3. Schwingungen von FK

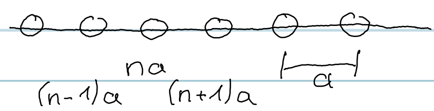
09.05.12

3.1 Dispersionsbeziehung

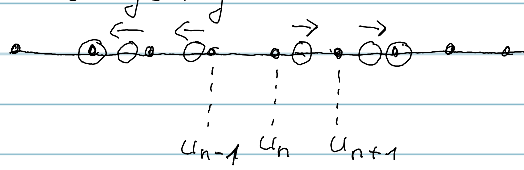
gesucht: $\omega = f(k)$

1. dim. Kette aus gleichen Atomen

in Ruhe: ~~Auf~~ Atome auf Gitterpl. x_n $(x_n = na)$



in Bewegung:



$$F = -K(u_n - u_{n+1} + u_n - u_{n-1})$$
$$= -K(2u_n - u_{n+1} - u_{n-1})$$

Bewegungsgl.

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

Lsg.: $u_n = u_0 \cos(\omega t - k x_n)$ $\quad x_n = na$

u_n = longitudinale Auslenkung

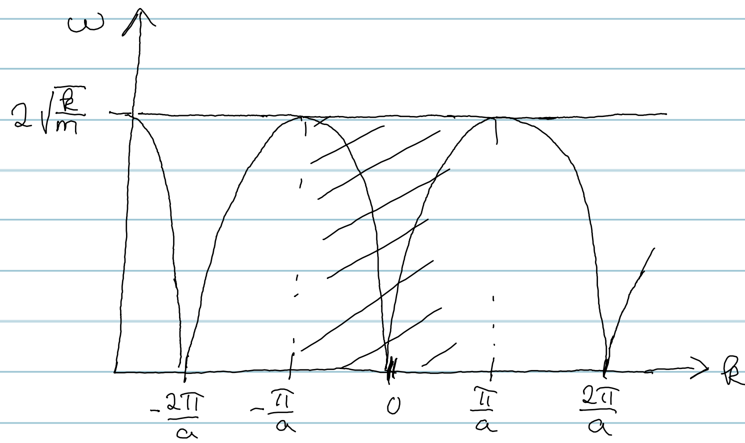
u_0 = Amplitude

mit $\cos(\omega t - k(n-1)a) + \cos(\omega t - k(n+1)a) = 2\cos(ka)\cos(\omega t - kna)$

$\Leftrightarrow -m\omega^2 n_0 = -K(2 - 2\cos ka)n_0 = -4K\sin^2\left(\frac{ka}{2}\right)n_0$

$$\boxed{\omega = 2\sqrt{\frac{k}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

Anm.: $1 - \cos\alpha = 2\sin^2\left(\frac{\alpha}{2}\right)$



<u>Konsequenzen</u>

- großes λ:

$$\omega \simeq a\sqrt{\frac{k}{m}}\,|k| \qquad v = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi}\lambda = \nu\cdot\lambda$$

$$\hookrightarrow v \simeq a\sqrt{\frac{k}{m}}$$

Ausbreitungsgeschw. unabh. $\lambda(k)$

- kleines λ ($<10a$)

Ausbreitungsgeschw. $\downarrow$ $\lambda\downarrow (k\uparrow)$

- ω_{max} für $k = \frac{\pi}{a}$

$$\hookrightarrow u_n = u_0 \cos(\omega t - n\pi) = u_0(-1)^n \cos(\omega t)$$

- ω_{max}: $k = \frac{\pi}{a}$, $\lambda = 2a$

z.B.: $k' = k + \frac{2\pi}{a}p \qquad p = 1, 2, 3, \ldots$

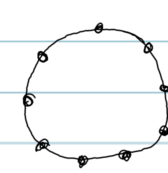
$$\hookrightarrow u = u_0 \cos\left(\omega t - kna - \frac{2\pi}{a}pna\right)$$

$$= u_0 \cos(\omega t - kna)$$

$\hookrightarrow$ k-Werte $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ beschreiben alle Schwingungen

- period. Randbedingungen:

(zykl.) $\qquad L = N\cdot a \qquad (N = \text{Anzahl Atome})$

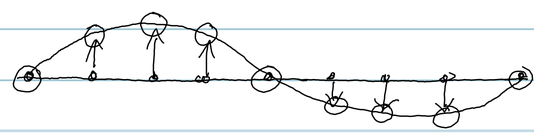


$$\hookrightarrow \lambda = L, \frac{L}{2}, \frac{L}{3}, \ldots, 2a$$

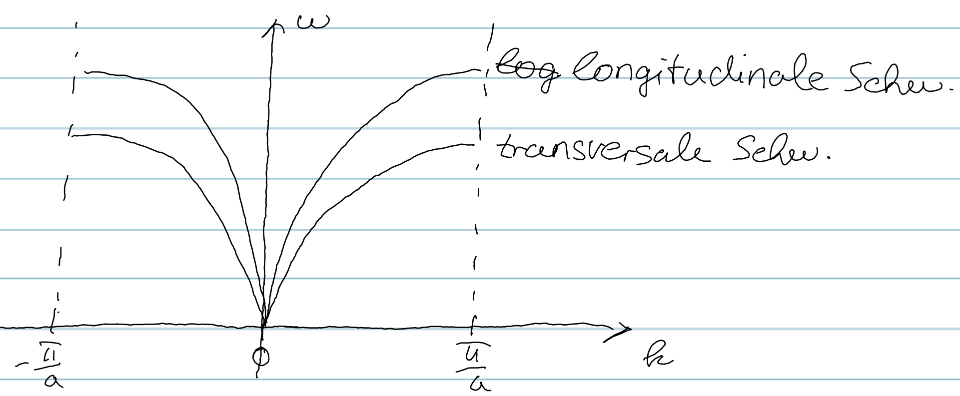
$$\hookrightarrow k = \underbrace{\pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \pm\frac{6\pi}{L}, \ldots, \pm\frac{\pi}{a}}_{N \text{ Longitudinalschw.}}$$

3.2. Verschiedene Schwingungsarten

bisher: longitudinale Schwingungen → Auslenkung in Kettenrichtung
transversale " → Auslenkung ⊥ Kettenrichtung

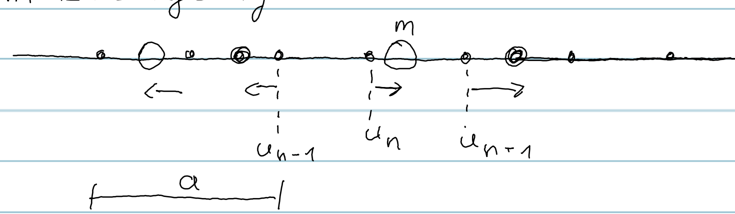


N Atome → 3N Schwingungsmoden
N longitudinale Schwingungen
2N transversale "



1 dim. Kette aus zwei verschiedenen Atomen

in Bewegung



Bewegungsgl.

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

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

Lsg.: $u_n = U_1 \cos\left(\omega t - k\frac{na}{2}\right)$

$u_{n+1} = U_2 \cos\left(\omega t - k\frac{(n+1)a}{2}\right)$

$$(2K - m\omega^2)U_1 - 2K\cos\left(\frac{ka}{2}\right)U_2 = 0$$
$$-2K\cos\left(\frac{ka}{2}\right)U_1 + (2K - M\omega^2)U_2 = 0$$

hom. lin. Gl.system: Koeff.det $= 0$

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

Lsg. 1: akust. Zweig

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

• großes λ: $\omega_a \approx a\sqrt{\frac{k}{2(m+M)}}\,|k|$

$m = M$ $\quad v_a \approx \frac{a}{2}\sqrt{\frac{k}{m}}$

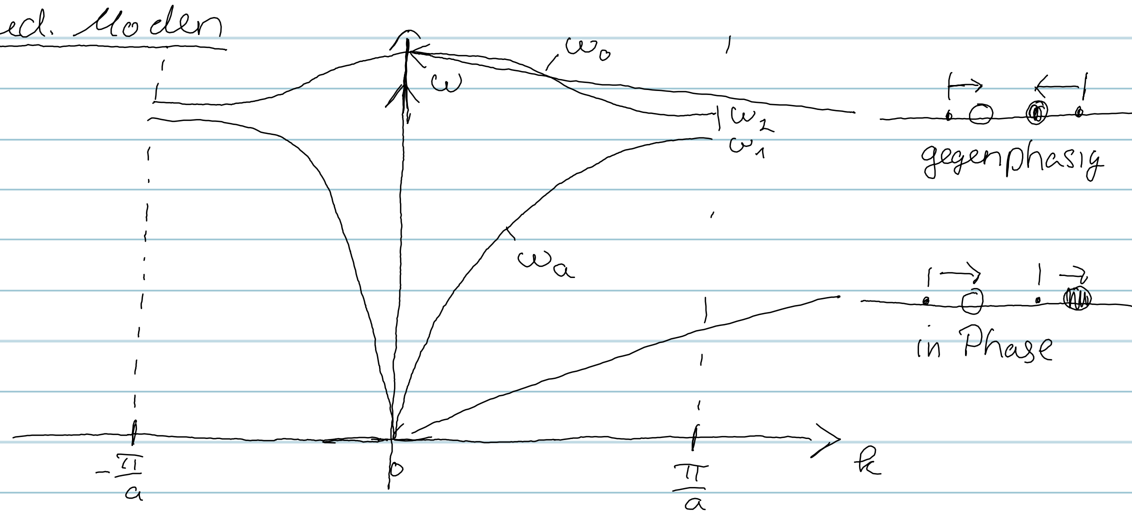
Lsg. 2: opt. Zweig

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

• ω_{max} für $k = 0$

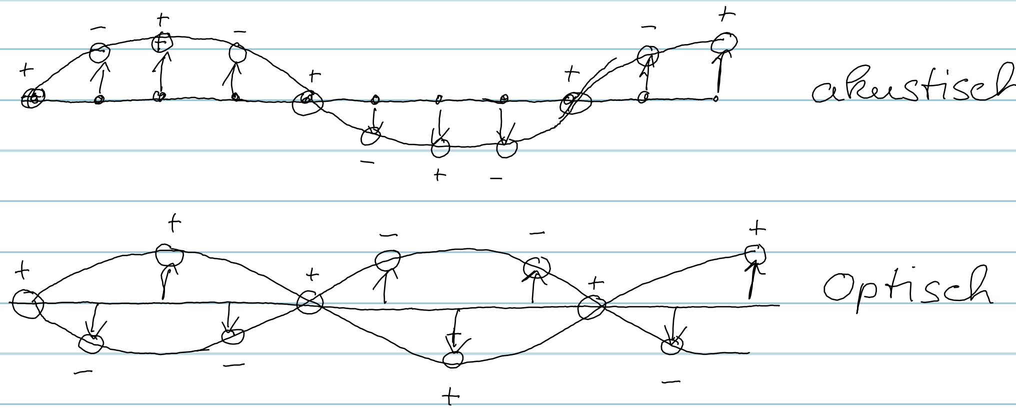
$\hookrightarrow \omega_o = \sqrt{\frac{2k(m+M)}{mM}}$

Longitud. Moden



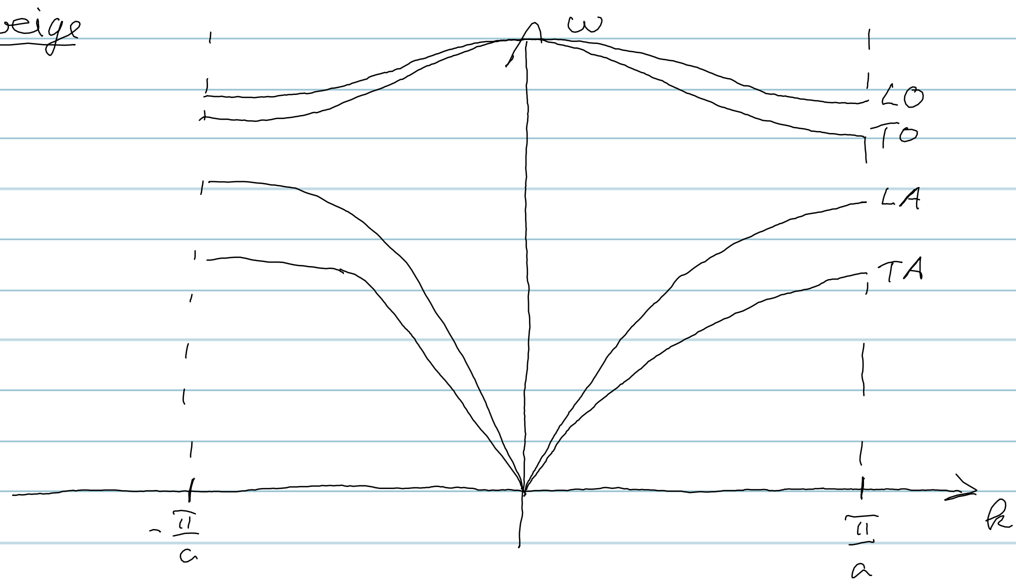
Transversalschw.

z.B. NaCl



2 atom. Kette:

Zweige



Bsp.: Dispersionskurven Ge, KBr

1 dim. Kette → 3 dim. Kristall

p Atome in EZ → 3p Zweige
3 akustische, 3p−3 optische
z.B. Ge, KBr p=2: 1LA, 2TA, 1LO, 2TO
N·EZ → 3p·N
3N akustische, (3p−3)N optische

3.3. Quantisierung

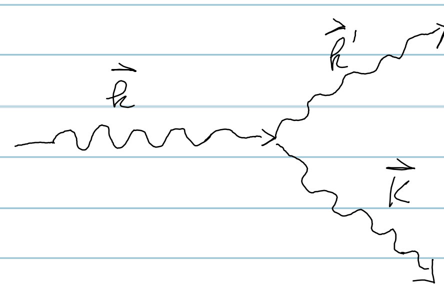
FKschwingungen sind gequantelt
Quantum = Phonon

$E = (n + \frac{1}{2})\hbar\omega$
n = Anzahl Phononen in Mode eines Zweiges
$n \equiv n(\omega, T) = \frac{1}{\exp(\hbar\omega/(kT)) - 1}$ Planksche Verteilungsfkt.

$E_{ges} = \sum_{k,p} (n_{k,p} + \tfrac{1}{2})\hbar\omega_{k,p}$

3.4. Inelastische Streuprozesse

inelast.: $|\vec{k}'| \neq |\vec{k}|$
↳ $\boxed{\vec{k}' = \vec{k} - \vec{K}}$



- Neutronenstreuung
  $k \simeq 4\cdot10^{10}\,m^{-1}$ (300 K) vgl. $\frac{2\pi}{a}$ (1. BZ): $k = \frac{\pi}{a} \simeq 10^{9}\,m^{-1}$
  ↳ Phononenspektrum

- Photonenstreuung (VIS)
  $k \simeq 1{,}2\cdot10^{7}\,m^{-1}$ (514 nm)
  akustische Phononen → Brillouin-Streuung
  optische Phononen → Raman