FYS3410 - Vår 2011 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

Course content

- **Periodic structures, understanding of diffraction experiment and reciprocal lattice**
- **Imperfections in crystals: diffusion, point defects, dislocations**
- **Crystal vibrations: phonon heat capacity and thermal conductivity**
- **Free electron Fermi gas: density of states, Fermi level, and electrical conductivity**
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- **Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions**
- **Metals: Fermi surfaces, temperature dependence of electrical conductivity**

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FYS3410 lecture schedule and exams: Spring 2011

W/19/1/2011:	Introduction and motivation. Periodicity and lattices	1h
M/24/1/2011:	Index system for crystal planes. Crystal structures	2h
W/26/1/2011:	Reciprocal space, Laue condition and Ewald construction	1h
M/31/1/2011:	Brillouin Zones. Interpretation of a diffraction experiment	2h
W/02/2/2011:	Crystal binding, elastic strain and waves	1h
M/07/2/2011:	Elastic waves in cubic crystals; defects in crystals	2h
W/09/2/2011:	Defects in crystals; case study – vacancies; diffusion	2h
M/14/2/2011:	Crystal vibrations and phonons	2h
W/16/2/2011:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
M/21/2/2011:	Phonon density of states (DOS) and Debye model	2h
W/23/2/2011:	General result for DOS; role of anharmonic interactions	2h
M/28/2/2011:	Thermal conductivity and repetition of crystal vibrations	2h
W/02/3/2011:	no lectures	
M/07/3/2011:	no lectures	
W/09/3/2011:	no lectures	
M/14/3/2011:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/17/3/2011:	Density of states, effect of temperature – FD distribution	1h
M/21/3/2011:	Heat capacity of FEFG	2h
W/23/3/2011:	Repetition	1h
M/28/3/2011:	Mid-term exam	

M/04/4/2011:	**Electrical and thermal conductivity in metals**	**2h**
W/06/4/2011:	**Bragg reflection of electron waves at the boundary of BZ**	**2h**
M/11/4/2011:	**Energy bands, Kronig - Penny model**	**2h**
W/13/4/2011:	**Empty lattice approximation; number of orbitals in a band**	**2h**
Påsk uppehåll		
W/27/4/2011	**no lectures**	
M/02/5/2011:	**no lectures**	
W/04/5/2011:	**no lectures**	
M/09/5/2010:	**Semiconductors, effective mass method, intrinsic carriers**	**2h**
W/11/4/2010:	**Impurity states in semiconductors and carrier statistics**	**2h**
M/16/5/2010:	**p-n junctions, Schottky contacts and heterojunctions**	**2h**
W/18/5/2010:	**Metals and Fermi surfaces**	**1h**
M/23/5/2010:	**Repetition**	**2h**
26-27/5/2010:	**Final Exam (sensor:???)**	

Lecture 9: Crystal vibrations and phonons

• **Examples of phonon-assisted processes**

• **Vibrations of crystals with monatomic basis**

• **Vibrations in a lattice with two atoms per primitive basis**

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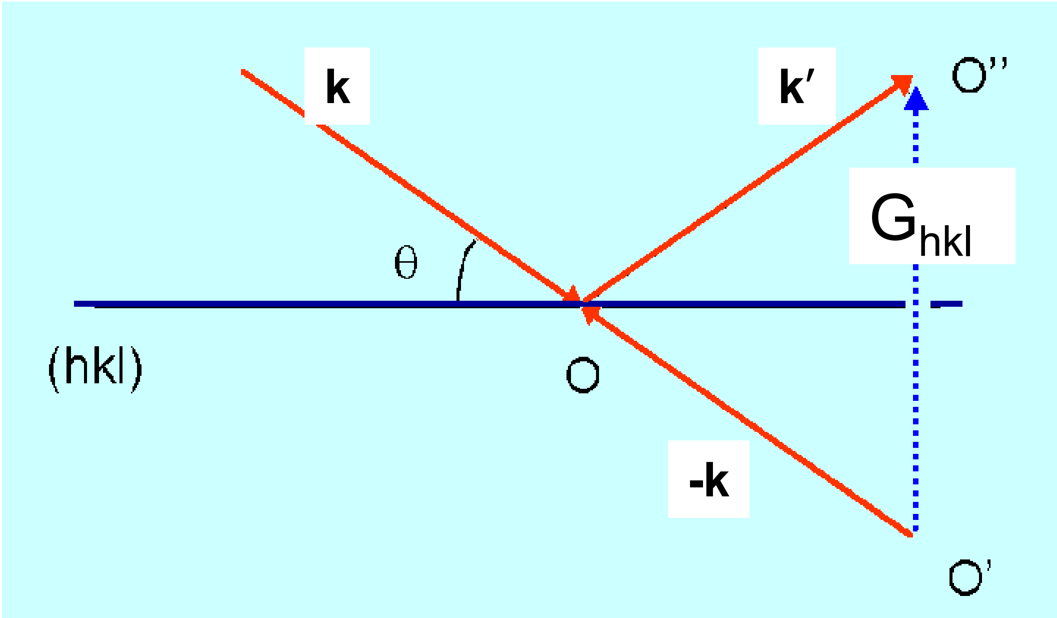
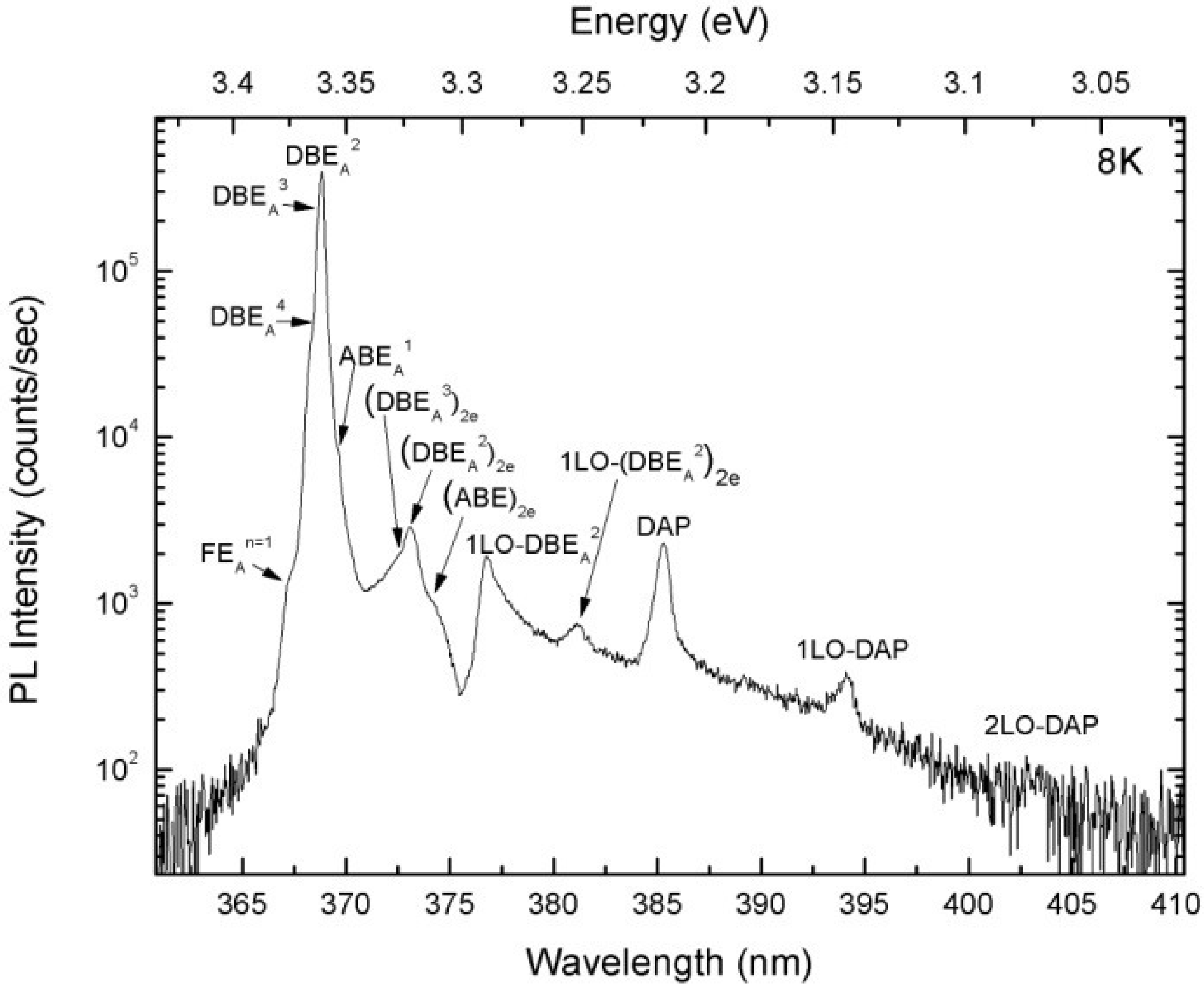
Diffraction



$$\mathbf{k}' \pm \mathbf{K} = \mathbf{k} + \mathbf{G}$$

Photoluminescence



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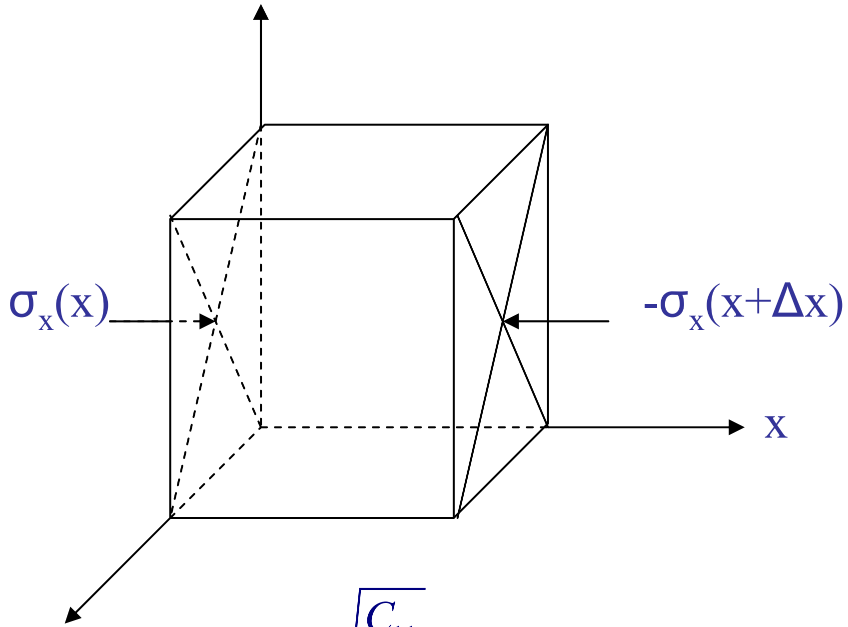
Vibrations in a continuous approximation (repetition)

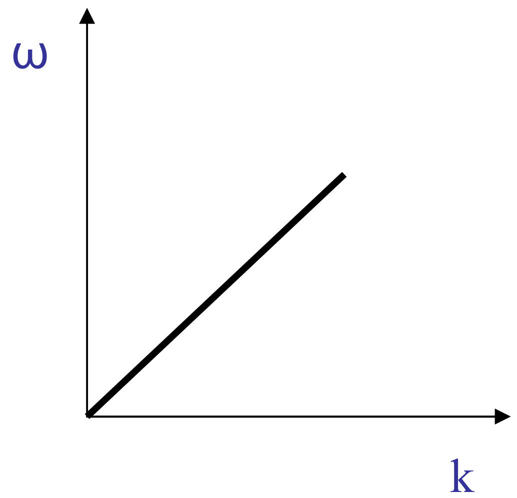


$$\omega_L = \sqrt{\frac{C_{11}}{\rho}}\, k$$

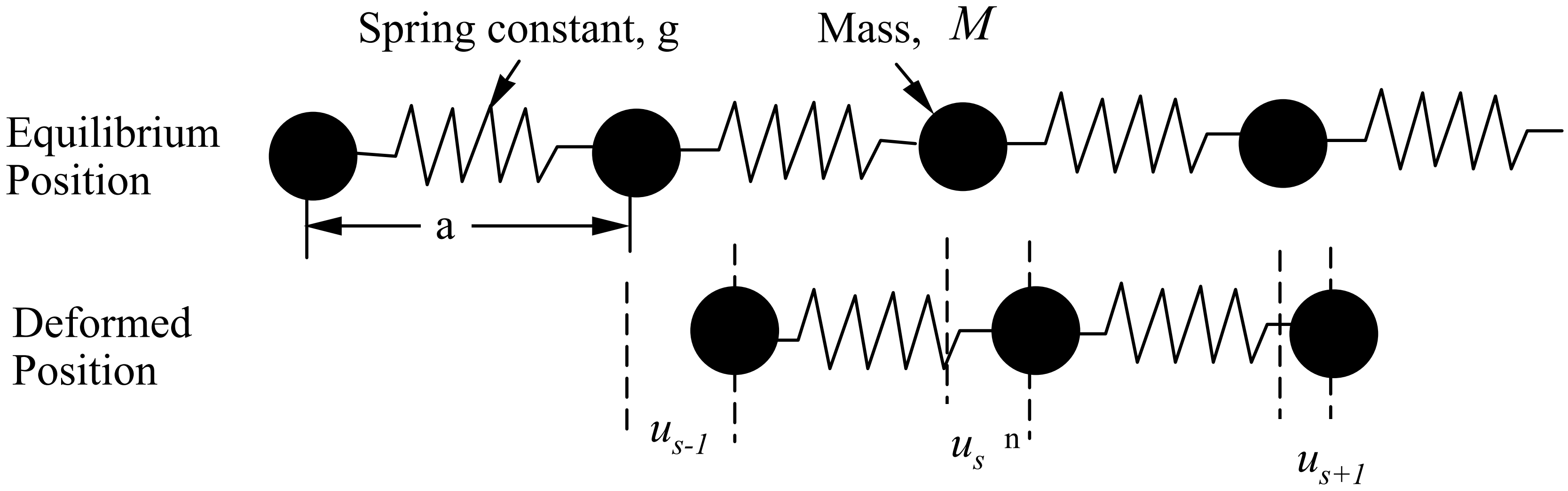
Longitudinal

$$\omega_T = \sqrt{\frac{C_{44}}{\rho}}\, k$$

Transverse

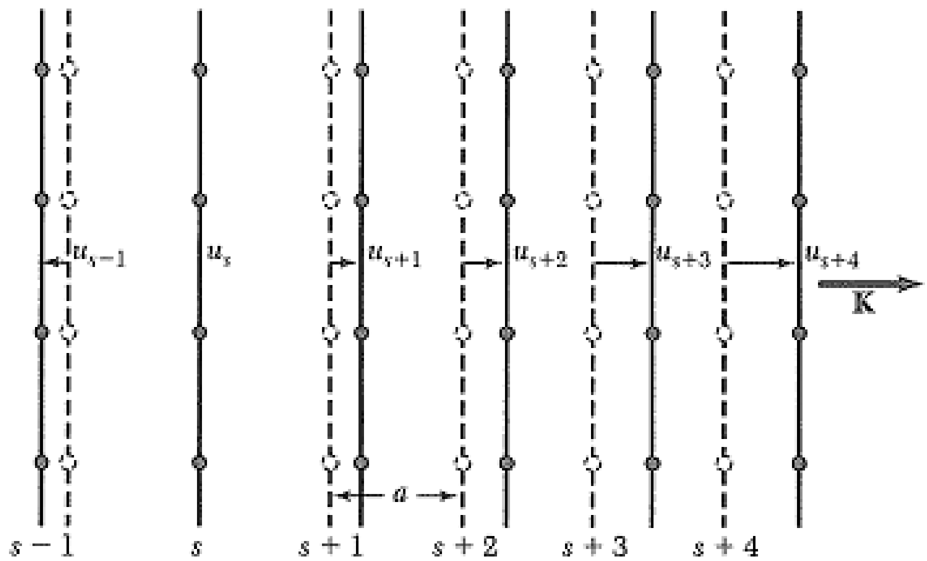


Vibrations of crystals with monatomic basis

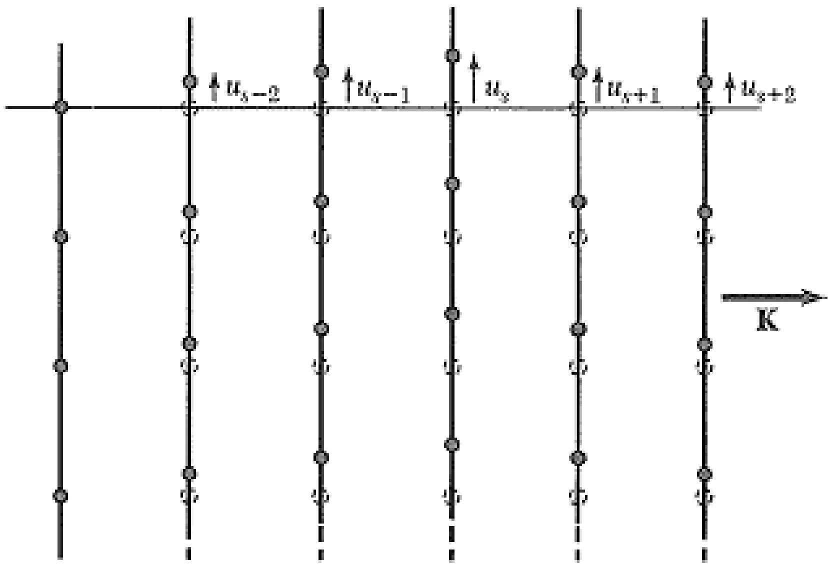


u_s: displacement of the sth atom from its equilibrium position

Propagation along high symmetry directions → 1-D problem
E.g. , [100], [110], [111] in sc lattice.



longitudinal wave



transverse wave

Entire plane of atoms moving in phase → 1-D problem

Force on s^{th} plane = $F_s = -C(u_s - u_{s+1}) - C(u_s - u_{s-1})$ (only neighboring planes interact)

Equation of motion: $M\dfrac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$

$u_s(t) = u_s\, e^{-i\omega t} \quad \rightarrow \quad -M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$

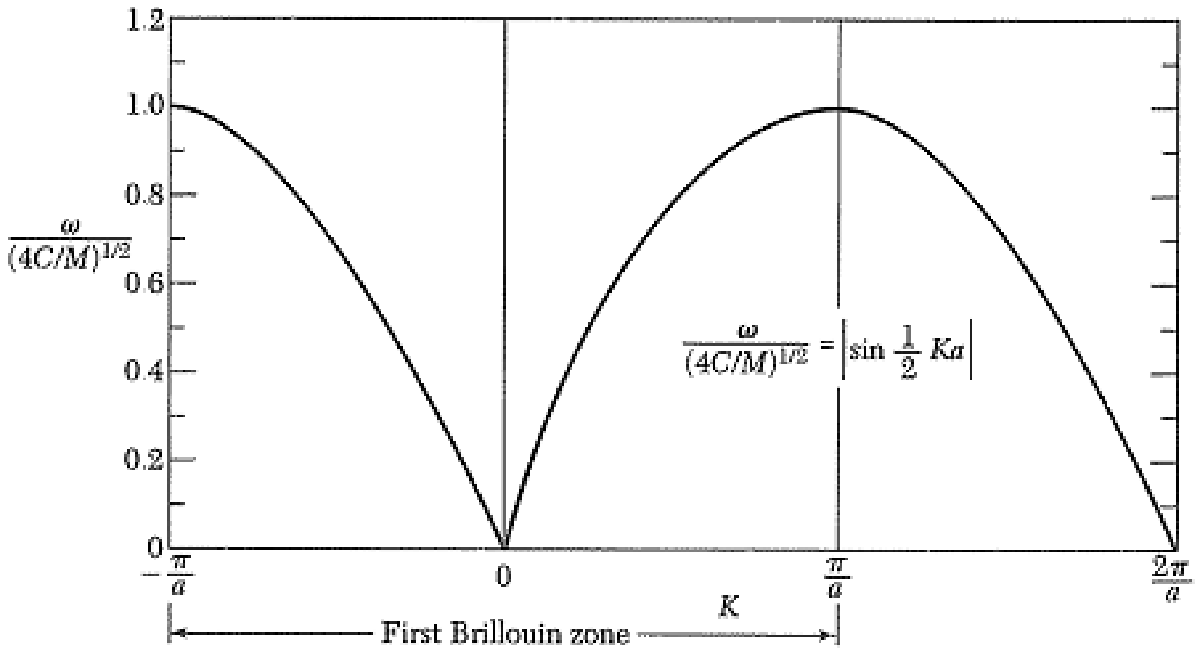
$u_s = u_0\, e^{iKas} \quad \rightarrow \quad -M\omega^2 = C(e^{iKa} + e^{-iKa} - 2)$

$$\omega^2 = \frac{2C}{M}(1 - \cos Ka)$$

Dispersion relation

$$\omega^2 = \frac{4C}{M}\sin^2\frac{1}{2}Ka$$

$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{1}{2}Ka\right|$$

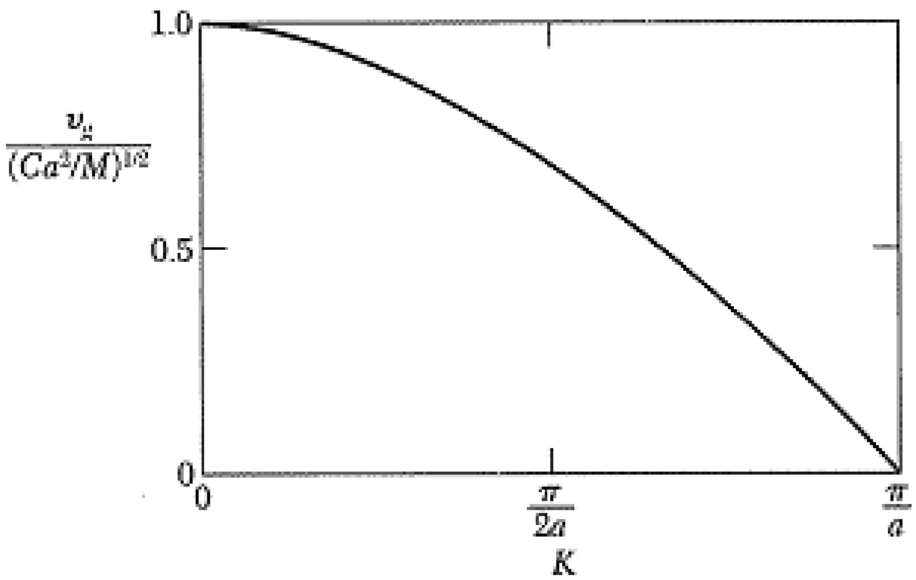


Group Velocity

Group velocity: $\mathbf{v}_g = \nabla_{\mathbf{K}} \omega$

1-D: $v_G = \left| \frac{d\omega}{dK} \right| = \sqrt{\frac{Ca^2}{M}} \left| \cos \frac{1}{2} Ka \right|$ $\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{1}{2} Ka \right|$

$v_G = 0$ at zone boundaries



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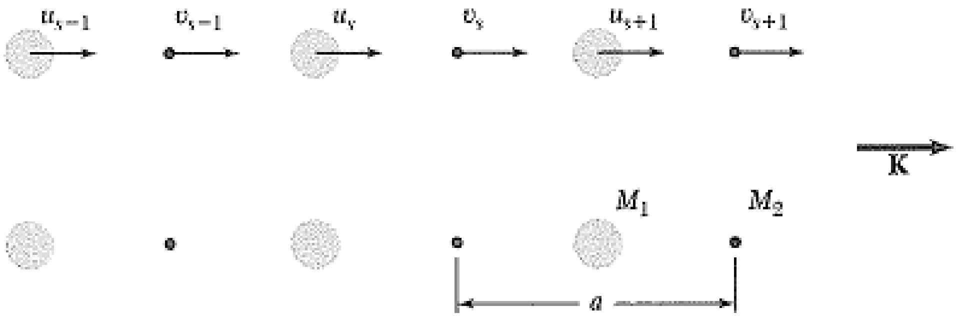
Two Atoms per Primitive Basis



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

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

$$u_s = u e^{isKa - i\omega t}$$

$$v_s = v e^{isKa - i\omega t}$$

$$\rightarrow$$

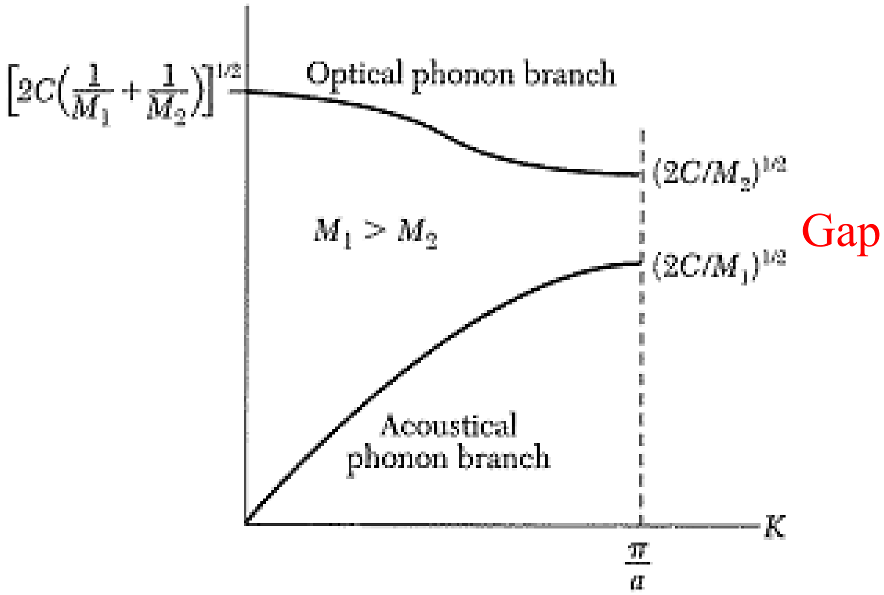
$$-M_1\omega^2 u = Cv\left(1 + e^{-iKa}\right) - 2Cu$$

$$-M_2\omega^2 v = Cu\left(1 + e^{iKa}\right) - 2Cv$$

$$\begin{vmatrix} 2C - M_1\omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2\omega^2 \end{vmatrix} = 0 \quad = M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1 - \cos Ka\right)$$

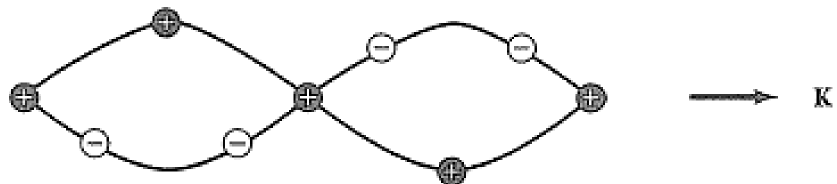
$$M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1 - \cos Ka\right) = 0$$

$Ka \to 0$: $$\omega^2 \approx \begin{cases} 2C\left(\dfrac{1}{M_1} + \dfrac{1}{M_2}\right) & optical \\ \dfrac{C}{2\left(M_1 + M_2\right)} K^2 a^2 & acoustical \end{cases}$$



$Ka \to \pi$:
$(M_1 > M_2)$ $$\omega^2 \approx \begin{cases} \sqrt{2C / M_2} & optical \\ \sqrt{2C / M_1} & acoustical \end{cases}$$

$$\begin{pmatrix} 2C - M_1 \omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2 \omega^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

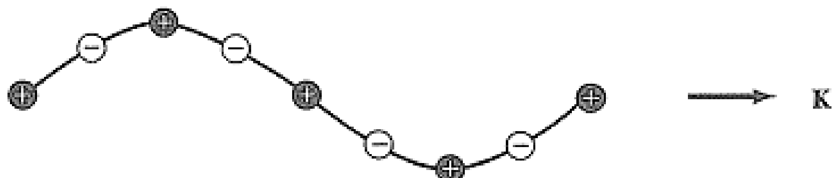


Optical mode

Transverse case:

TO branch, $Ka \to 0$: $$\frac{u}{v} = -\frac{M_2}{M_1}$$

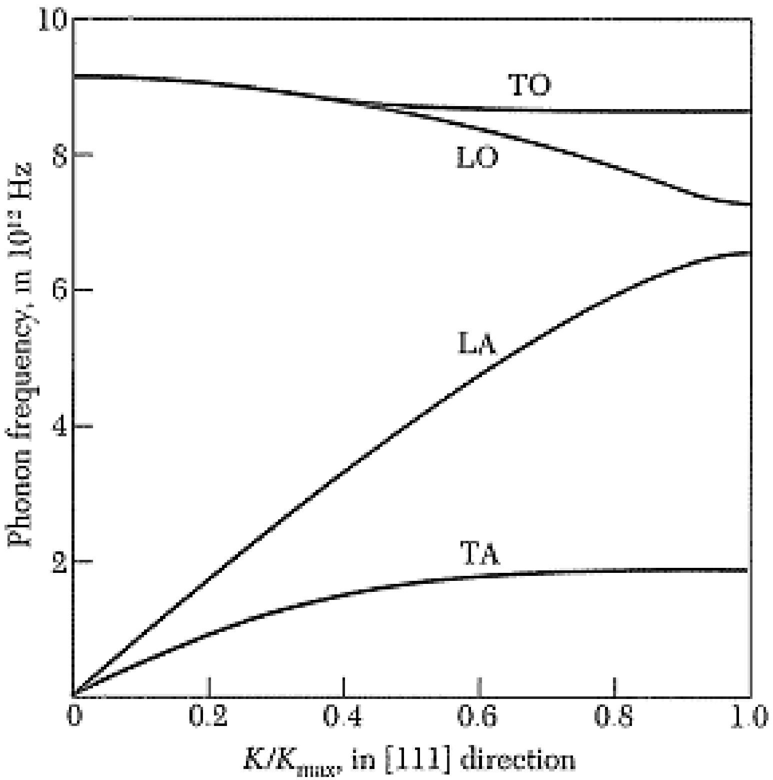
TA branch, $Ka \to 0$: $$\frac{u}{v} = 1$$



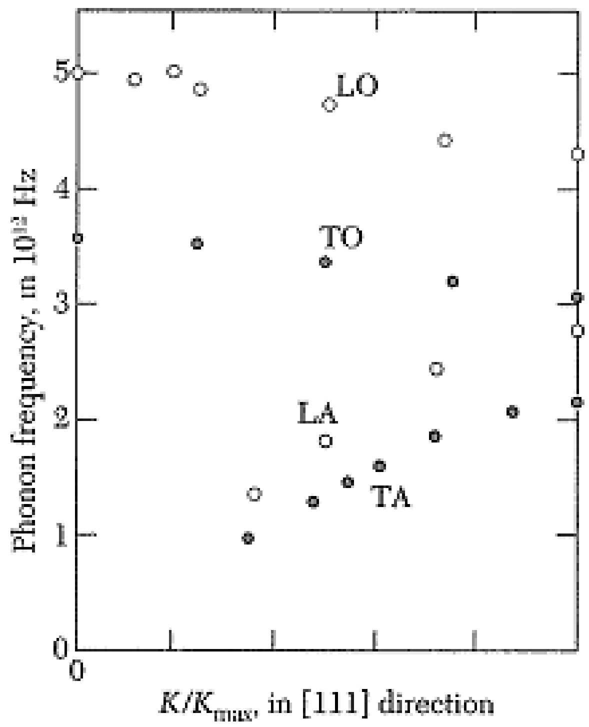
Acoustical mode

p atoms in primitive cell → $d\,p$ branches of dispersion.
$d = 3$ → 3 acoustical : 1 LA + 2 TA
(3p –3) optical: (p–1) LO + 2(p–1) TO

E.g., Ge or KBr: $p = 2$ → 1 LA + 2 TA + 1 LO + 2 TO branches



Ge



KBr

Number of allowed K in 1st BZ = N

Quantization of Elastic Waves

Quantization of harmonic oscillator of angular frequency ω → $\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega$

Classical standing wave: $u(x,t) = u_0 \sin kx \cos \omega t$ $\quad kL = \pi n$

$$K.E.density = \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 = \frac{1}{2}\rho\omega^2 u_0^2 \sin^2 kx \sin^2 \omega t$$

$$\langle K.E.\rangle = L^2 \int_0^L dx \, \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \; K.E.density = \frac{1}{8}\rho\omega^2 u_0^2 V \qquad V = L^3$$

Virial theorem: For a power-law potential $V \sim x^p$ $\quad 2\langle K.E.\rangle = p\langle P.E.\rangle$

For a harmonic oscillator, $p = 2$, $\quad \langle K.E.\rangle = \langle P.E.\rangle = \frac{1}{2}\varepsilon_n = \frac{1}{8}\rho\omega^2 u_0^2 V$

$$u_0^2 = \frac{4\hbar}{\rho V \omega}\left(n + \frac{1}{2}\right)$$

Phonon Momentum

Phonon DOFs involve relative coordinates
$\rightarrow$ phonons do not carry physical linear momenta (except for $\boldsymbol{K} = \mathbf{G}$ modes)
Reminder: $\boldsymbol{K} = \mathbf{G} \rightarrow \boldsymbol{K} = \mathbf{0}$ when restricted to 1st BZ .

Proof:
See 7th ed.

Scattering of a phonon with other particles behaves as if it has momentum $\eta\, \mathbf{K}$

E.g., elastic scattering of X-ray: $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ $\quad$ $\mathbf{G}$ = reciprocal lattice vector

(whole crystal recoil with momentum $\eta\, \mathbf{G}$ / Bragg reflection)

Inelastic scattering with a phonon created: $\mathbf{k}' + \mathbf{K} = \mathbf{k} + \mathbf{G}$

Inelastic scattering with a phonon absorbed: $\mathbf{k}' = \mathbf{k} + \mathbf{G} + \mathbf{K}$

Normal Process: $\mathbf{G} = \mathbf{0}$.
Umklapp Process: $\mathbf{G} \neq \mathbf{0}$.

Inelastic Scattering by Phonons

Neutron scattering:

Conservation of momentum:

$$\mathbf{k}' \pm \mathbf{K} = \mathbf{k} + \mathbf{G}$$

Conservation of energy:

$$\frac{\hbar^2 k^2}{2M_n} = \frac{\hbar^2 k'^2}{2M_n} \pm \hbar\omega$$