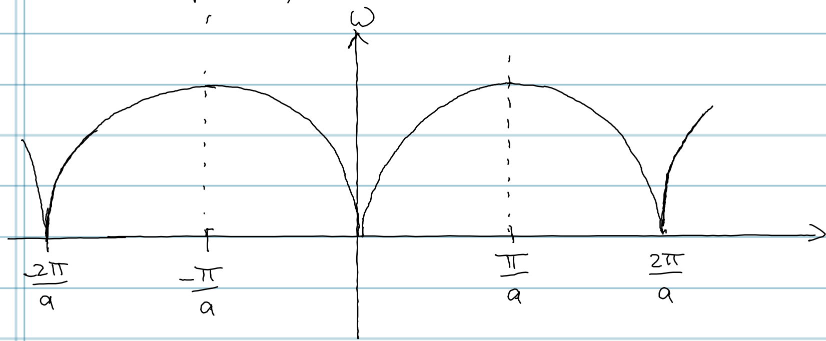
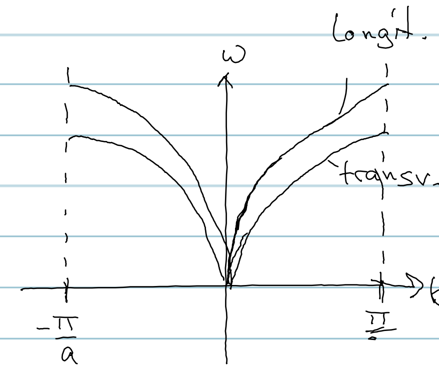
1-dim Kette aus identischen Atomen

$\omega = f(\vec{k})$



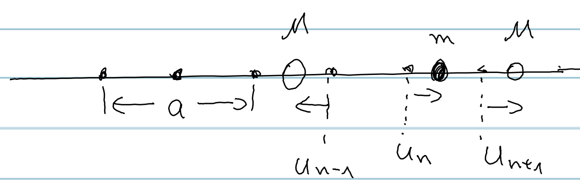


1-dim Kette mit 2 verschiedenen Atomen

z.B. KBr

$x_n = \frac{na}{2}$

in Bew.



Bew. gl. $m \frac{d^2 u_n}{dt^2} = -K(u_n - u_{n+1} + u_n - u_{n-1}) = -K(2u_n - u_{n+1} - u_{n-1})$

$M \frac{d^2 u_{n+1}}{dt^2} = -K(u_{n+1} - u_{n+2} + u_{n+1} - u_n) = -K(2u_{n+1} - u_{n+2} - u_n)$

Lsg: $u_n = \overset{u_1}{\cancel{u_0}} \cos(\omega t - kx) = \overset{u_1}{\cancel{u_0}} \cos\left(\omega t - \frac{kna}{2}\right)$

$u_{n+1} = u_2 \cos(\omega t - kx) = u_2 \cos\left(\omega t - \frac{k(n+1)a}{2}\right)$

$(2K - m\omega^2)u_1 - 2K\cos\frac{ka}{2}\, u_2 = 0$

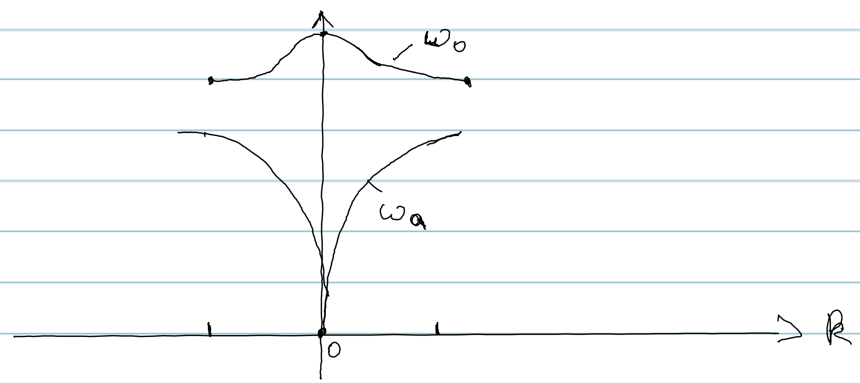
$-2K\cos\frac{ka}{2}\, u_1 + (2K - M\omega^2)\, u_2 = 0$

lineare homogenes Gleichungssystem: Lösung ? → Det = 0

$mM\omega^4 - 2K(m + M)\omega^2 + 4K^2 \sin\frac{ka}{2} = 0$

1. Lösung: akustischer Zweig

$$\omega_a^2 = K\left(\frac{m+M}{mM} - \frac{\left[(m-M)^2 + 4mM\cos^2\frac{ka}{2}\right]^{1/2}}{mM}\right)$$



$k \to 0$:

$$\omega_a^2 = K\left(\frac{m+M}{mM} - \frac{\left[(m-M)^2 + 4mM\right]^{1/2}}{mM}\right)$$

$$= K\left(\frac{m+M}{mM} - \frac{(m+M)}{mM}\right) = 0$$

ω_{max}? für $k = \frac{\pi}{a}$ $\qquad \left[\cos\frac{\pi}{2} = 0\right.$

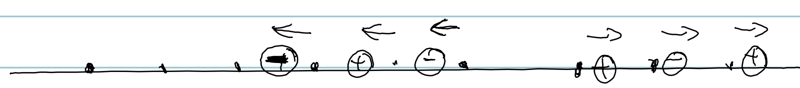
2. Lösung: optischer Zweig

$$\omega_o^2 = K\left(\frac{m+M}{mM} + \frac{\left[(m-M)^2 + 4mM\right]^{1/2}}{mM}\right)$$

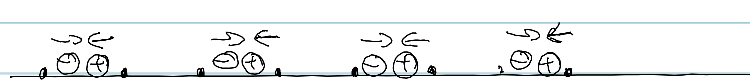
ω_o min? $\quad k = \frac{\pi}{a}$

max? $\quad k = 0$

Longitudinale Schwingungen

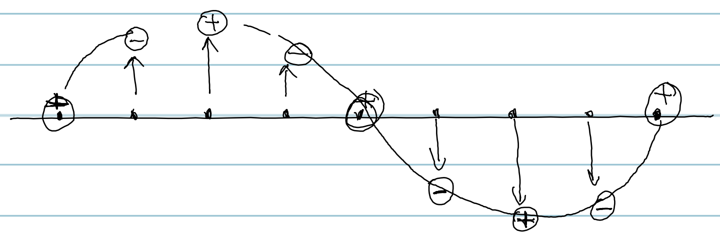


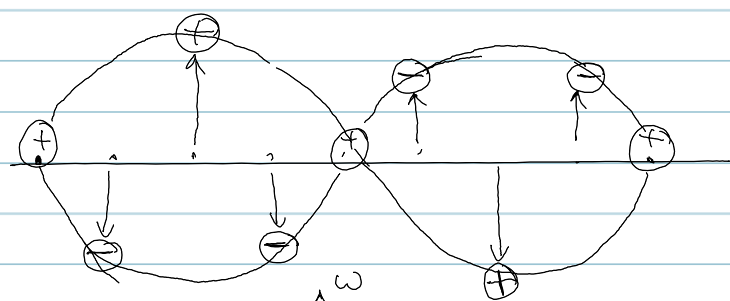
akustisch
„in Phase"

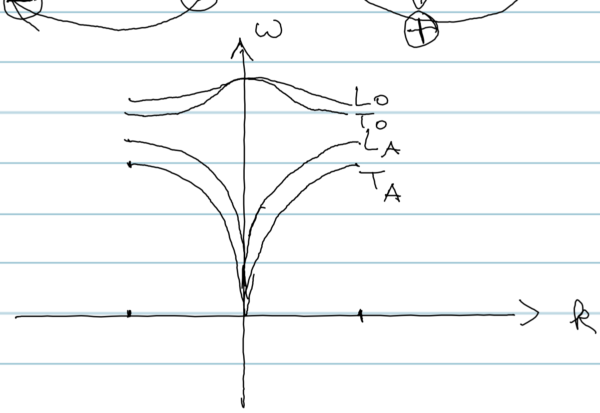


optisch
„außer Phase"

transversale Schwingungen







1-dim Kette → 3-dim Kristall

p Atome in Elementarzelle (EZ) → 3p Zweige
3 akustische, (3p−3) optische Zweige

z.B. KBr: p = 2: 1 LA, 2 TA, 1 LO, 2 TO

z.B. TiO_2 2 Moleküle / EZ → 6 Atome / EZ
3 akust, 15 opt.
→ 1 LA, 2 TA, 5 LO, 10 TO

N · EZ → ~~N~~ N · 3p Schwingungen

3.3 Quantisierung

Energie der Gitterschwingung ist quantisiert

Energiequant? = Phonon

Energie $E = (n + 1/2)\,\hbar\omega$

~~n= Anzahl angeregter Phononen in~~

Anzahl Phononen in Gitterschwingung

$n = n(\omega, T) = \frac{1}{e^{\hbar\omega/kT} - 1}$

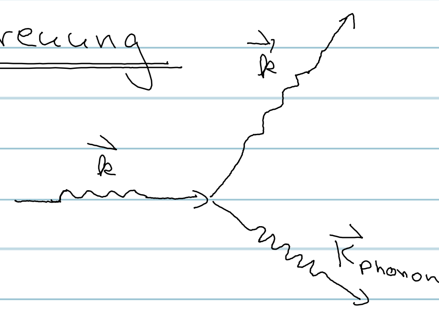
(Zustandssumme Harmon. Oszillator = plancksche Verteilungs Fkt.)

$\Rightarrow$ Gesamtes Gitter: $E_{ges} = \sum_{p,k} (n_{p,k} + 1/2)\,\hbar\,\omega_{p,k}$

3.4 Inelastische Streuung

inelastisch: $|\vec{k}| \neq |\vec{k}'|$

$\boxed{\vec{k} = \vec{k}' + \vec{K}_{Phonon}}$



Phononenerzeugung

experimentell: inelast. Neutronenstreuung

$k \simeq 4 \cdot 10^{10}\ m^{-1}$ (bei 300K) $\rightarrow$ vgl. 1BZ $k = \frac{\pi}{a} \simeq 10^{9}\ m^{-1}$

$\Rightarrow$ Phononenspektrum

exp: Photonenstreuung (VIS)

$k \simeq 1{,}2 \cdot 10^{7}\ m^{-1}$ (514 nm)

akust. Phononen $\rightarrow$ Brillouin

opt. " $\rightarrow$ Raman