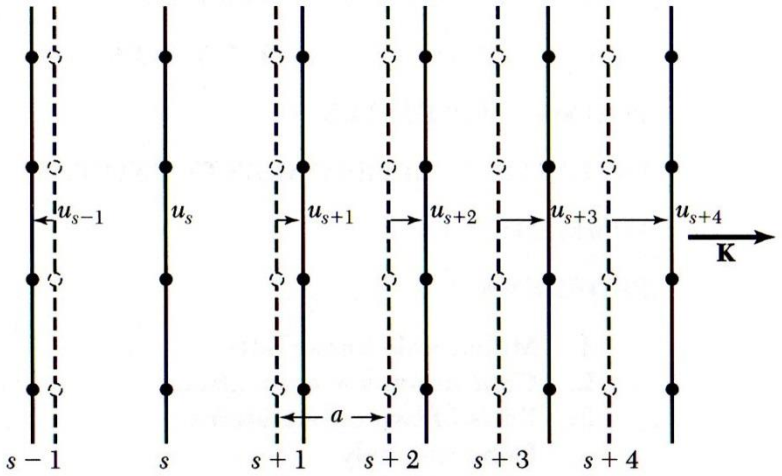
Solid state physics for Nano

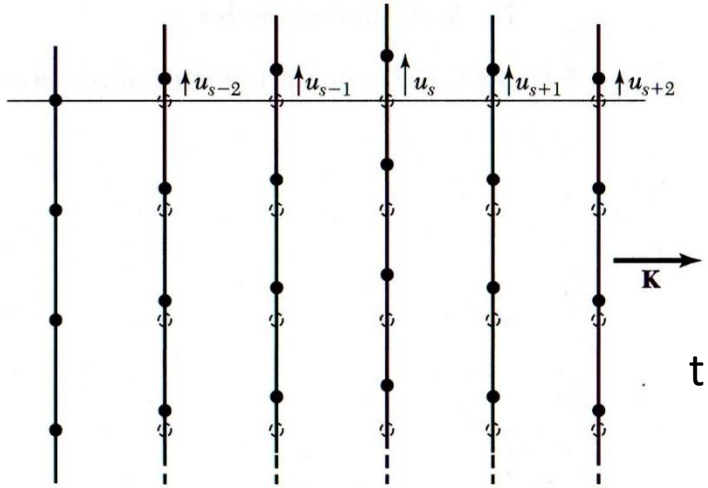
Lecture 4: Phonons

Prof. Dr. U. Pietsch

Crystal lattice vibration



longitudinal



transversal

Hook´s law

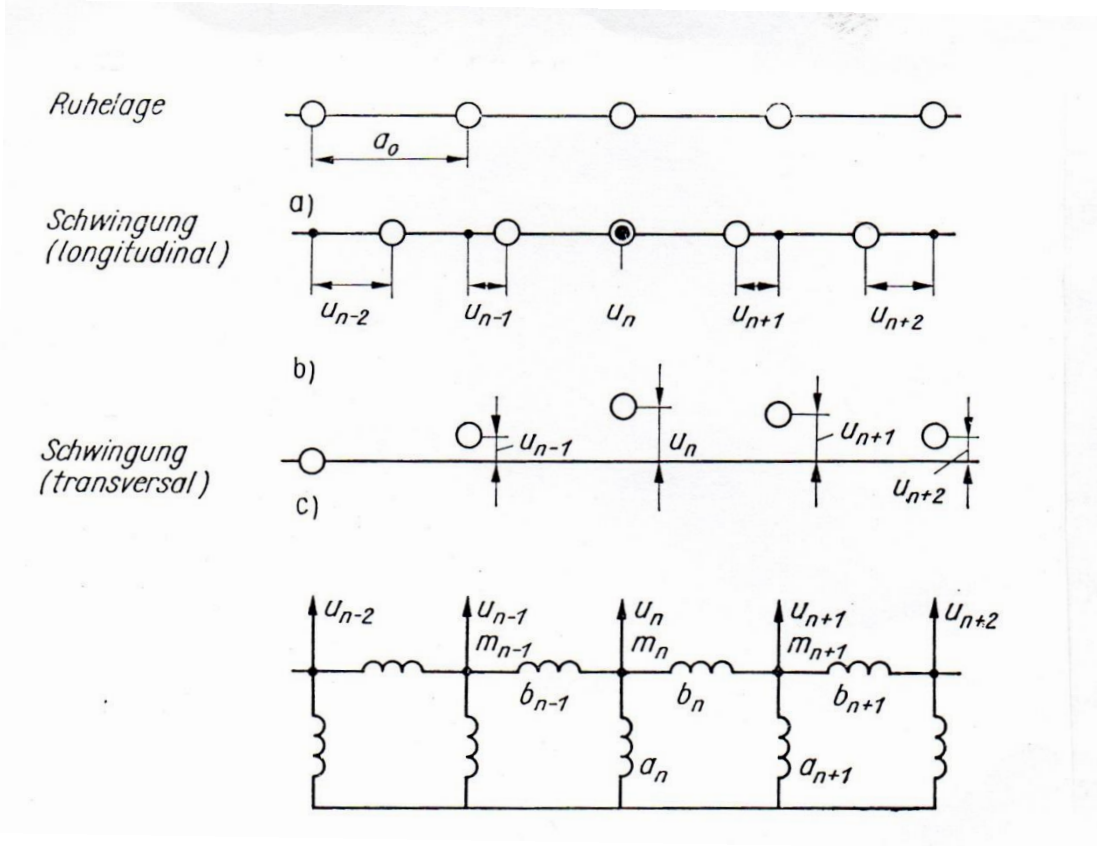
$$F_n = \sum_p C_p (u_{n+p} - u_n)$$

F_n – Force on plane n;
C_p – force constant between planes of distance p

lattice vibration of 1D monoatomic chain

Equation of motion

$$M\frac{d^2u_n}{dt^2}=\sum_{p=-\infty}^{+\infty}C_p(u_{n+p}-u_n)$$



Ansatz:

$$u_{n+p}=u_0e^{i[(n+p)\vec{q}\vec{a}-\omega t)]}$$

a – lattice spacing; q – wave number, $\vec{q}$ - wave vector

Solution of 1D wave equation

→(*)

$$M\frac{d^2u_n}{dt^2} = -\omega^2 M u_0 e^{i[(nqa-\omega t)]} = \sum_p [e^{i[(n+p)qa]} - e^{i[nqa]}]e^{-i\omega t}$$

$$\omega^2 M = -\sum_p C_p (e^{ipqa} - 1)$$

$C_{-p} = -C_p$

$$\omega^2 M = -\sum_{p>0} [C_p (e^{ipqa} - 1) + C_p (e^{-ipqa} - 1)]$$

$$\omega^2 M = -\sum_{p>0} C_p (e^{ipqa} + e^{-ipqa} - 2) = -\sum_{p>0} C_p (2\cos(pqa) - 2)$$

Dispersion relation

$$\omega^2 = \frac{2}{M}\sum_{p>0} C_p (1 - \cos(pqa))$$

$\omega(q)$ – dispersion – nonlinear function

Only nearest neighbours , p=1

$$\omega^2 = \frac{2C_1}{M}(1-\cos(pa) = \frac{2C_1}{M}(2\sin^2\frac{qa}{2})$$

$$\omega^2 = \frac{4C_1}{M}\sin^2(\frac{qa}{2})$$

Small q $$\omega^2 = \frac{2C}{M}(1-\cos(pqa) = \frac{2C}{M}(1-1+\tfrac{1}{2}q^2p^2a^2...)$$

$$\omega^2 = \frac{C_1}{M}q^2a^2 \qquad \omega \sim q$$

1st Brillouin zone contains all information : $\omega(q)$ is periodic in q*a

$$\frac{u_{n+1}}{u_n} = \frac{e^{i[(n+1)qa-\omega t]}}{e^{i[nqa-\omega t]}} = e^{i(qa-\omega t)}$$

Only in range $|qa| < 2\pi$ independent values of q

$$-\frac{\pi}{a} \le q \le \frac{\pi}{a}$$

Range of 1st Brillouin zone

$$\omega^2 = \frac{4C_1}{M}\sin^2\left(\frac{qa}{2}\right)$$

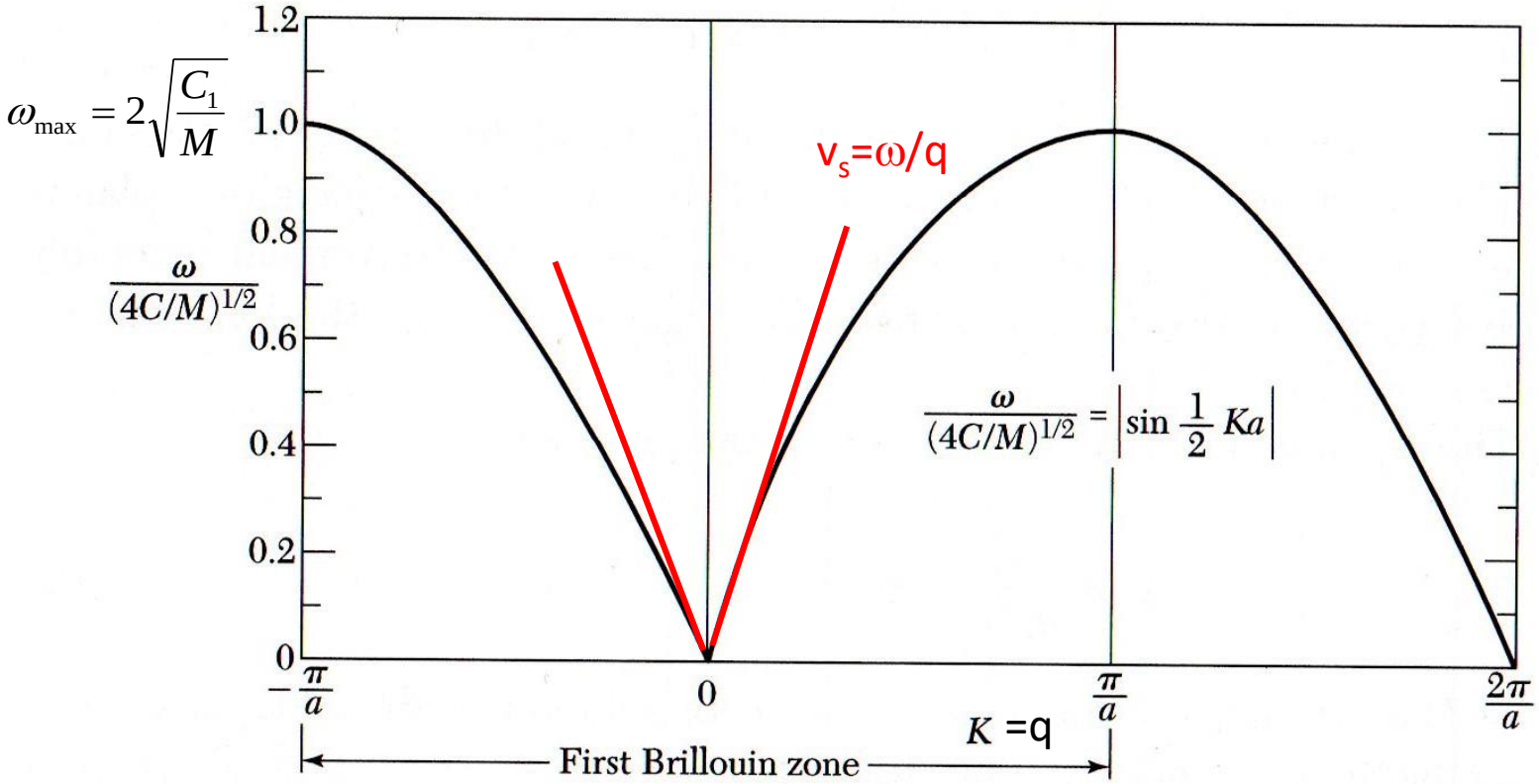


Figure 4 Plot of ω versus K. The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K.

C.Kittel

$$q_{\max} = \pm\frac{\pi}{a} \approx 10^{10} m^{-1}$$

$$\lambda_{\min} = \frac{2\pi}{q_{\max}} = 2a$$

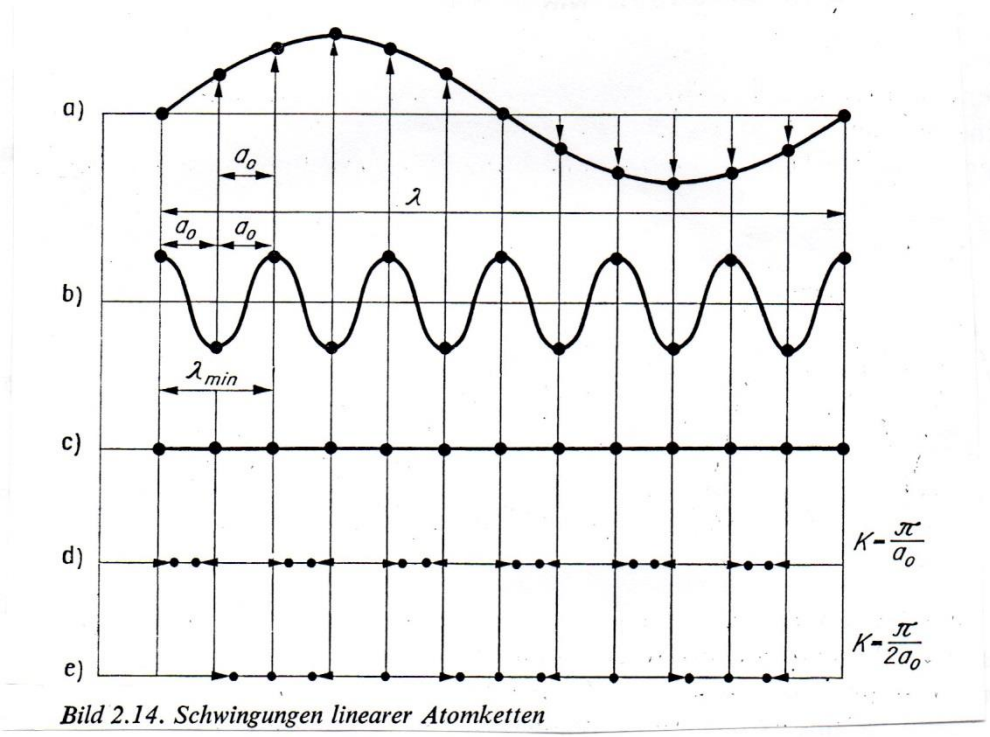


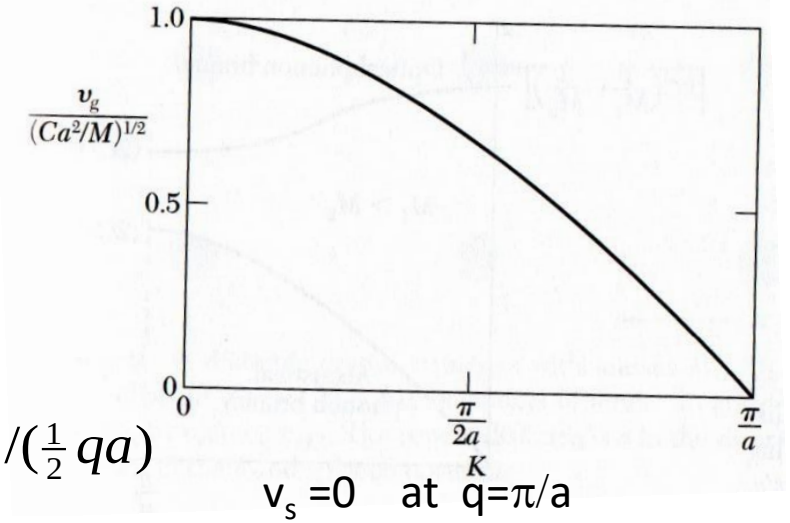
Bild 2.14. Schwingungen linearer Atomketten

Group velocity= signal velocity of a wave packet

$$v_g = \frac{d\omega}{dq} \qquad v_g = \sqrt{\frac{Ca^2}{m}}\cos(\tfrac{1}{2}qa)$$

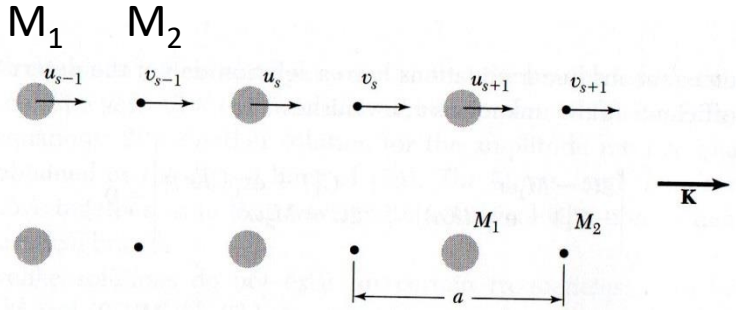
phase velocity > group velocity

$$v_p = \frac{\omega}{q} \qquad v_p = \sqrt{\frac{Ca^2}{m}}\sin(\tfrac{1}{2}qa)/(\tfrac{1}{2}qa)$$



$v_s = 0$ at $q=\pi/a$

lattice vibration of 1D bi-atomic chain



$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

$$u_s = u_0 e^{i(sqa-\omega t)} \qquad v_s = v_0 e^{i(sqa-\omega t)}$$

$$-\omega^2 M_1 u = Cv\,[1+e^{iqa}] - 2Cu$$

$$-\omega^2 M_2 v = Cu\,[e^{iqa}+1] - 2Cv$$

$$\begin{vmatrix} 2C - M_1\omega^2 & -C[1+e^{iqa}] \\ -C[1+e^{iqa}] & 2C - M_1\omega^2 \end{vmatrix} = 0$$

Quadratic equation in ω^2

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1-\cos qa) = 0$$

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

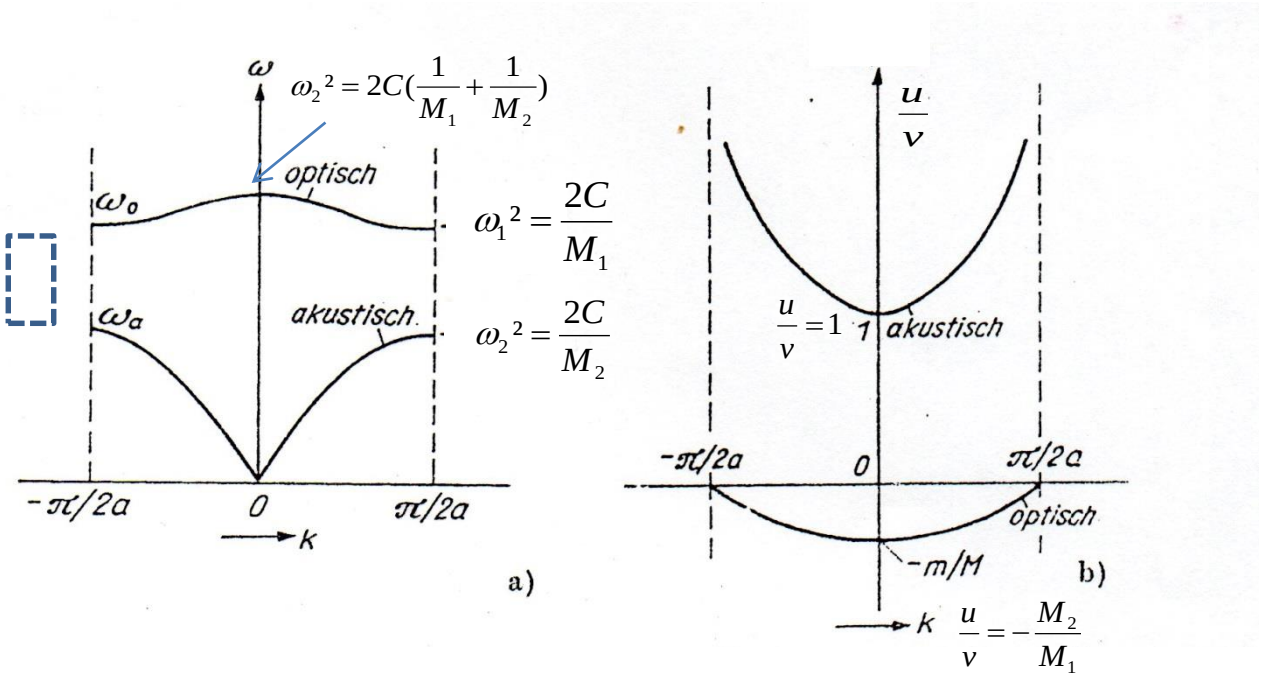
Acoustic branch

For q=0 $\omega_1^2 = 0$ For sin(qa) ≈ qa $\omega_1^2 = \frac{\frac{1}{2}C}{M_1+M_2}(qa)^2$

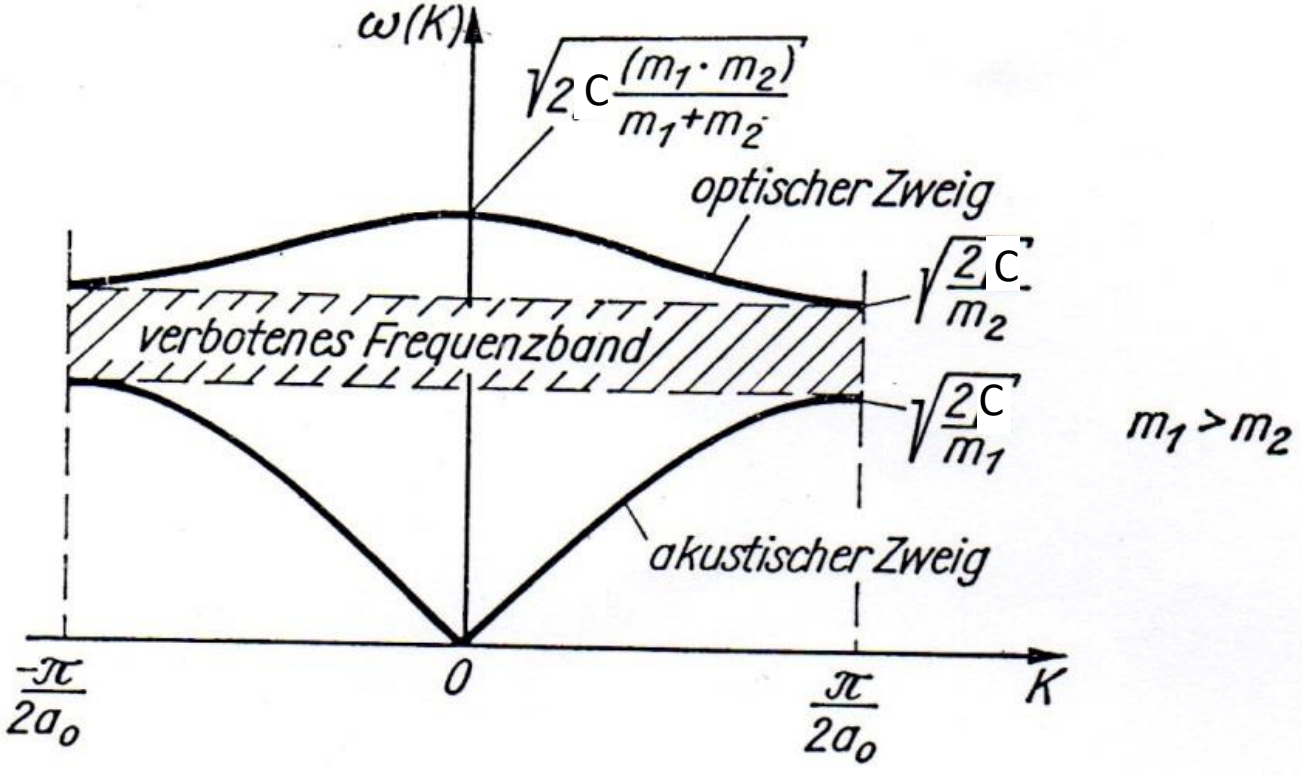
Optical branch

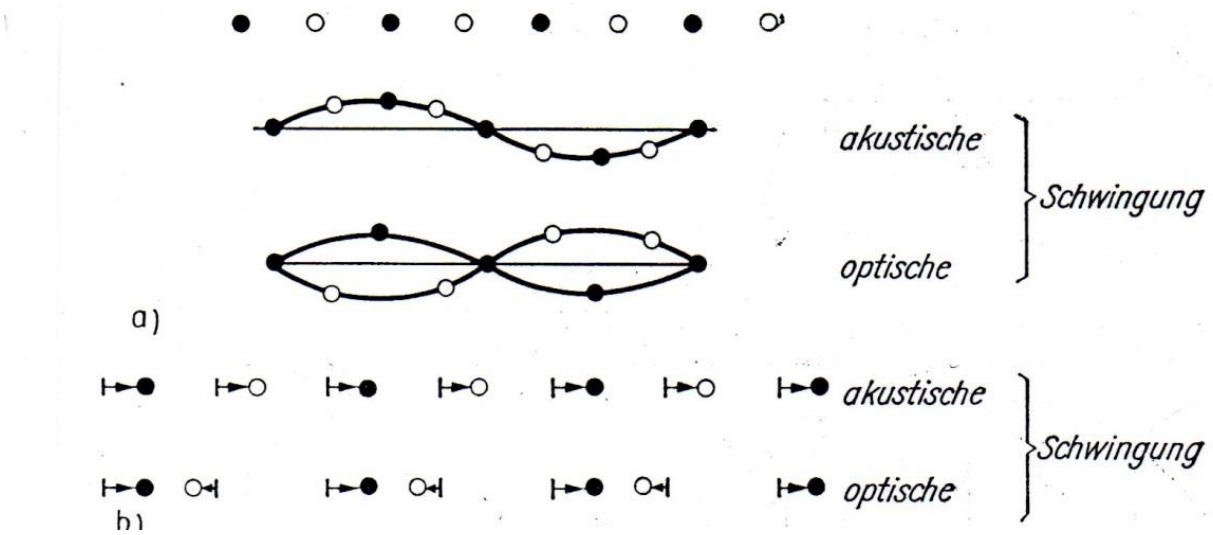
$$\omega_2^2 = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

Optical frequency gap

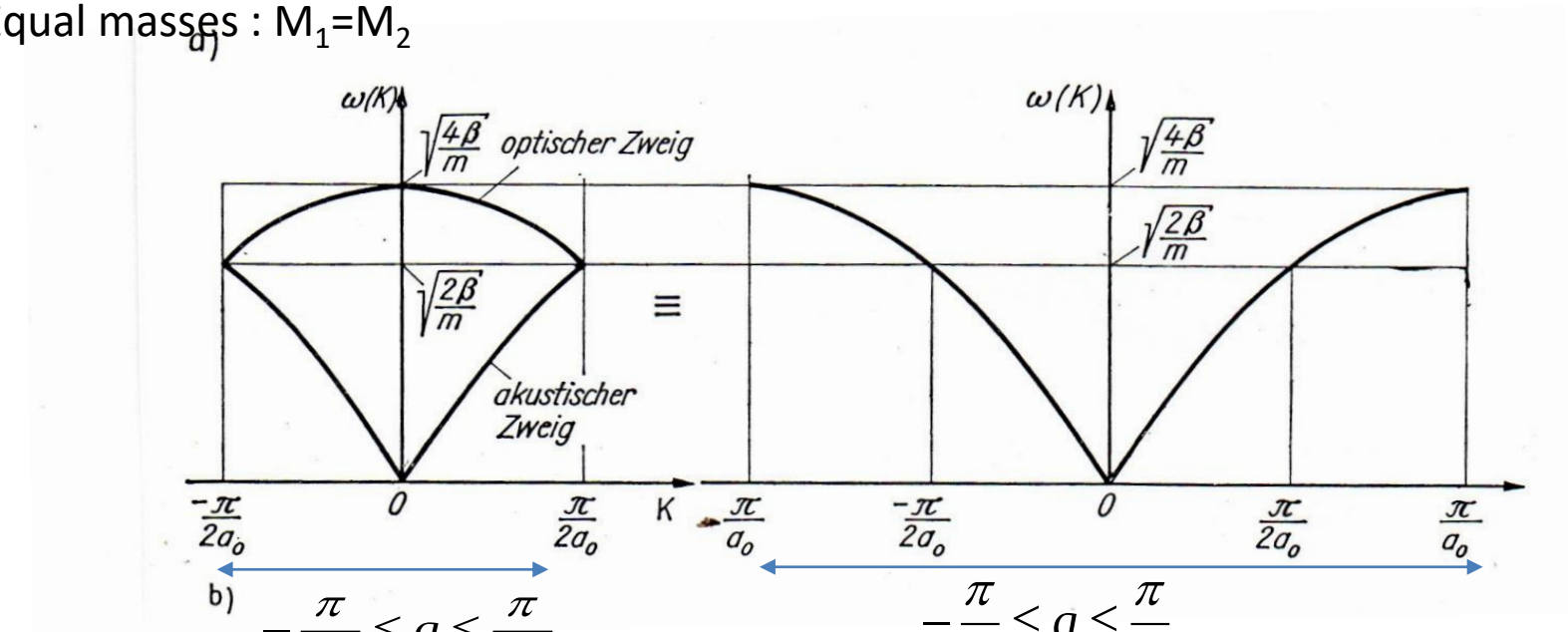


	$q = 0$	$q = \pm\frac{\pi}{2a}$
$acoustic\_branch$	$\omega = 0; u = v$	$\omega = \sqrt{\frac{2C}{M_1}}; v = 0 \quad ; u_{n-1} = -u_{n+1}$
$optical\_branch$	$\omega = \sqrt{2C(\frac{1}{M_1} + \frac{1}{M_2})}, \frac{u}{v} = -\frac{M_2}{M_1}$	$\omega = \sqrt{\frac{2C}{M_2}}; u = 0; v_{n-1} = -v_{n+1}$





Equal masses : $M_1=M_2$



$$-\frac{\pi}{2a} \le q \le \frac{\pi}{2a}$$

$$-\frac{\pi}{a} \le q \le \frac{\pi}{a}$$

Phonons in 3D

- 3D crystal of size Pa_1, Pa_2, Pa_3 may contain S different atoms per unit cell
- Each atoms has $3SP^3=3SN$ degrees of freedom for displacements
- Each displacement results in 1D equations of motion
- → 3SN differential equation with 3SN solutions
- Direction of wave propagation given by vector **K**
- Displacement $u= u_0 \exp(i(K'a_n-\omega t))$ using

$$\vec{K}' = \vec{K} + \vec{G} \qquad \vec{G} = hb_1 + kb_2 + lb_3$$

$$\vec{K}'\vec{a}_n = \vec{K}\vec{a}_n + (hb_1 + kb_2 + lb_3)\vec{a}_n = \vec{K}\vec{a}_n + m2\pi$$

K´ periodic in 3D

$$-\pi \le \vec{K}\vec{a}_n \le \pi$$

- Valid values in 1st BZ
- Number of solutions is 3S
- 3S equation give 3S branches $\omega_j(\mathbf{K})$, j=1,2,3, corresponds to 1 long + 2 trans modes

- In total 3 acoustic branches and 3(S-1) optical branches

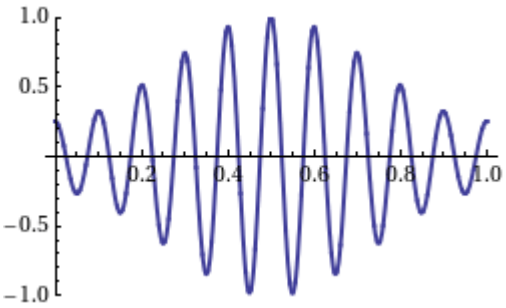
Group and phase velocities

Group velocity = signal velocity

$$v_{gr} = \frac{d\omega}{dq} = v_0(\cos\frac{qa}{2})$$

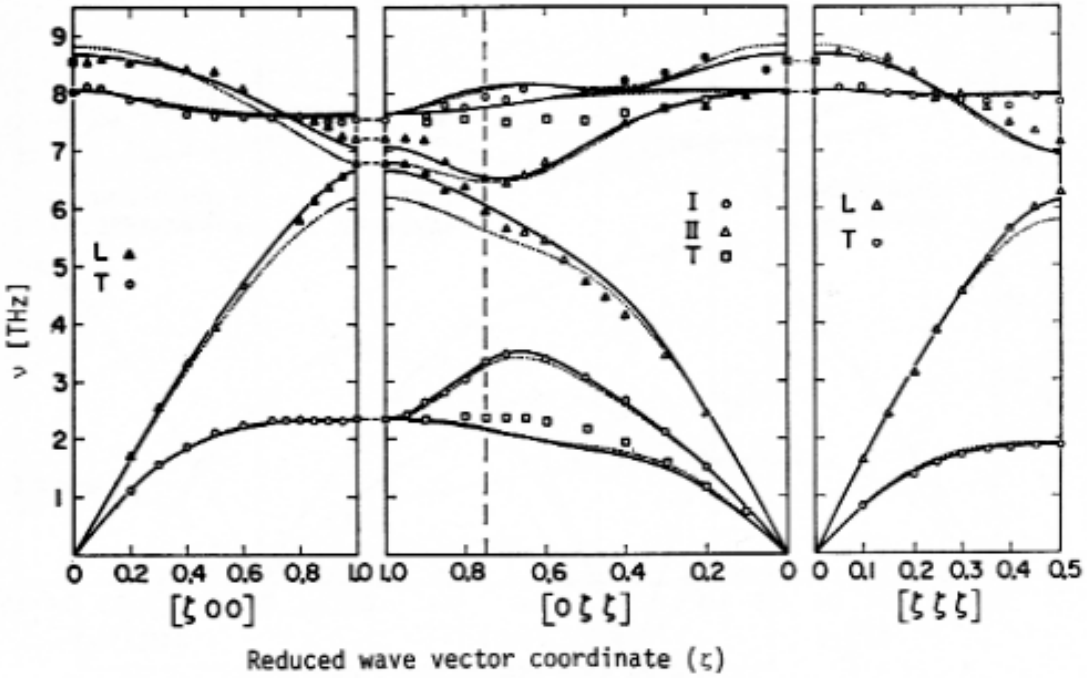
Phase velocity

$$v_{ph} = \frac{\omega}{q} = v_0 \left| \frac{\sin(qa/2)}{qa/2} \right|$$



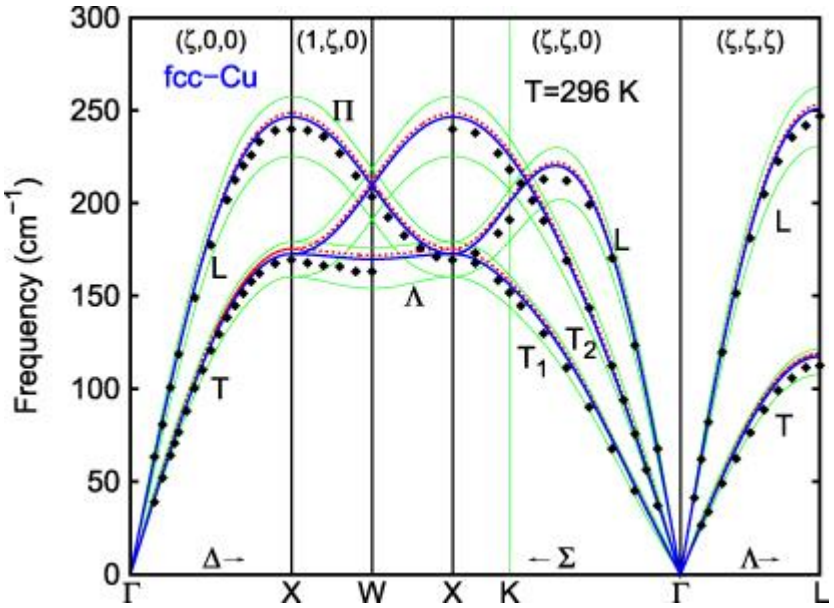
This shows a wave with the group velocity and phase velocity going in different directions. The group velocity is positive, while the phase velocity is negative.

https://en.wikipedia.org/wiki/Phase_velocity#/media/File:Wave_opposite-group-phase-velocity.gif



http://wolf.ifj.edu.pl/phonondb/gaas.htm

Phonon dispersion
of GaAs



***Ab initio* phonon dispersions of transition and noble metals: effects of the exchange and correlation functional**
Andrea Dal Corso

Phonon dispersion
of Cu