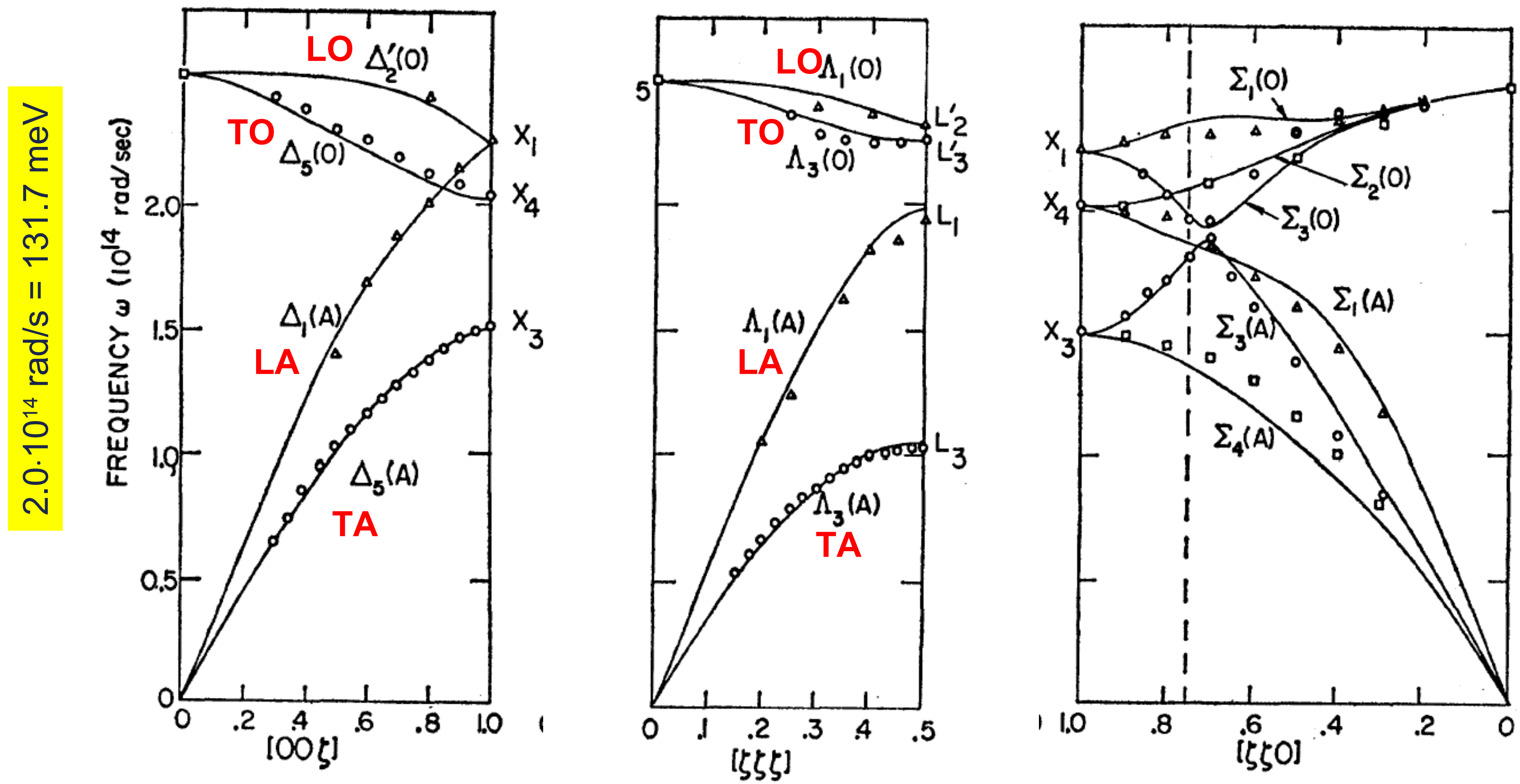
- lattice constant for crystal with $m \neq M$: a
- lattice constant for crystal with $m = M$: ½a (gap vanishes)

5 Reminder: Longitudinal and transverse phonons



5 Inelastic scattering: Phonon dispersion diamond

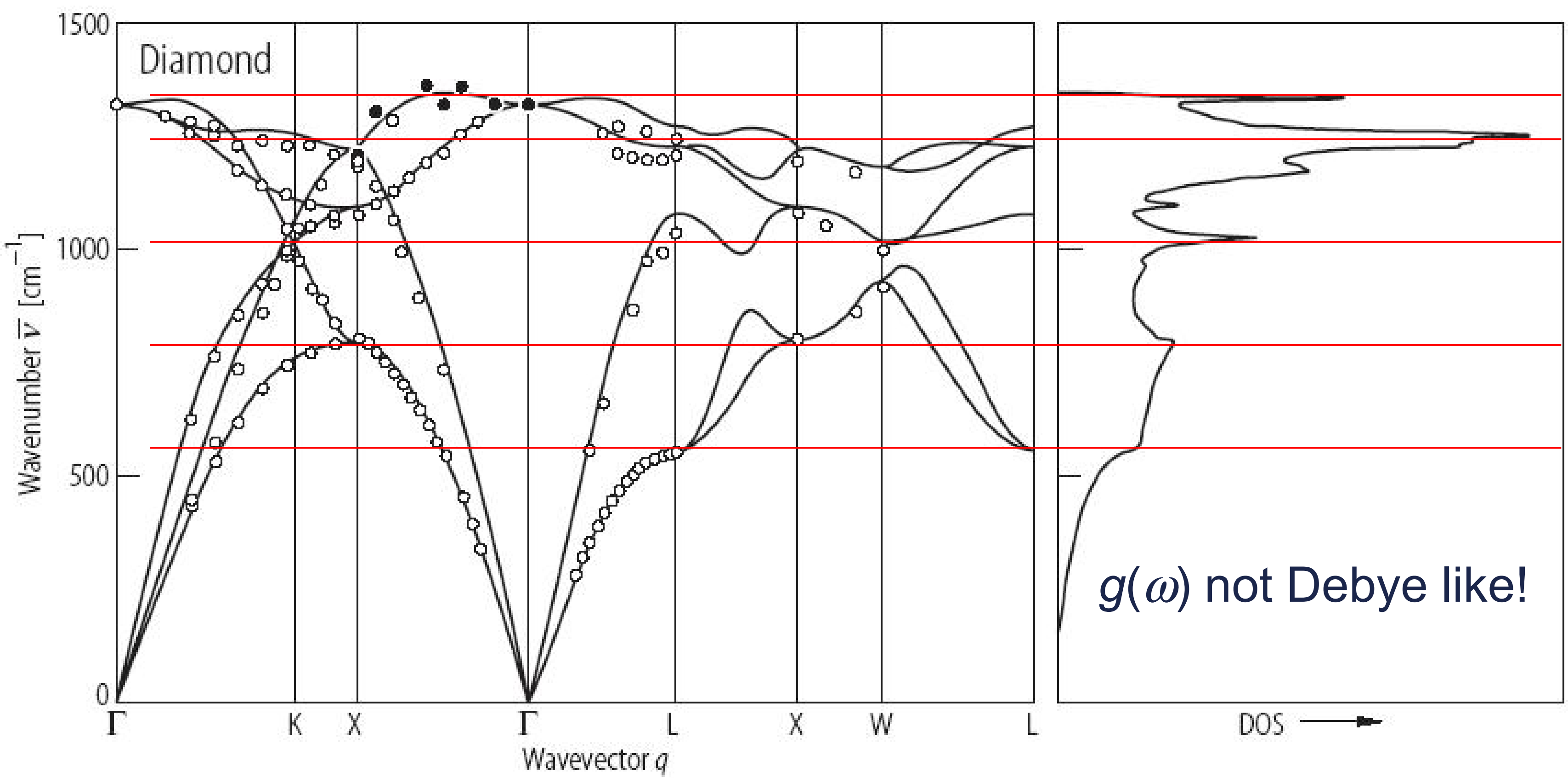
diamond: fcc, basis: (000), (¼ ¼ ¼) , *T* = 296 K, shell model fits



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

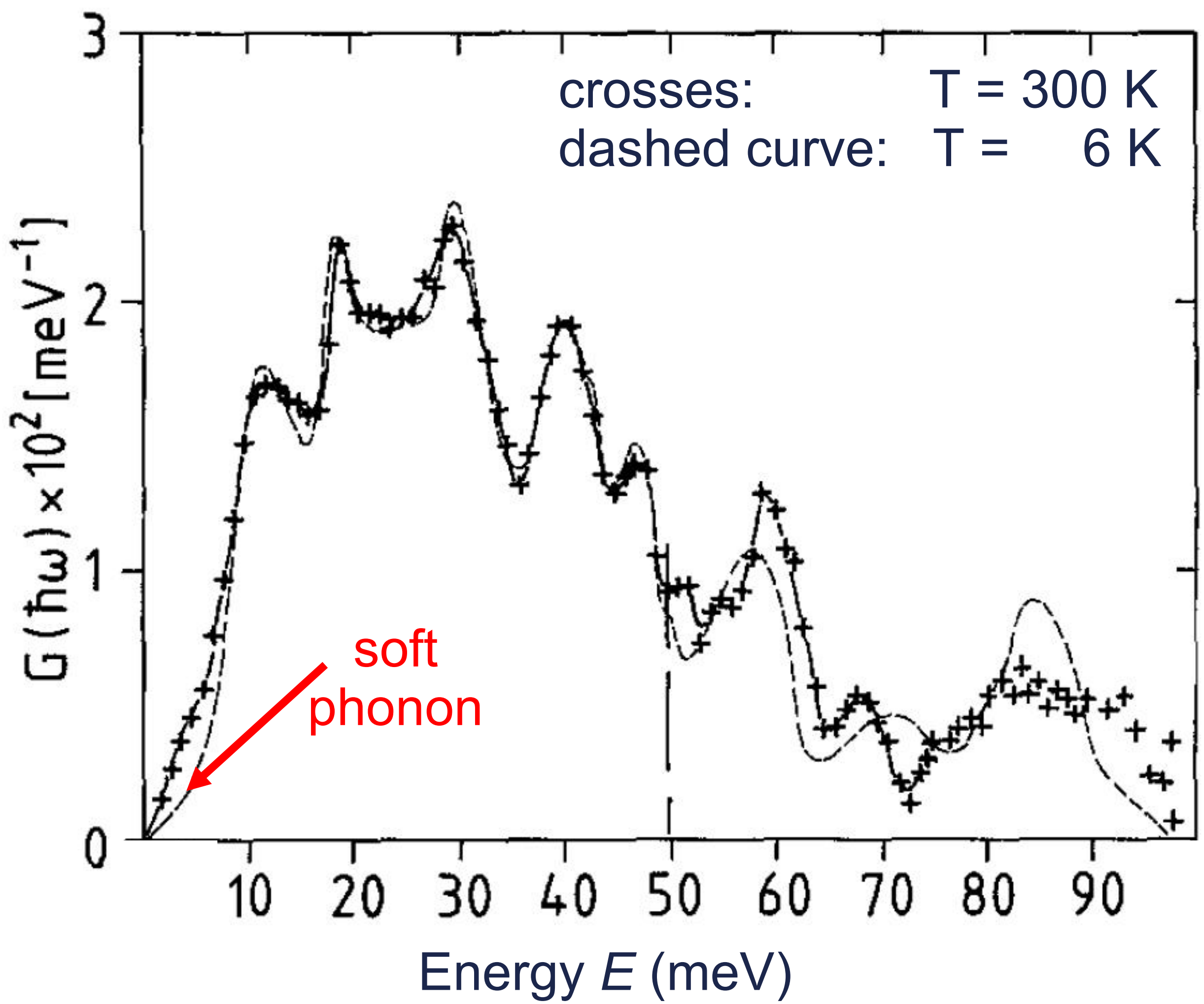
For X-ray data see: E. Burkel, Inelastic Scattering of X-Rays with Very High Energy Resolution, Springer Berlin (1991)

5 Reminder: Phonon DOS, specific specific heat, Debye approximation



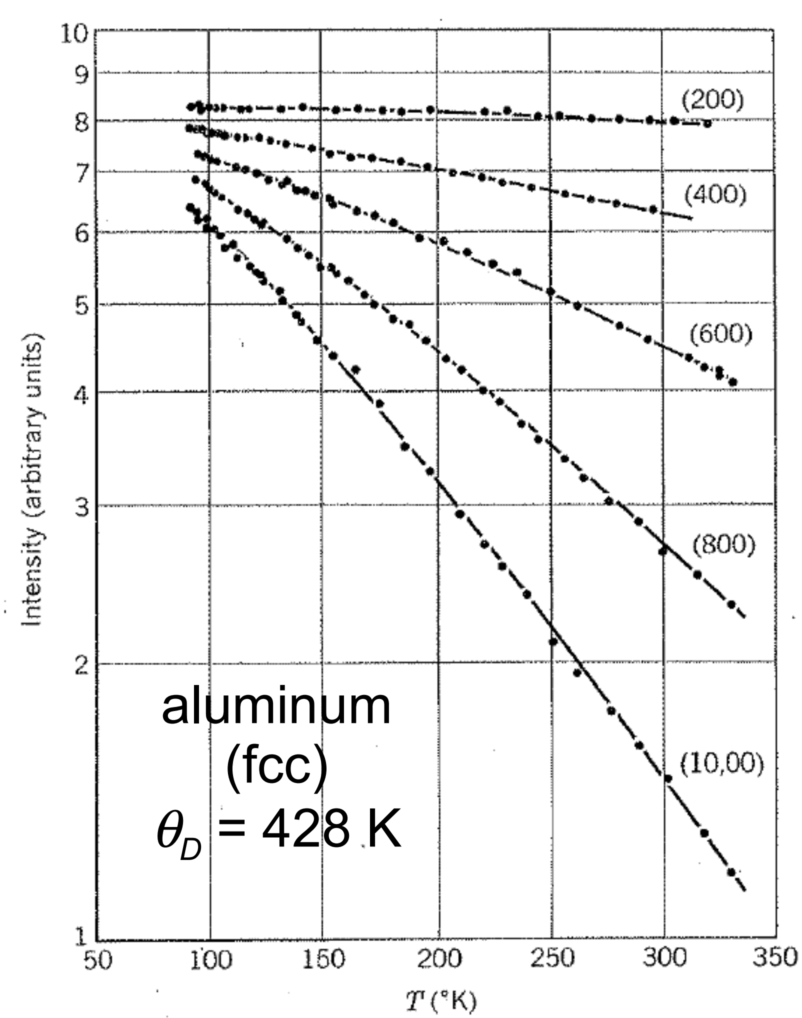
Van Hove singularities are kinks or discontinuities in the density of states due to flat portions of the dispersion curves.

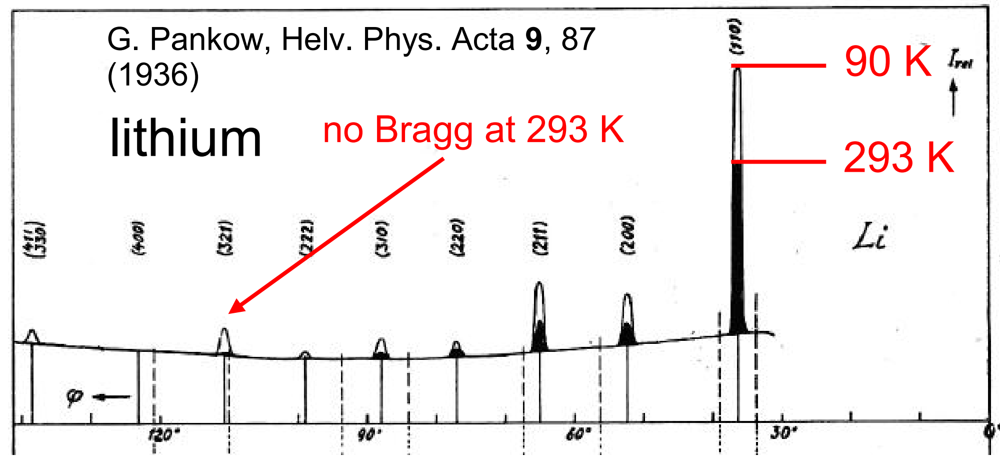
5 Reminder: Phonon DOS, specific specific heat, Debye approximation

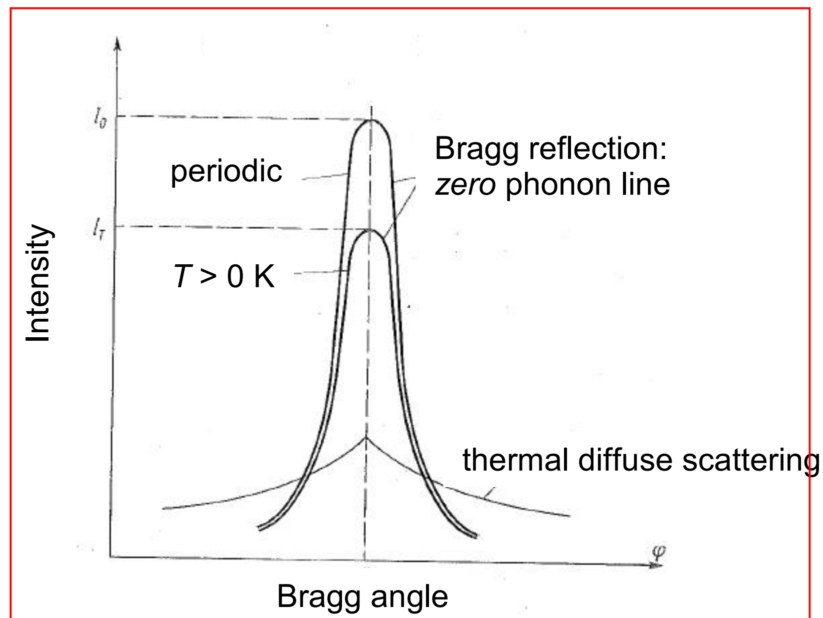


after: B. Renker et al., Z. Phys. B – Condensed Matter **67**, 15 (1987).

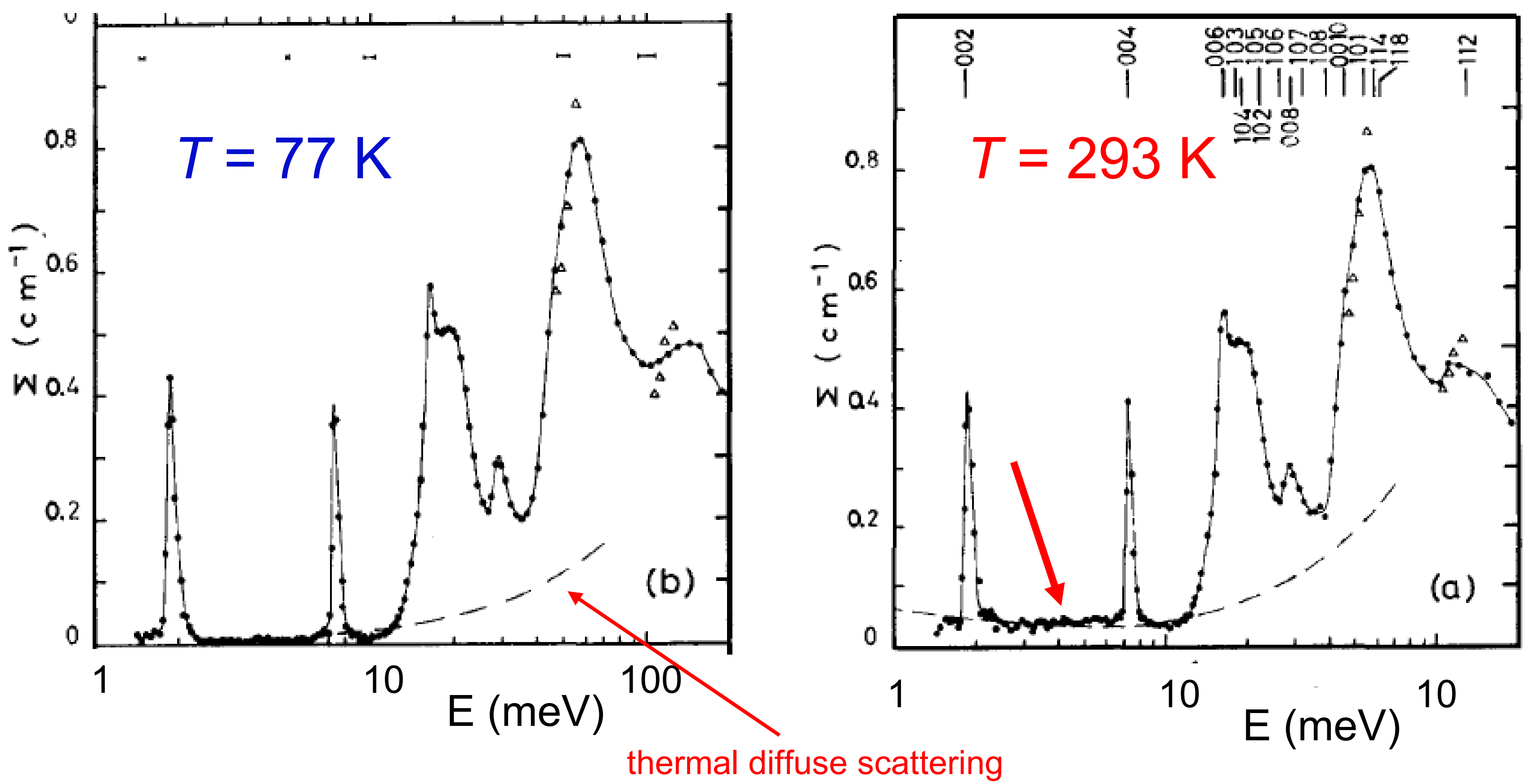
5 Inelastic scattering: Debye Waller factor: Aluminium/Lithium







5 Inelastic scattering: Thermal diffuse scattering of pyrolytic graphite



J. Bergsma and C. Van Dijk, Nucl. Instrum. Methods **51**, 121 (1967).

5 Inelastic scattering: Cross-section for phonon emission/absportion

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

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

5 Inelastic scattering: Cross-section for phonon emission/absportion

Abbreviaton of the exponents

$$\hat{A} = -\imath \boldsymbol{Q} \cdot \hat{\boldsymbol{u}}_{j'}(0) = -\imath \sum_{s,\boldsymbol{q}} \left(\alpha_s(\boldsymbol{q})\hat{a}_s(\boldsymbol{q}) + \alpha_s^*(\boldsymbol{q})\hat{a}_s^+(\boldsymbol{q})\right)$$

$$\alpha_s(\boldsymbol{q}) = \sqrt{\frac{\hbar}{2MN}} \sum_{s,\boldsymbol{q}} \frac{\boldsymbol{Q} \cdot \boldsymbol{e}_s(\boldsymbol{q})}{\sqrt{\omega_s(\boldsymbol{q})}} e^{\imath \boldsymbol{q} \cdot \boldsymbol{l}_{j'}},$$

$$\hat{B} = \imath \boldsymbol{Q} \cdot \hat{\boldsymbol{u}}_j(t) = \imath \sum_{s,\boldsymbol{q}} \left(\beta_s(\boldsymbol{q})\hat{a}_s(\boldsymbol{q}) + \beta_s^*(\boldsymbol{q})\hat{a}_s^+(\boldsymbol{q})\right),$$

$$\beta_s(\boldsymbol{q}) = \sqrt{\frac{\hbar}{2MN}} \sum_{s,\boldsymbol{q}} \frac{\boldsymbol{Q} \cdot \boldsymbol{e}_s(\boldsymbol{q})}{\sqrt{\omega_s(\boldsymbol{q})}} e^{\imath[\boldsymbol{q} \cdot \boldsymbol{l}_j - \omega_s(\boldsymbol{q})t]}$$

Taylor expansion of the time evolution

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

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

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

5 Inelastic scattering: Cross-section for phonon emission/absportion

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)

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

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

Phonon emission

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

Phonon absorption

5 Inelastic scattering: Scattering „triangle“ for inelastic scattering

Example:
phonon creation

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

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