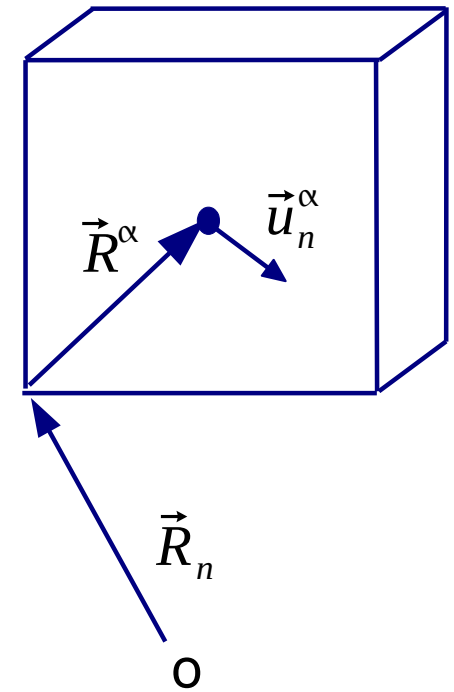


Phonons in a 3D Lattice

Potential: $\Phi = \Phi(\dots, \vec{R}_\alpha^n + \vec{u}_\alpha^n, \dots)$

$$= \Phi(\dots, \vec{R}_\alpha^n, \dots) + \frac{1}{2} \sum_{ij\alpha\beta nm} \frac{\partial^2 \Phi}{\partial R_{\alpha i}^n \partial R_{\beta j}^m} \cdot u_{\alpha i}^n u_{\beta j}^m + \dots$$

$$M_\alpha \ddot{u}_{\alpha i}^n = \sum_{m\beta j} \Phi_{\alpha i \beta j}^{n m} \cdot u_{\beta j}^m \quad \Phi_{\alpha i \beta j}^{n m} = \frac{\partial^2 \Phi}{\partial R_{\alpha i}^n \partial R_{\beta j}^m}$$



Coupling constants: Force constant at atom n, α in i -direction for displacement of atom m, β in j -direction

$$\Phi_{\alpha \beta}^{n m} = \Phi_{\alpha \beta}^{n-m \ 0} \quad \text{Translational invariance}$$

$$\sum_{m\beta j} \Phi_{\alpha \beta}^{n m} = 0 \quad \text{no force, if } u_{\beta j}^m = d \text{ for all } m, \beta, j, \text{ i. e. rigid shift of crystal}$$

3D-Equation of Motion

(i, j hidden in arrow)

$$M_{\alpha} \ddot{\vec{u}}_{\alpha}^n + \sum_{m\beta} \Phi_{\alpha\beta}^{nm} \vec{u}_{\beta}^m = 0$$

plane wave
solutions:

$$\vec{u}_{\alpha}^n = \frac{1}{\sqrt{M_{\alpha}}} \vec{u}_{\alpha}(\vec{k}) \exp\left(i(\vec{k} \cdot \vec{R}_{\alpha}^n - \omega t)\right)$$

↑ independent of n

$$-\omega^2 \vec{u}_{\alpha} + \sum_{\beta} D_{\alpha\beta} \vec{u}_{\beta} = 0$$

Dynamical matrix

$$D_{\alpha\beta} = \sum_m \frac{1}{\sqrt{M_{\alpha} M_{\beta}}} \Phi_{\alpha\beta}^{n0} \exp(i\vec{k} \cdot \vec{R}_m)$$

$$(\mathbf{D} - \omega^2 \mathbf{1}) \vec{u} = 0$$

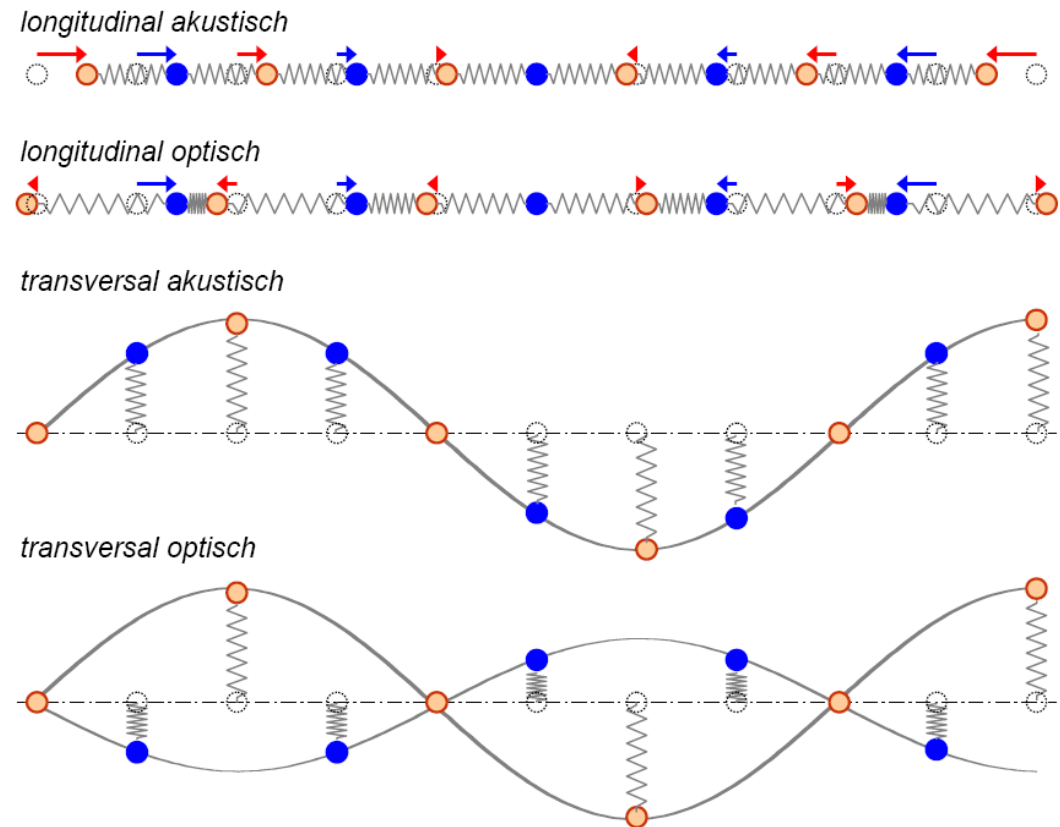
\mathbf{u} has $3r$ components

$D_{\alpha\beta}$: Force on atom α in ref. unit cell,

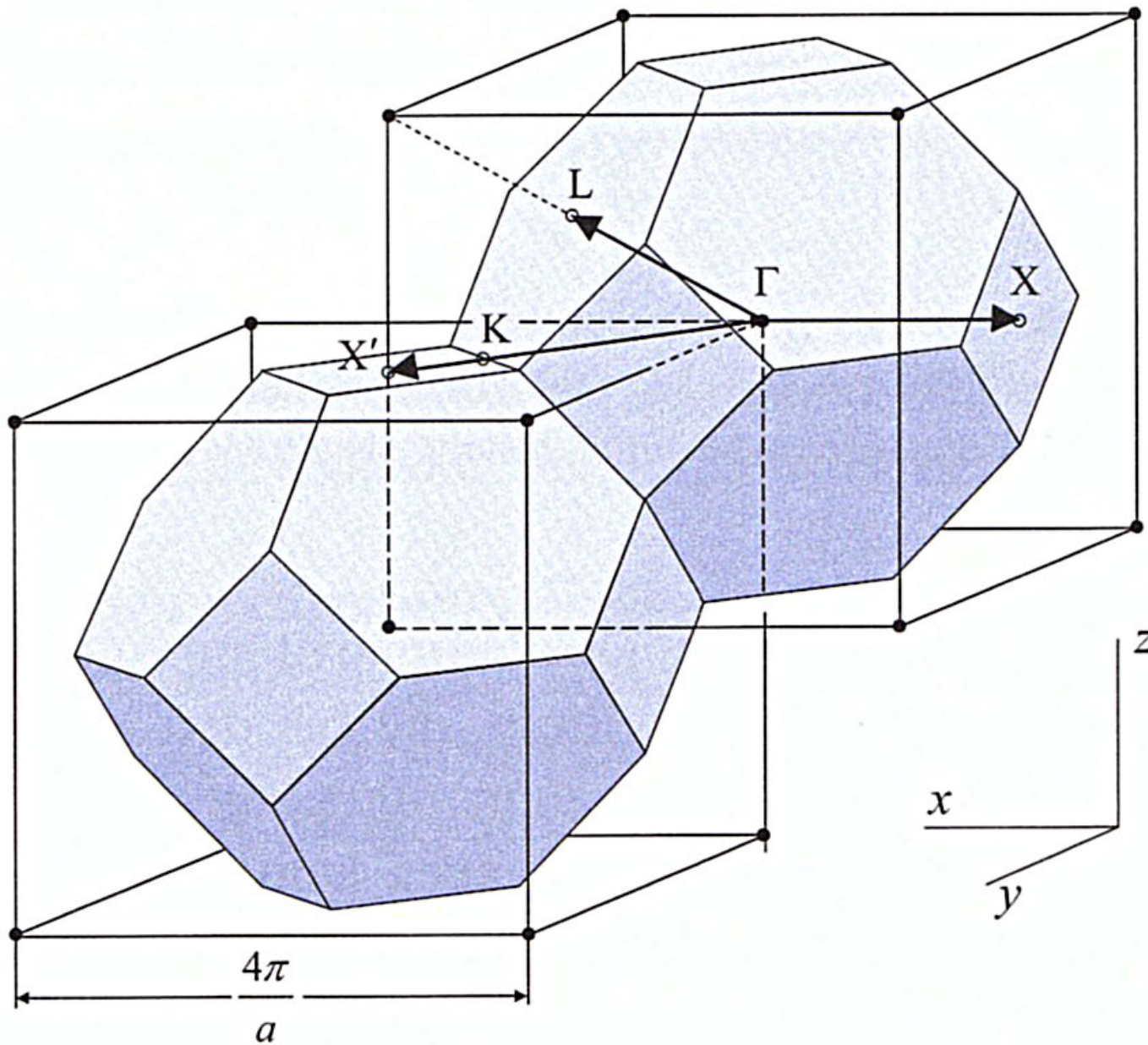
resulting from phase-shifted elongations of atoms β in cells m ²

- Matrix **D** is symmetric
- Eigenvalues yield $\omega(\mathbf{k})$
- Eigenvectors describe displacements (polarisation vectors)
uncoupled, normal modes – called Phonons

- 3 acoustic branches
- $3(r-1)$ optical branches
- transverse modes $\vec{u} \perp \vec{k}$
- longitudinal modes $\vec{u} \parallel \vec{k}$



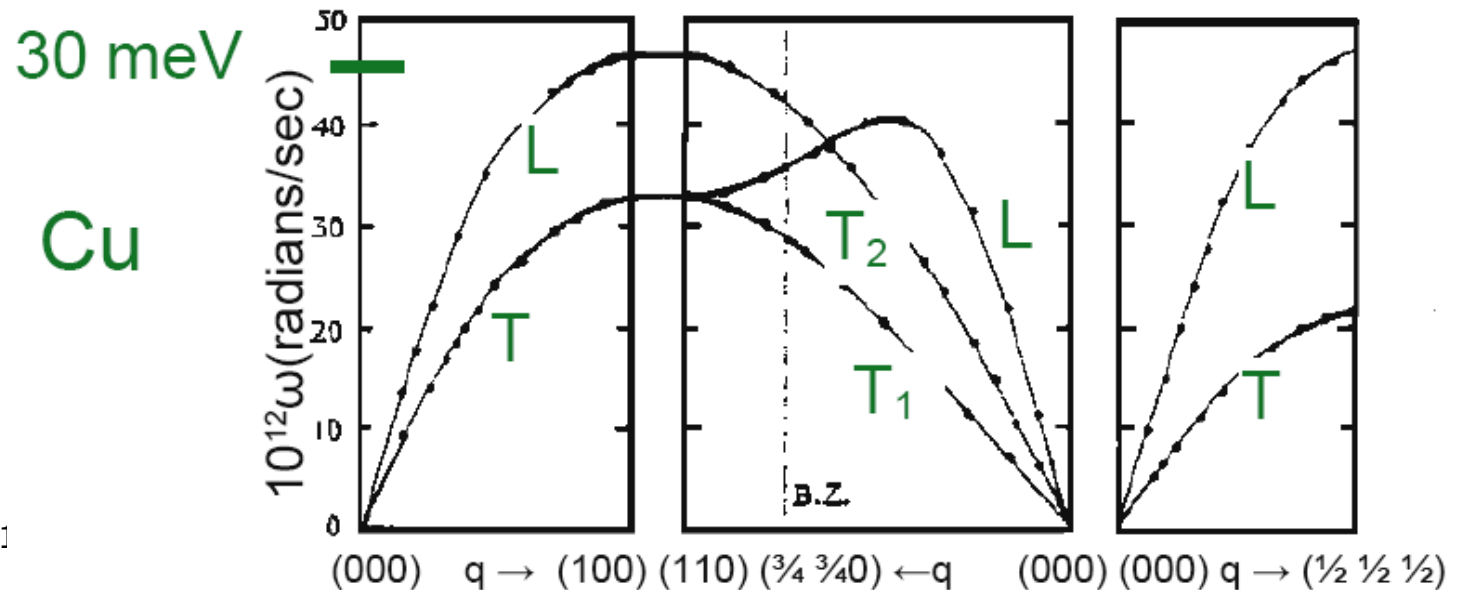
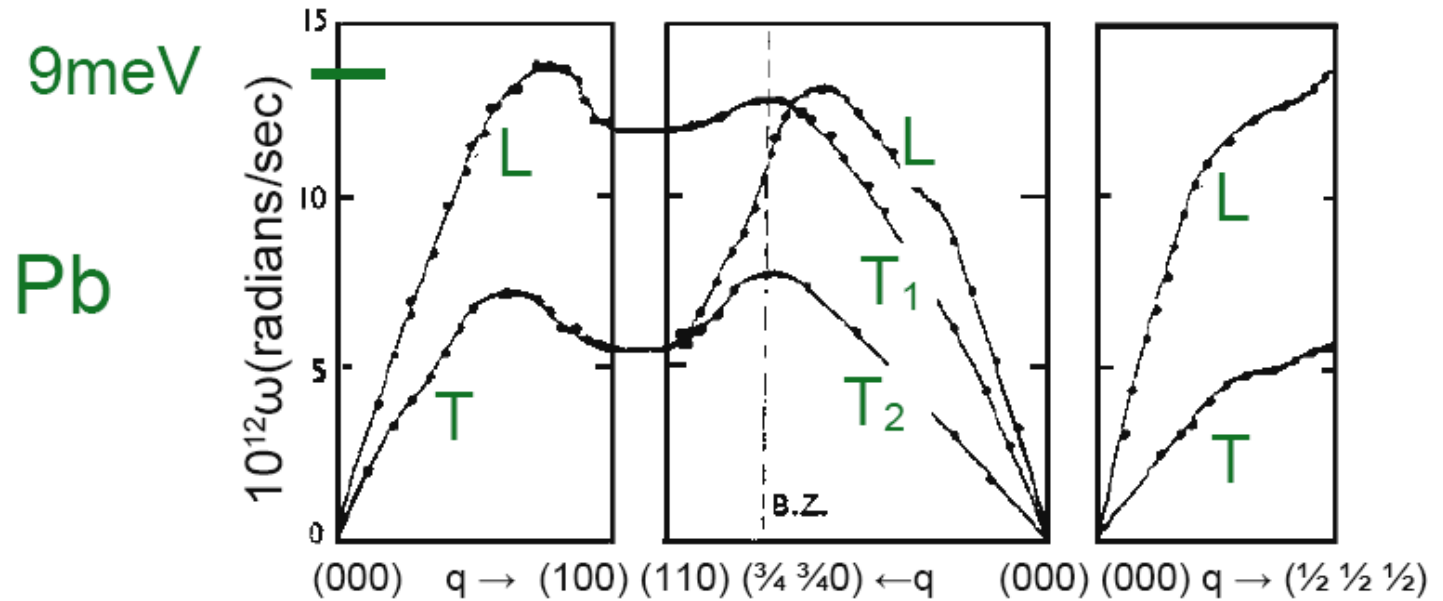
Two neighboring FCC Brillouin zones



Phononen- dispersion

Inelastische Neutronenstreuung

Pb, Cu sind fcc → nur akustische Zweige

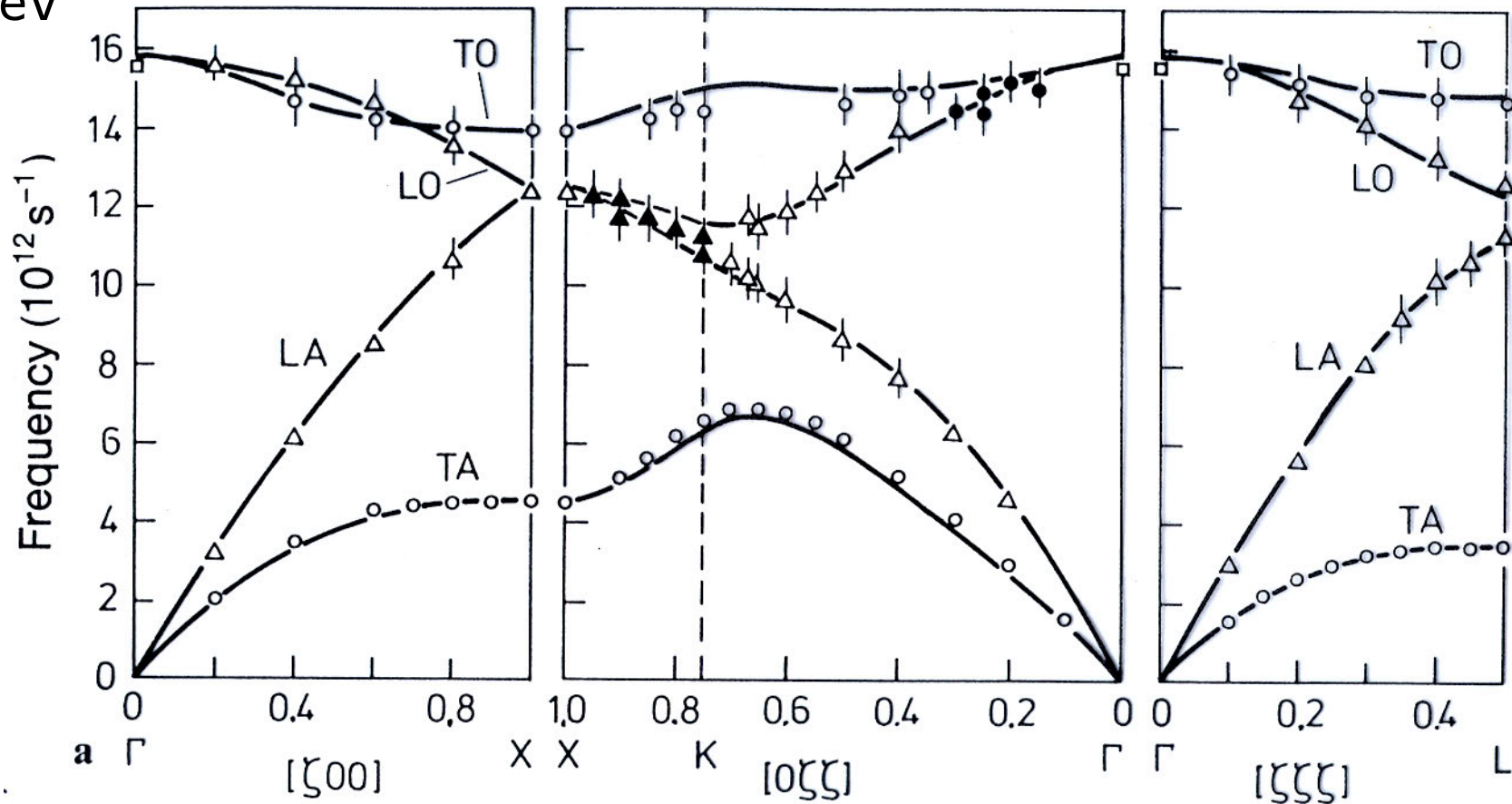


Pb data: Brockhouse et al.,
Phys. Rev. 128, 1099 (1957)

Cu data: Svensson et al.,
Phys. Rev. 155, 619 (1967)

Silizium: optische & akustische Zweige

65 meV



$$\zeta := k \frac{a}{2\pi}$$

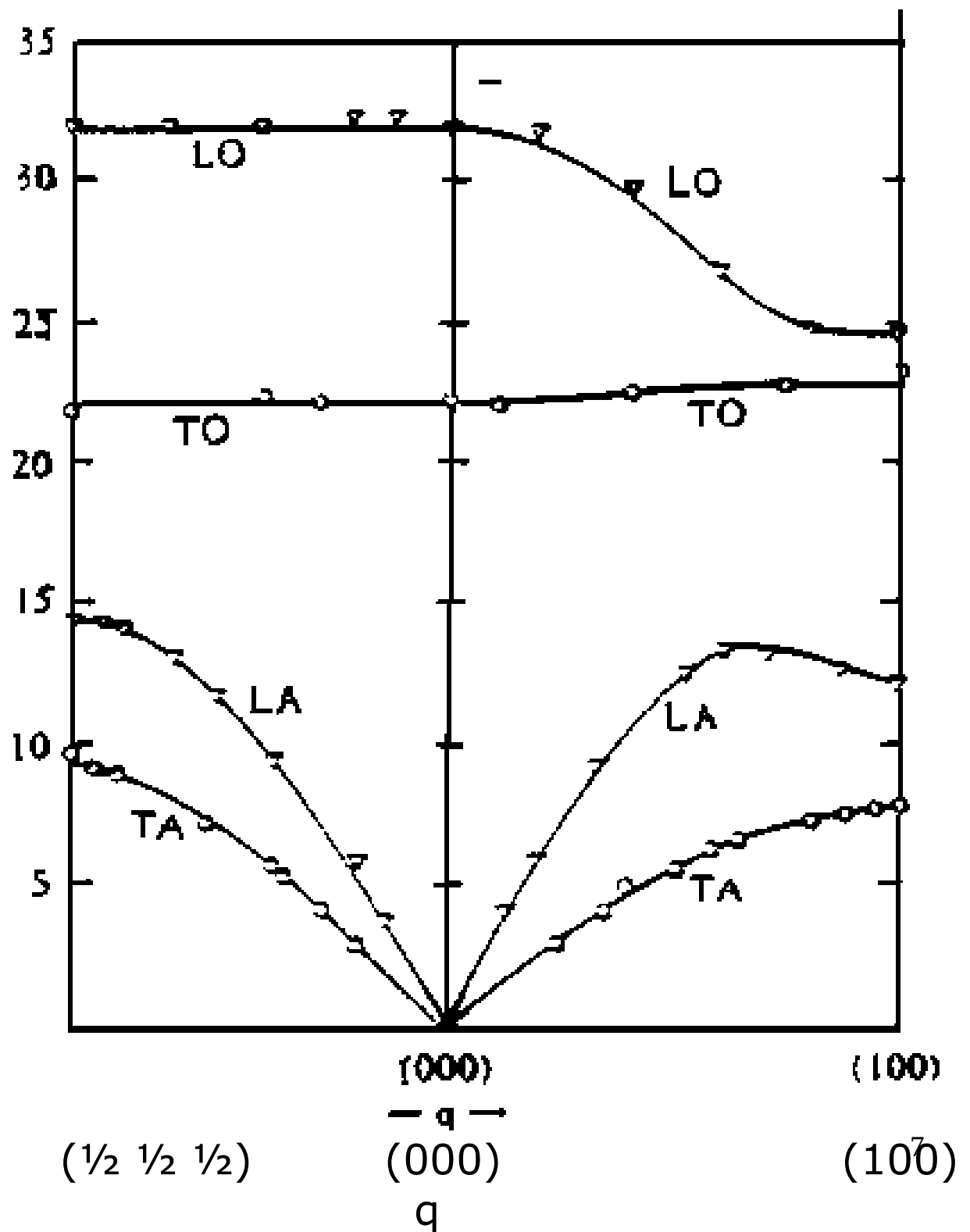
TA entartet in $[100]$, $[111]$

NaJ

J: Z=53

Na: Z=11

$\omega_{\text{Optisch}} \gg \omega_{\text{Akustisch}}$



Longitudinal, **T**ransverse
Optical, **A**coustic

Data taken at 100 K

Woods et al., Phys. Rev. **131**, 1025 (1963)

Quantisierung der Gitterschwingungen

- $3nN$ Gitterschwingungsmoden, charakterisiert durch ω , \mathbf{k} , s
- entkoppelte harmonische Oszillatoren $E_{\vec{k}s} = \left(n_{\vec{k}s} + \frac{1}{2}\right) \hbar \omega_{\vec{k}s}$
- Sprachregelung:

statt 'Oszillator ist n -fach angeregt' sagt man

' n Phononen vom Typ s mit Wellenvektor \mathbf{k} sind vorhanden'

- Warum? Ist das nicht unnötig kompliziert?

Nein, denn in Streuexperimenten verhalten sich Phononen als

Quasiteilchen

- Bsp.: Neutron mit E , \mathbf{p} trifft Probe, anschließend E' , \mathbf{p}' mit

Energieerhaltung

$$E' - E = \sum_{\vec{k}s} \hbar \omega_{\vec{k}s} \Delta n_{\vec{k}s}$$

Erhaltung des 'Kristallimpulses'

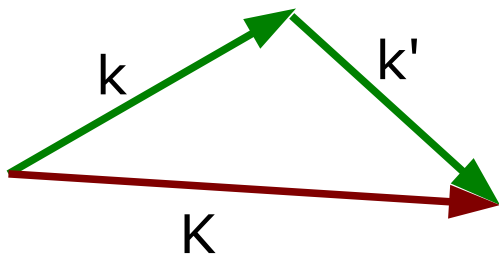
$$\vec{p}' - \vec{p} = - \sum_{\vec{k}s} \hbar \mathbf{k} \Delta n_{\vec{k}s} + \hbar \vec{G}$$

\mathbf{G} ist aus REL 8

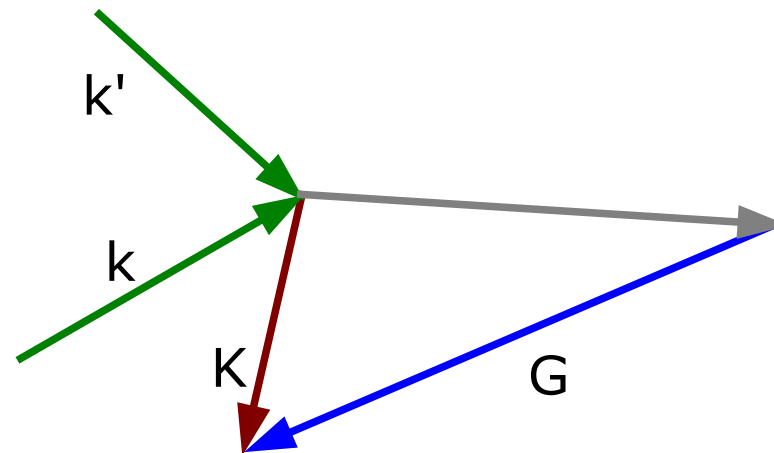
Quasiimpuls / Kristallimpuls

- Phonon existiert im diskreten Raum des Gitters
- Noether Theorem:
 - Symmetrie der Lagrangefunktion \leftrightarrow Erhaltungsgröße
 - ◆ Translationsinvarianz des Raumes \leftrightarrow Impuls
 - ◆ Translationsinvarianz der Zeit \leftrightarrow Energie
 - ◆ Rotationsinvarianz eines Raumes \leftrightarrow Drehimpuls
- Gitter-Translationsinvarianz:

$$\hbar k + \hbar k' = \hbar K + \hbar G; \quad G \in REL$$



n-Prozess



U-Prozess

n.b.
Streuprozess
erfordert
Anharmonizität o.ä.

Neutronenstreuung: E -, k -Bilanzen

0-Phonon-Streuung

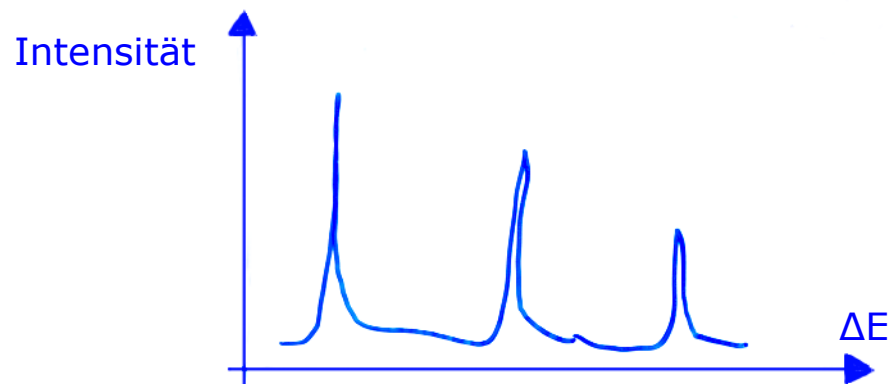
$$E' - E = \sum_{\vec{k}_s} \hbar \omega_{\vec{k}_s} \Delta n_{\vec{k}_s}$$
$$\vec{p}' - \vec{p} = - \sum_{\vec{k}_s} \hbar \vec{k}_s \Delta n_{\vec{k}_s} + \hbar \vec{G}$$
$$\vec{p} = \hbar \vec{k} \quad \vec{p}' = \hbar \vec{k}'$$
$$|k| = |k'|$$
$$\vec{k}' = \vec{k} + \vec{G} \quad \text{Laue-Bedingung}$$

1-Phonon-Streuung

$$\frac{p'^2}{2m} = \frac{p^2}{2m} \pm \hbar \omega_s(\vec{q})$$

$$\vec{p}' = \vec{p} + \hbar \vec{q} + \hbar \vec{G}$$

4 Gleichungen für \mathbf{q} , ω_s erzwingen eindeutige Lösung (bis auf \mathbf{G})
→ 1-Phonon-Prozesse ergeben scharfe Linien



$$\Gamma = \frac{\hbar}{\tau}$$

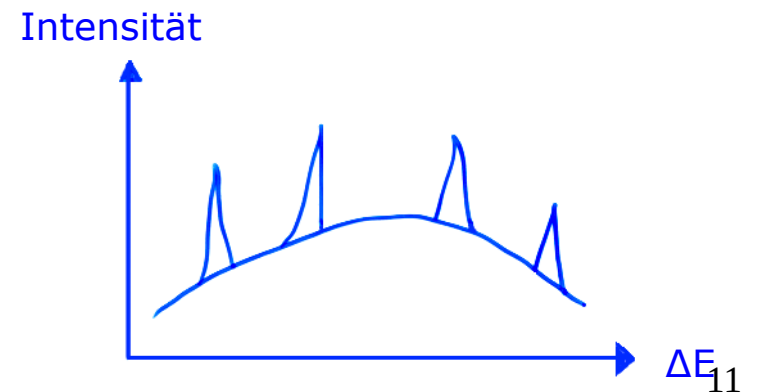
2-Phononen-Streuung

$$E' = E + \hbar\omega_s(\vec{q}) + \hbar\omega_{s'}(\vec{q}')$$

$$\vec{p}' = \vec{p} + \hbar\vec{q} + \hbar\vec{q}' + \hbar\vec{G}$$

2 Phononenimpulse in Impulsbilanz

- beliebig viele Lösungen
- breiter Hintergrund in Energieverteilung der gestreuten Neutronen

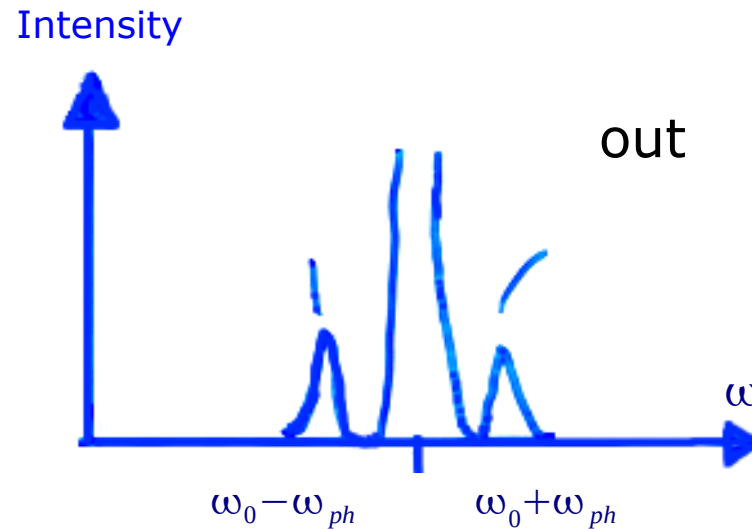
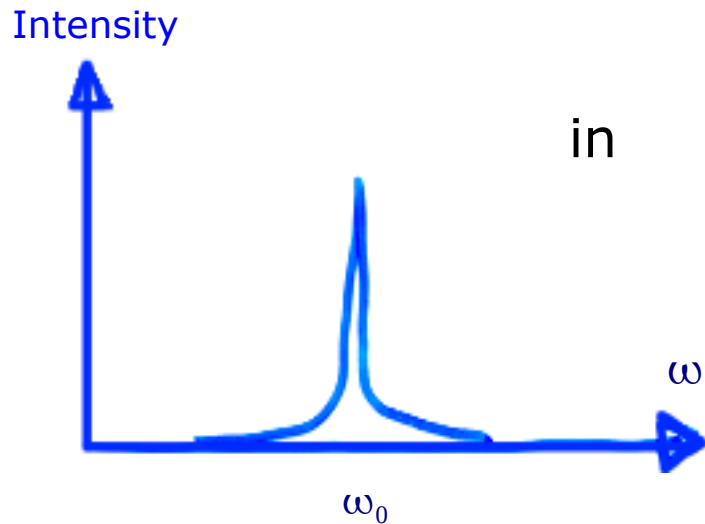


Raman Spectroscopy

Thermal neutrons, phonons: similar energies (meV)
similar momenta ($1/\text{\AA}$)

(This is why neutron-phonon scattering works well)

Photons: momentum much smaller - even in VIS (~ 2 eV) range



Stokes line / anti-Stokes line

$$q = 0$$

Ramanstreuung

Inelastische Lichtstreuung (1. Ordnung) zur Charakterisierung von Elementaranregungen wie Phononen, Magnonen, ...

liefert Energie und Symmetrie einer Anregung

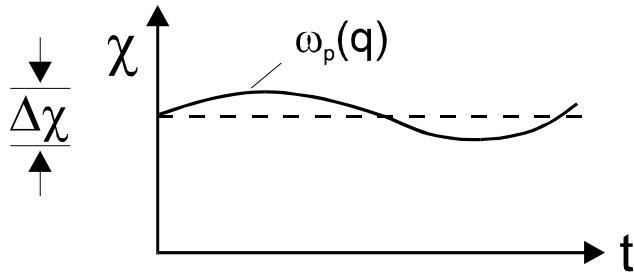
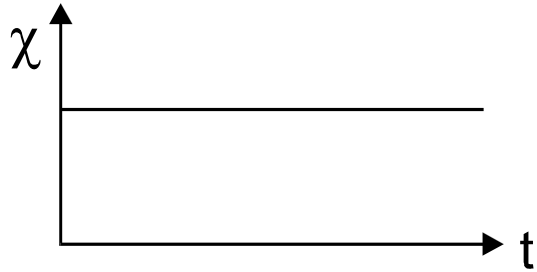
elektronische Polarisation: $\vec{\mathbf{P}} = \frac{\sum_i p_i}{V} = \chi \vec{\mathbf{E}}$

einfallende Welle \rightarrow oszillierende Polarisation

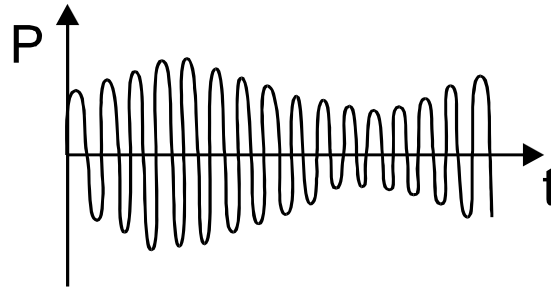
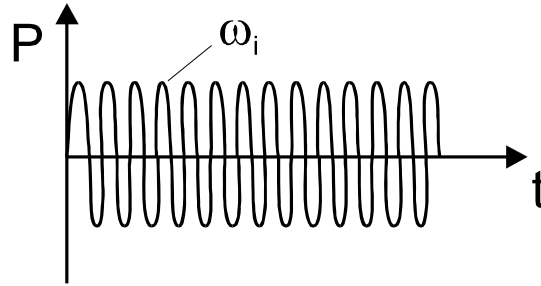
\rightarrow Abstrahlung einer Streuwelle $I \propto |\ddot{\mathbf{P}}|^2$

atomare Auslenkungen $u = u_0 \cos(\omega_p t)$ modulieren Suszeptibilität χ

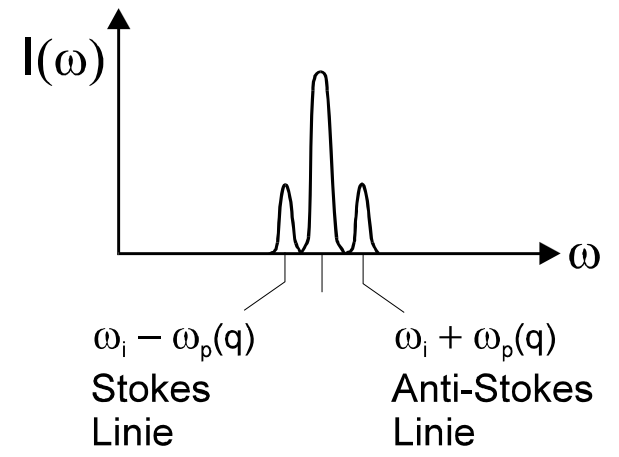
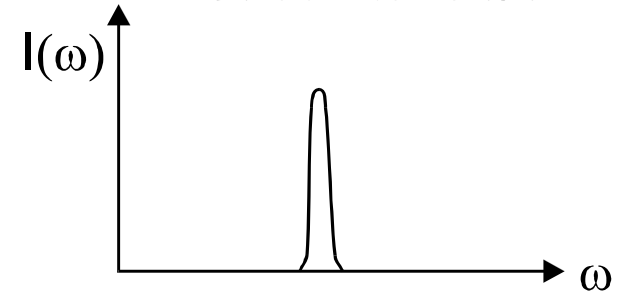
Suszeptibilität



Polarisation

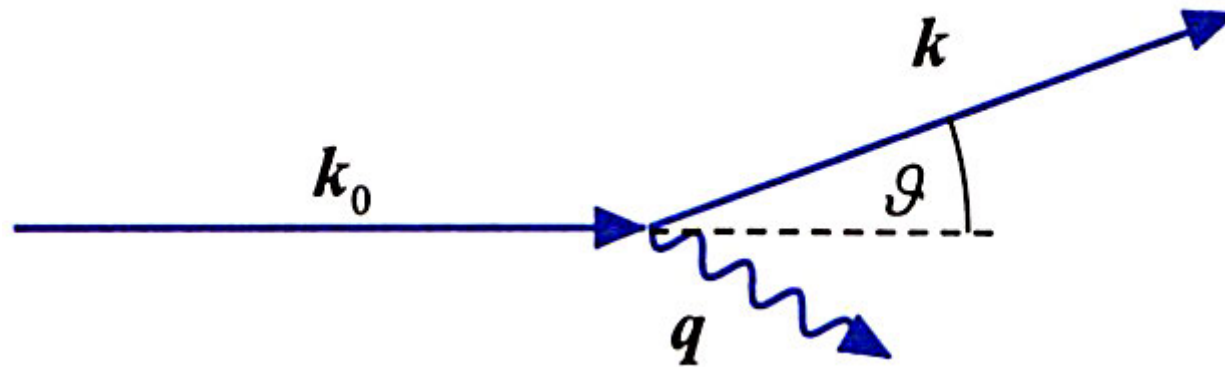


Spektrum der Streuintensität

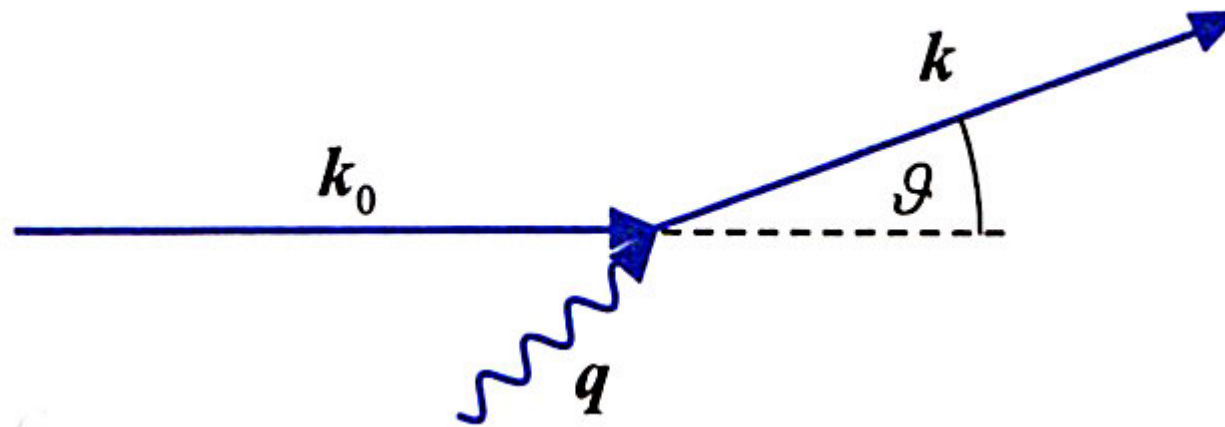


'AM Seitenbänder'

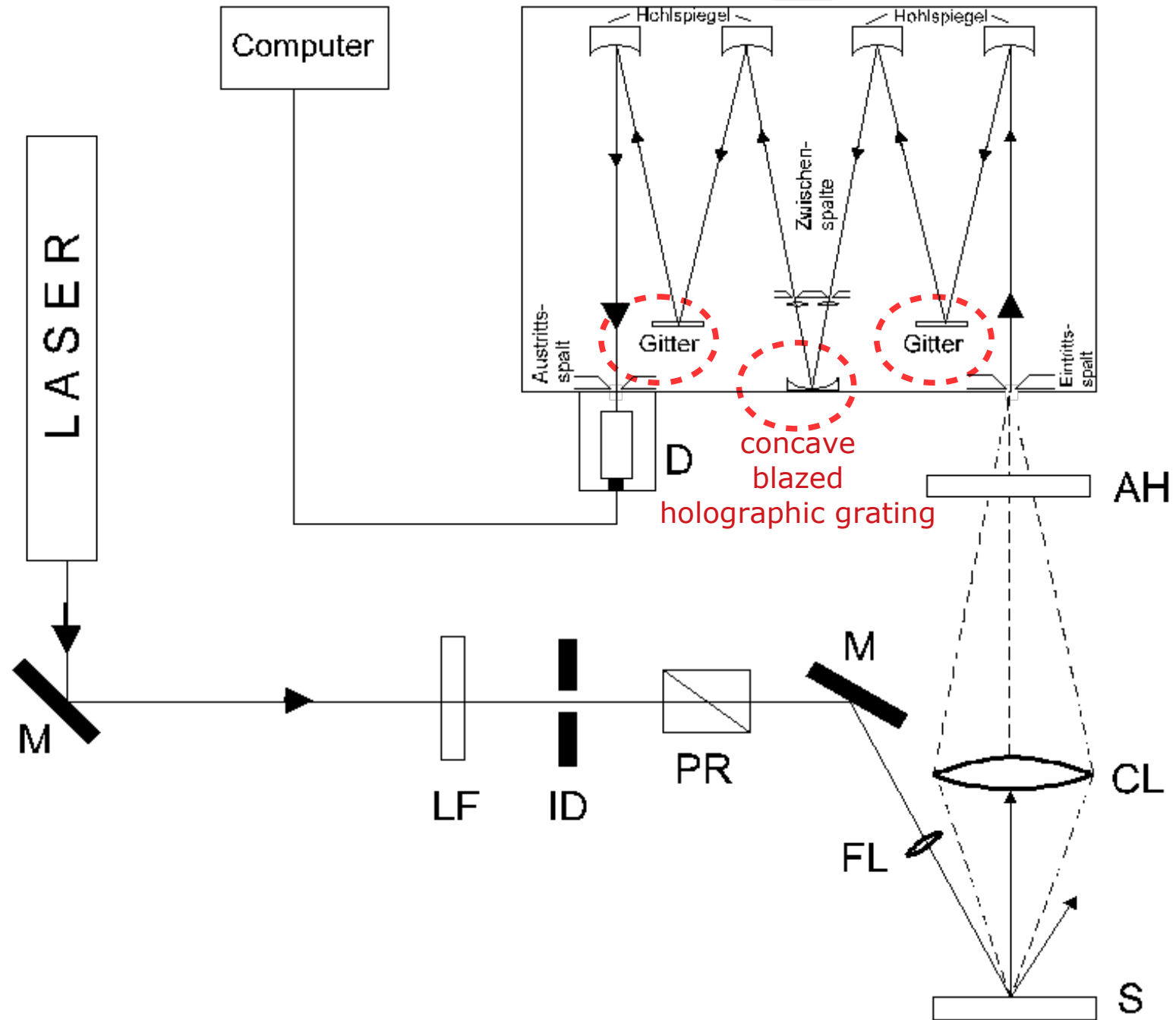
Stokes-Prozess



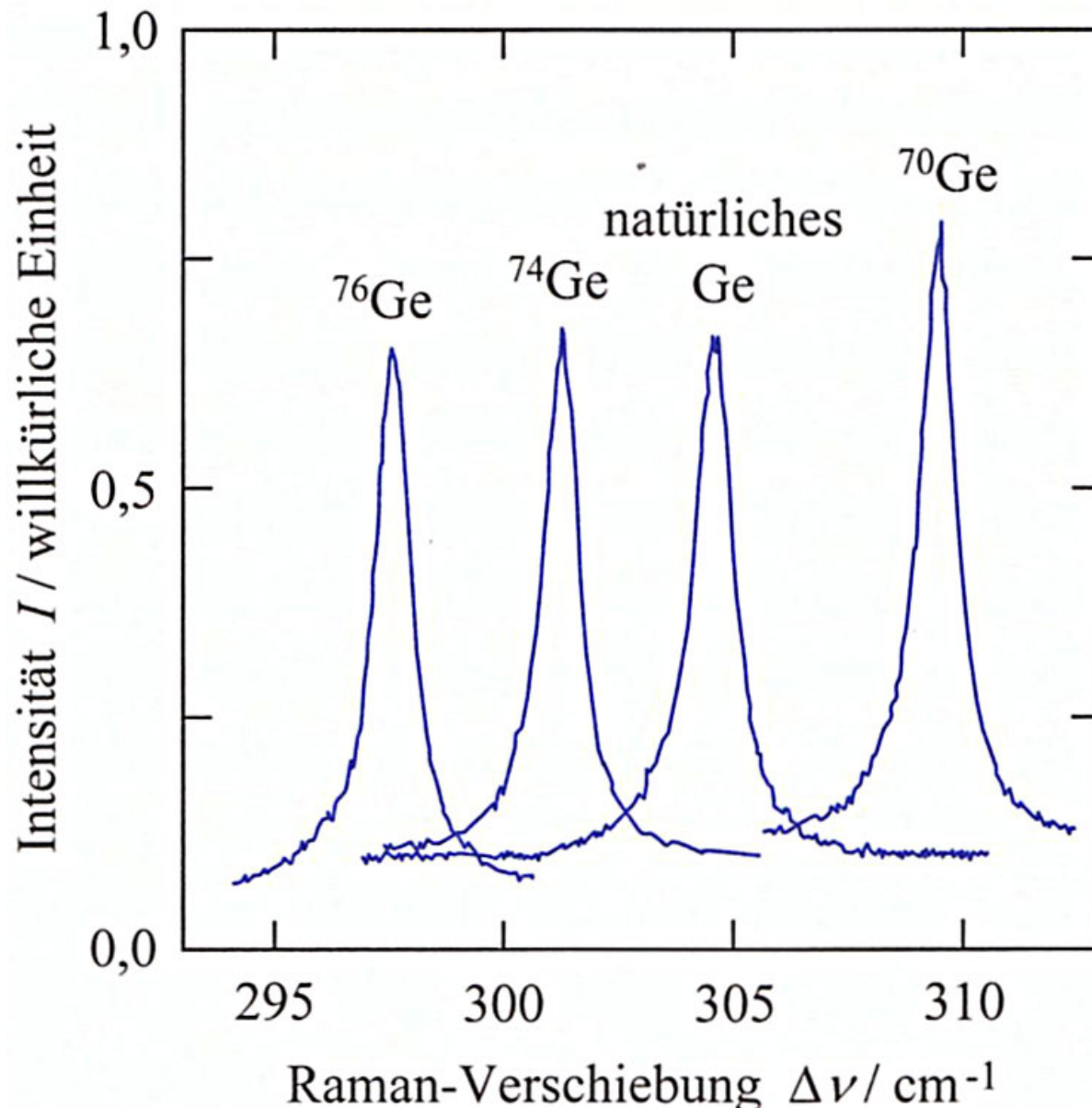
Anti-Stokes-Prozess



Dreitrittermonochromator



Raman-Spektren von Ge: isotopenrein vs. natürlich



Verschiebung $\Delta\nu$
der Ramanlinien
bzgl. Rayleighlinie

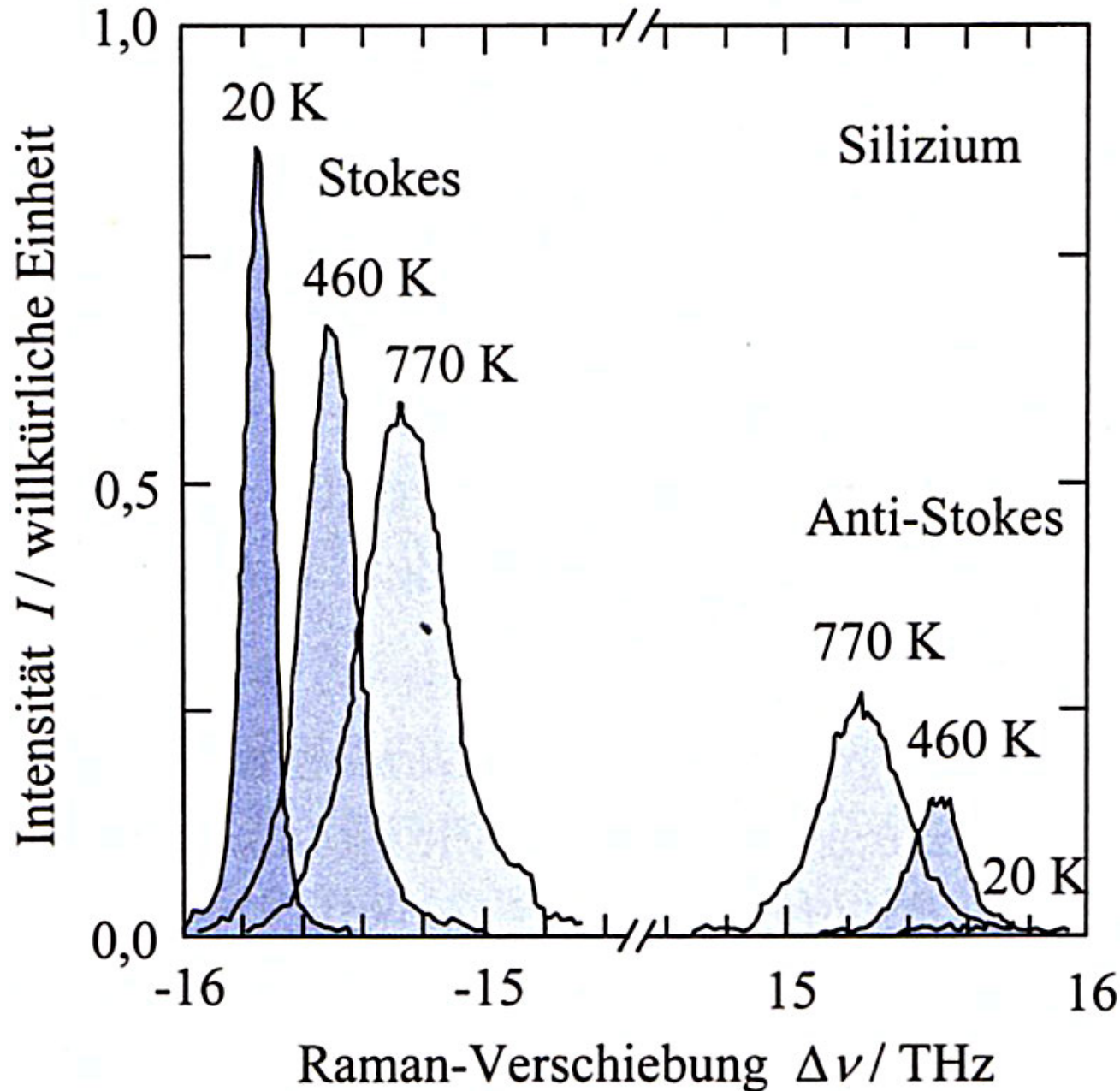
ungefähr $\Delta\nu \sim M^{-1/2}$

$T = 80 \text{ K}$

T. Ruf et al., Phys. Bl. 52, 1115 (1996)

$1 \text{ cm}^{-1} = 0.123985 \text{ meV} \sim 1/8 \text{ meV}$

Ramanspektrum von Si bei unterschiedlichen Temperaturen



1 THz = 4. 1357 meV