FYS3410 - Vår 2010 (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
- Crystal binding, elastic strain and waves
- Imperfections in crystals: point defects and diffusion
- **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 2010

M/18/1/2010:	Introduction and motivation. Periodicity and lattices	2h
W/20/1/2010:	Index system for crystal planes. Crystal structures	1h
M/25/1/2010:	Reciprocal space, Laue condition and Ewald construction	2h
W/27/1/2010:	Brillouin Zones. Interpretation of a diffraction experiment	1h
M/01/2/2010:	Crystal binding, elastic strain and waves	2h
W/03/2/2010:	Elastic waves in cubic crystals; defects in crystals	1h
M/08/2/2010:	Defects in crystals; case study - vacancies	2h
W/10/2/2010:	Diffusion	1h
M/15/2/2010:	Crystal vibrations and phonons	2h
W/17/2/2010:	Crystal vibrations and phonons	1h
M/22/2/2010:	Planck distribution and density of states	2h
W/24/2/2010:	Debye model	1h
M/01/3/2010:	Einstein model and general result for density of states	2h
W/03/3/2010:	Thermal conductivity	1h
M/08/3/2010:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/10/3/2010:	Density of states, effect of temperature – FD distribution	1h
M/15/3/2010:	Heat capacity of FEFG	2h
W/17/3/2010:	Repetition	1h
22/3/2010:	Mid-term exam	

M/14/4/2010:	Electrical and thermal conductivity in metals	2h
W/12/4/2010:	Bragg reflection of electron waves at the boundary of BZ	1h
M/19/4/2010:	Energy bands, Kronig - Penny model	2h
W/21/4/2010:	Empty lattice approximation; number of orbitals in a band	1h
M/26/4/2010:	Semiconductors, effective mass method, intrinsic carriers	2h
W/28/4/2010:	Impurity states in semiconductors and carrier statistics	1h
M/03/5/2010:	p-n junctions and heterojunctions	2h
W/05/5/2010:	surface structure, surface states, Schottky contacts	2h
M/10/5/2010:	no lectures	
W/12/5/2010:	no lectures	
W/19/5/2010:	Repetition	2h
W26/5/2010:	Repetition	2h
27-28/5/2010:	**Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Aarhus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)**	

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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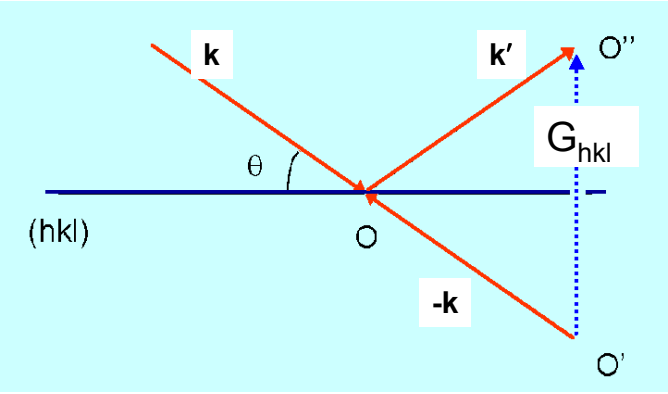
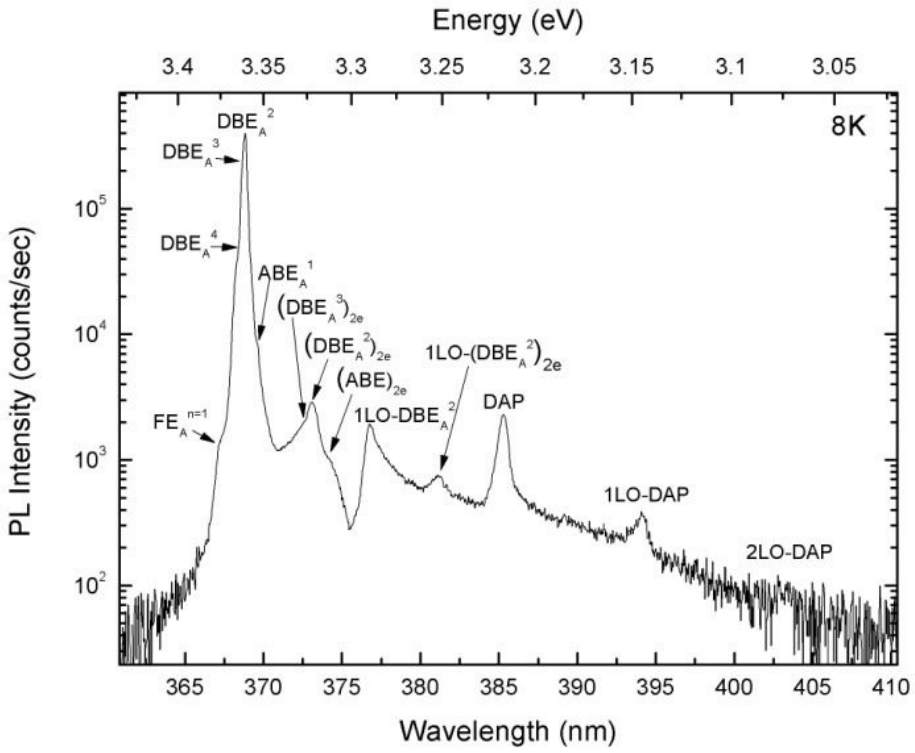
Diffraction



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

Photoluminescence



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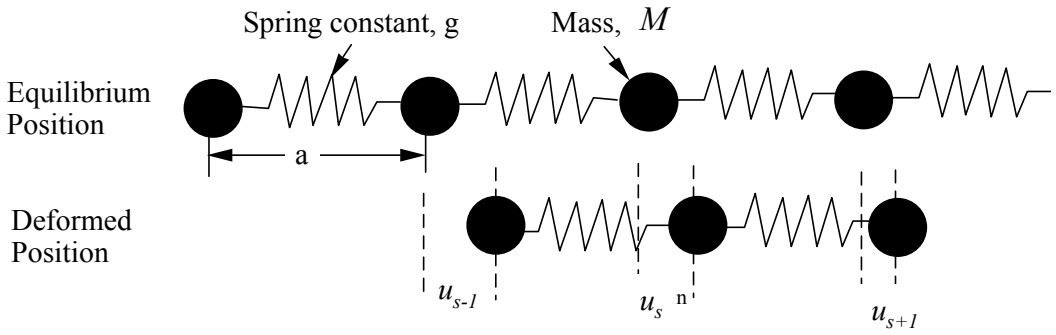
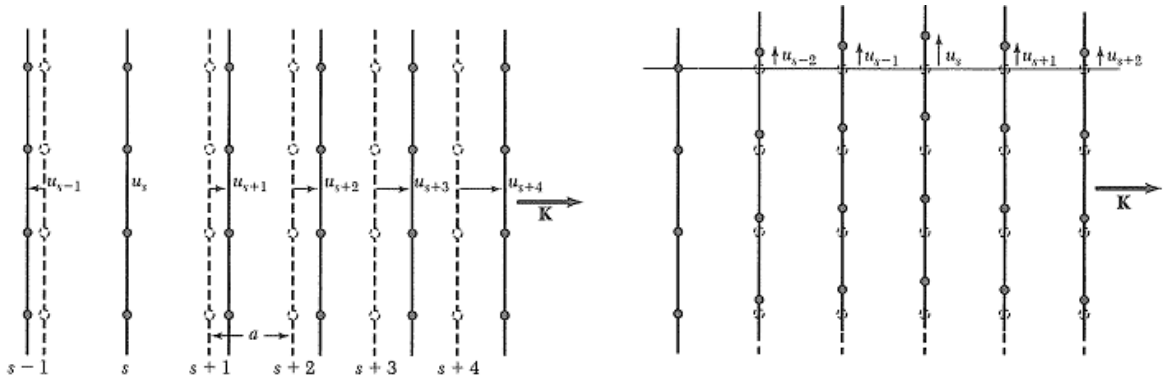
Vibrations of crystals with monatomic basis



u_s: displacement of the s[th] 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 = $F_s = -C\left(u_s - u_{s+1}\right) - C\left(u_s - u_{s-1}\right)$ (only neighboring planes interact)

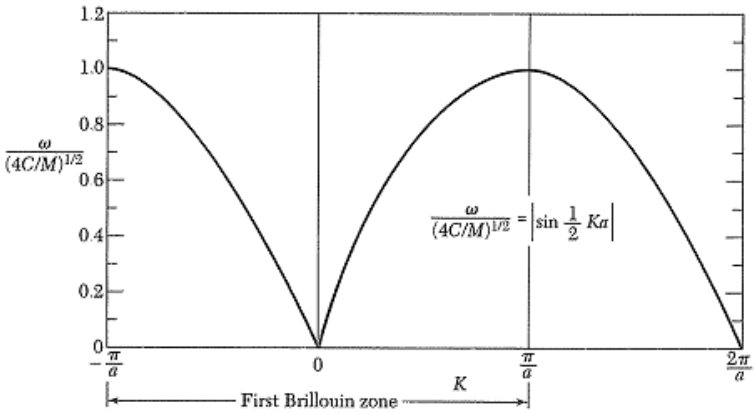
Equation of motion: $M\dfrac{d^2u_s}{dt^2} = C\left(u_{s+1} + u_{s-1} - 2u_s\right)$

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

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

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

Dispersion relation



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

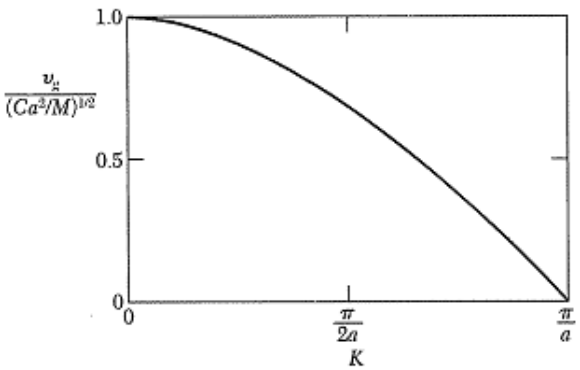
$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{1}{2}Ka\right|$$

Group Velocity

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

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

$v_G = 0$ at zone boundaries



Lecture 9: Crystal vibrations and phonons

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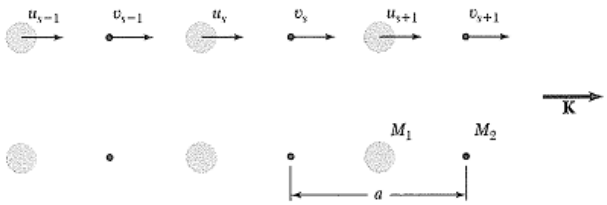
- **Vibrations in a lattice with two atoms per primitive basis**

Two Atoms per Primitive Basis



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

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

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

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

$$\rightarrow$$

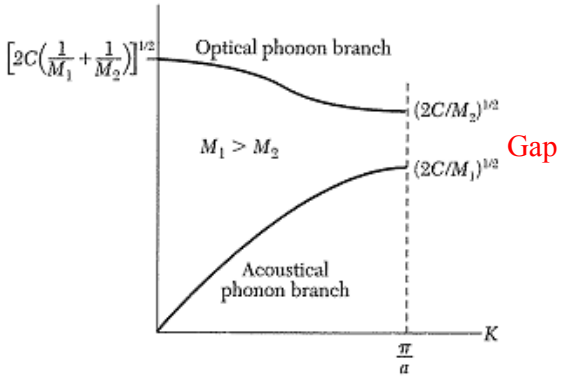
$$-M_1\omega^2 u = Cv\left(1 + e^{-iKa}\right) - 2Cu$$

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

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

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

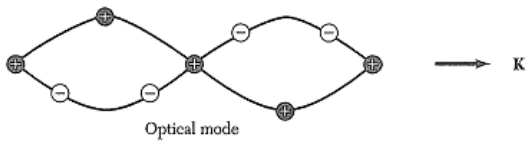
$Ka \to 0$: $\omega^2 = \begin{cases} 2C\left(\dfrac{1}{M_1} + \dfrac{1}{M_2}\right) & \textit{optical} \\ \dfrac{C}{2\left(M_1 + M_2\right)} K^2 a^2 & \textit{acoustical} \end{cases}$



Gap

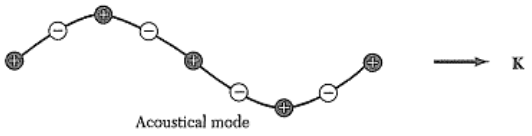
$Ka \to \pi$: ($M_1 > M_2$) $\omega^2 = \begin{cases} \sqrt{2C/M_2} & \textit{optical} \\ \sqrt{2C/M_1} & \textit{acoustical} \end{cases}$

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



Transverse case:

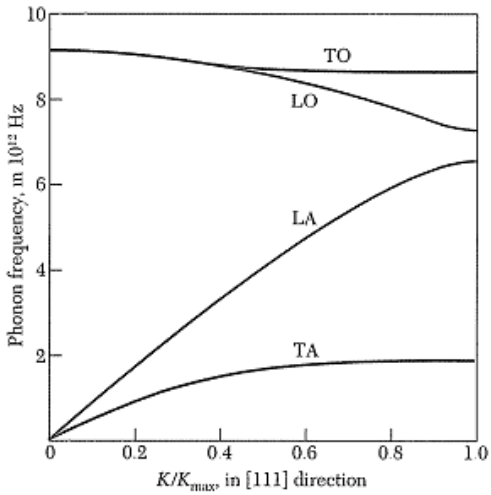
TO branch, $Ka \to 0$: $\dfrac{u}{v} = -\dfrac{M_2}{M_1}$



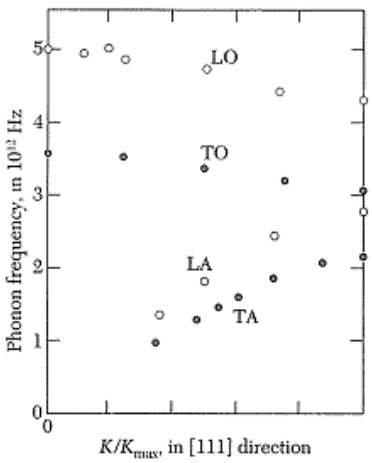
TA branch, $Ka \to 0$: $\dfrac{u}{v} = 1$

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: $u(x,t) = u_0 \sin kx \cos\omega t$ $\qquad kL = \pi n$

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

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

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

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

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

Phonon Momentum

Phonon DOFs involve relative coordinates
→ 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: $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ $\qquad$ **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:

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