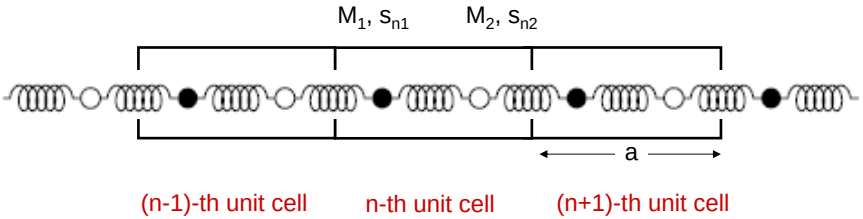
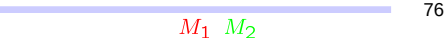
3.1. Linear chain with two atoms per unit cell



$$M_1\ddot{s}_{n1} + 2f\ s_{n1} - f\ s_{(n-1)2} - f\ s_{n2} = 0$$
$$M_2\ddot{s}_{n2} + 2f\ s_{n2} - f\ s_{(n+1)1} - f\ s_{n1} = 0$$



$M_1\ddot{s}_{n1} + 2f\ s_{n1} - f\ s_{(n-1)2} - f\ s_{n2} = 0$
$M_2\ddot{s}_{n2} + 2f\ s_{n2} - f\ s_{(n+1)1} - f\ s_{n1} = 0$

Ansatz:

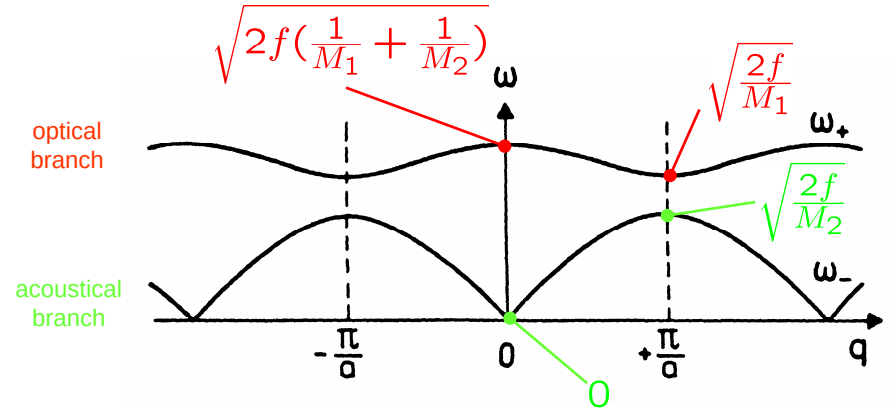
$$s_{n\alpha} = \frac{1}{M_\alpha} u_\alpha(q) e^{i(qna-\omega t)}$$

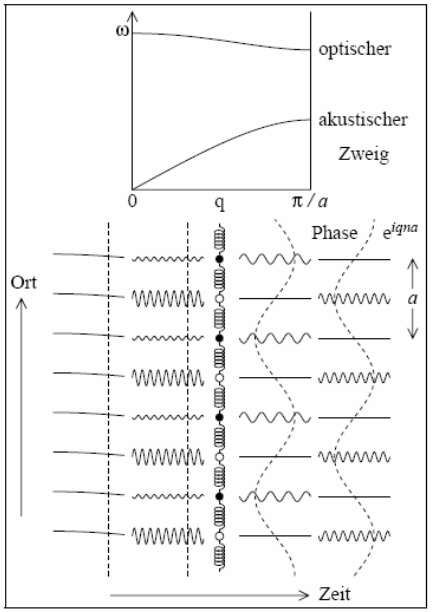
$$\begin{pmatrix} \frac{2f}{M_1} - \omega^2 & -\frac{f}{\sqrt{M_1 M_2}}(1+e^{-iqa}) \\ -\frac{f}{\sqrt{M_1 M_2}}(1+e^{iqa}) & \frac{2f}{M_2} - \omega^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = 0$$

$det(\ ) = 0$:

$$\omega^2_{1,2} = f\left(\frac{1}{M_1}+\frac{1}{M_2} \pm \sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\frac{qa}{2}}\right)$$

$$\omega^2_{1,2} = f\left(\frac{1}{M_1}+\frac{1}{M_2} \pm \sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\frac{qa}{2}}\right)$$





source: Th. Fauster

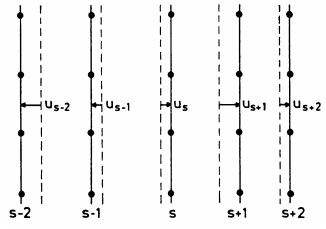
Dispersion relation for the diatomic linear chain.

Displacement of atoms in a diatomic linear chain for q ~ 0 and q = π/a.

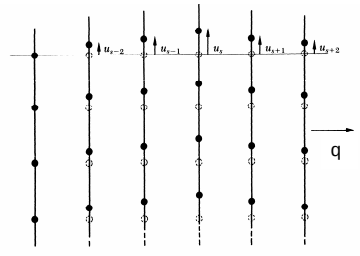
Note: to understand this figure most of us will need at least 10 minutes!

3.2. Lattice vibrations (3 dim.)

lattice planes

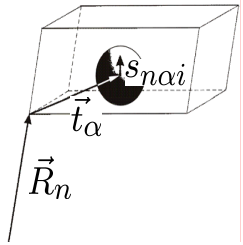


Longitudinal mode



Transversal mode

3.2. Lattice vibrations (3 dim.)



$$M_\alpha \ddot{s}_{n\alpha i} + \sum_{m\beta j} \Phi^{n\alpha i}_{m\beta j} s_{m\beta j} = 0$$

$$s_{n\alpha i} = \frac{1}{\sqrt{M_\alpha}} u_{\alpha i}(q) e^{i(\vec{q}\vec{R}_n - \omega t)}$$

$$-\omega^2 u_{\alpha i} + \sum_{\beta j} \underbrace{\sum_m \frac{1}{\sqrt{M_\alpha M_\beta}} \Phi^{n\alpha i}_{m\beta j} e^{i\vec{q}(\vec{R}_n - \vec{R}_m)}}_{\text{Dynamische Matrix : } D^{\alpha i}_{\beta j}(q)} u_{\beta j} = 0$$

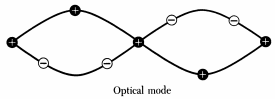
Loesung : $\det(D^{\alpha i}_{\beta j}(q) - \omega^2 \cdot 1) = 0 \;\Rightarrow\; 3N_\alpha$ Zweige

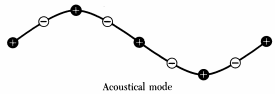
$$\omega(\vec{q}) = \omega(-\vec{q}),\ \omega(\vec{q} + \vec{G}) = \omega(\vec{q})$$

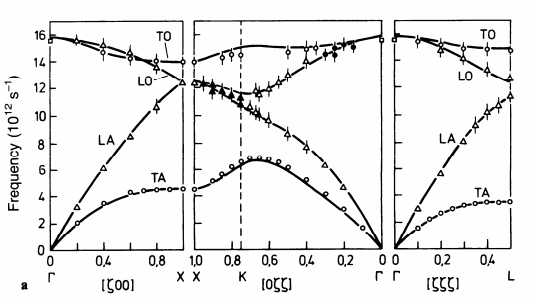
3.2. Lattice vibrations (3 dim.)

Example: (**Si,** Ge, diamond)
fcc lattice with basis of 2 atoms (a = 2)

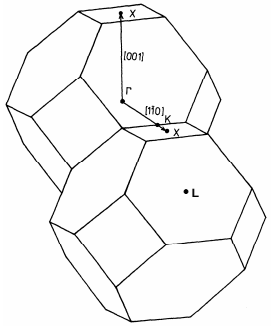
6 branches: 1x LA + 2x TA
1x LO + 2x TO







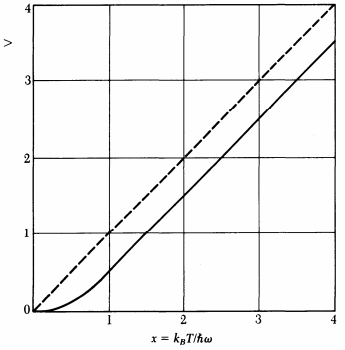
Data points stem from inelastic neutron diffraction



3.3. Thermal properties

Bose Verteilung

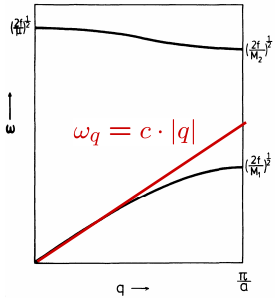
$$\langle n \rangle_T = \frac{1}{e^{\frac{\hbar\omega q}{k_B T}} - 1}$$



$$U(\omega_q, T) = \hbar\omega(\tfrac{1}{2} + \langle n \rangle_T)$$

3.3. Debye approximation

$$\omega_q = c \cdot |q|$$



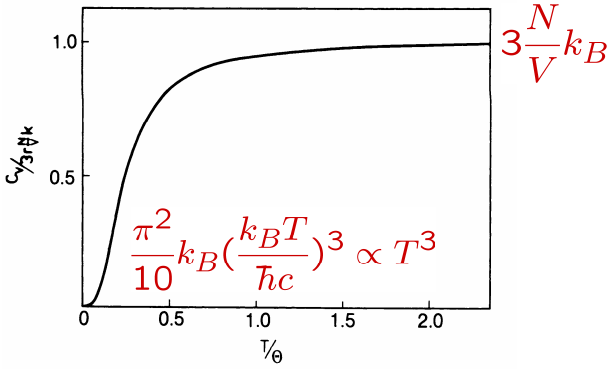
$$\int_{BZ} d^3q = 4\pi \int_0^{q_D} q^2 dq = \frac{4\pi}{3} q_D^3 = V_{BZ} = \frac{(2\pi)^3}{V_{WS}}$$

q_D Debye wave-vector

$\hbar c q_D = k_B \Theta_D$ Debye temperature (material property)

3.3. Debye specific heat

$$c_v = \frac{9 N_\alpha}{V_{WS}} k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\frac{\Theta_D}{T}} dx \frac{x^4 \, e^x}{(e^x - 1)^2}$$

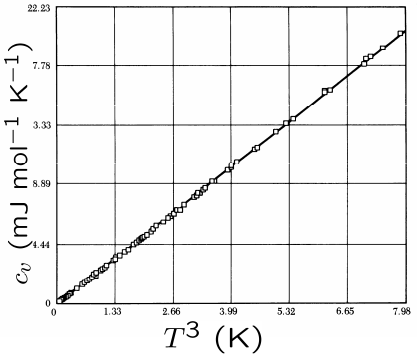


Good approximation for small and large T

3.3. Debye specific heat

T^3 – law at low temperatures

Specific heat of solid argon
Θ_D = 92 K



0 K 2 K

DEBYE TEMPERATURES FOR SELECTED ELEMENTS[a]

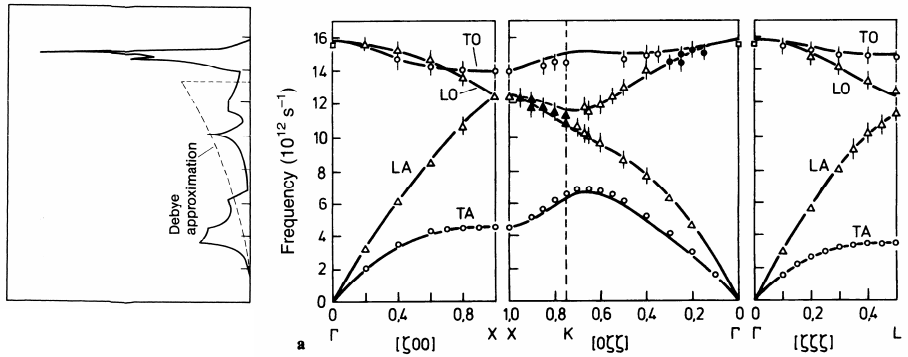
ELEMENT	Θ_D (K)	ELEMENT	Θ_D (K)
Li	400	A	85
Na	150	Ne	63
K	100		
		Cu	315
Be	1000	Ag	215
Mg	318	Au	170
Ca	230		
		Zn	234
B	1250	Cd	120
Al	394	Hg	100
Ga	240		
In	129	Cr	460
Tl	96	Mo	380
		W	310
C (diamond)	1860	Mn	400
Si	625	Fe	420
Ge	360	Co	385
Sn (grey)	260	Ni	375
Sn (white)	170	Pd	275
Pb	88	Pt	230
As	285	La	132
Sb	200	Gd	152
Bi	120	Pr	74

[a] The temperatures were determined by fitting the observed specific heats c_v to the Debye formula (23.26) at the point where $c_v = 3nk_B/2$. Source: J. de Launay, *Solid State Physics*, vol. 2, F. Seitz and D. Turnbull, eds., Academic Press, New York, 1956.

3.4. Density of states

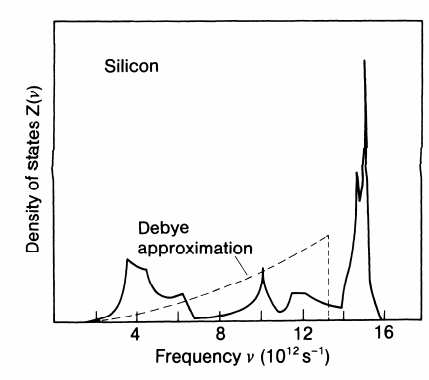
$$Z(\omega) d\omega = \frac{1}{(2\pi)^3} d\omega \sum_s \int_{\omega = const.} \frac{df_\omega}{|\nabla_q \omega|}$$

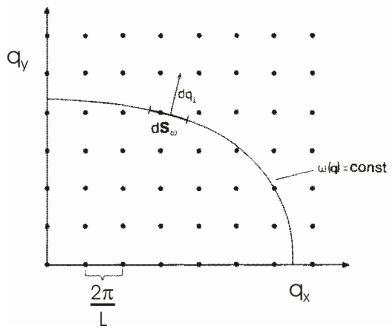
Example: Si



regions with low dispersion ω(q) ↔ high density of states

3.4. Debye approximation





Zustandsdichte:

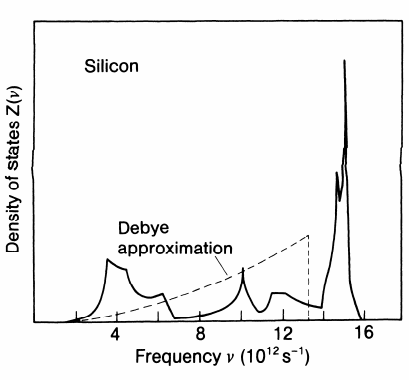
$$Z(\omega) = 3\frac{4\pi}{(2\pi)^3}\frac{\omega^2}{c^3}$$

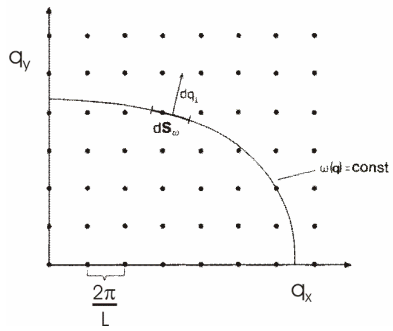
Volumen eines Zustands im q-Raum:

$$\frac{(2\pi)^3}{V}$$

3. Crystal vibrations
87

3.4. Debye approximation





Zustandsdichte:

$$Z(\omega) = 3\frac{4\pi}{(2\pi)^3}\frac{\omega^2}{c^3}$$

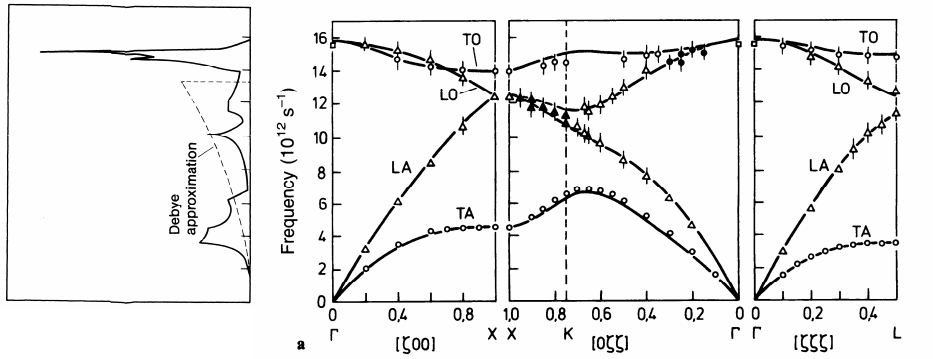
Volumen eines Zustands im q-Raum:

$$\frac{(2\pi)^3}{V}$$

3.4. Density of states

$$Z(\omega)d\omega = \frac{1}{(2\pi)^3}d\omega \sum_s \int_{\omega=const.} \frac{df_\omega}{|\nabla_q \omega|}$$

Example: Si

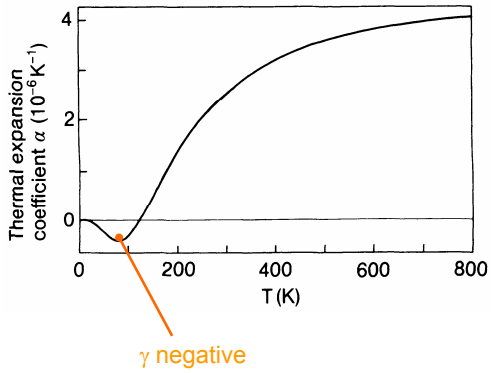


regions with low dispersion ω(q) ↔ high density of states

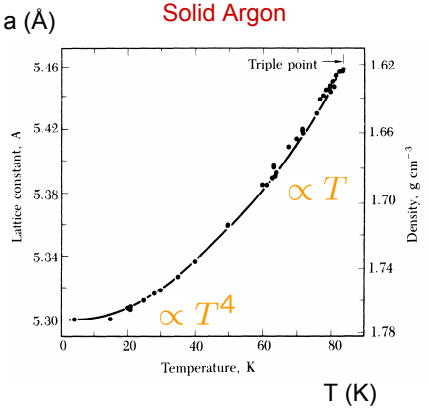
3.5. Anharmonic Effects

Thermal Expansion

Silicon

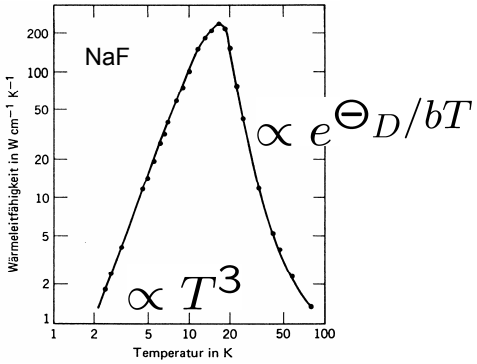


Solid Argon



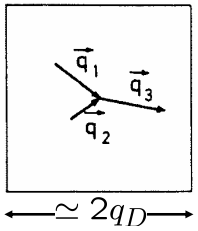
3.5. Anharmonic Effects

Heat conduction by phonons



$T \ll \Theta_D, q \ll q_D$

No umklapp: $\vec{q}_3 = \vec{q}_1 + \vec{q}_2$



$T < \Theta_D, q \simeq q_D$

Umklapp: $\vec{q}_3 = \vec{q}_1 + \vec{q}_2 - \vec{G}$