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:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
W/24/2/2010:	Phonon density of states (DOS) and Debye model	1h
M/01/3/2010:	General result for DOS; role of anharmonic interactions	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 14: Thermal conductivity

- **Repetition: anharmonic crystal interactions – thermal expansion**
- **Phenomenological description of thermal conductivity**
- **Temperature dependence of thermal conductivity as a cause of phonon scattering**
- **Phonon collisions: N and U processes**

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Anharmonic Properties of Solids

Two important physical properties that ONLY occur because of anharmonicity in the potential energy function:

1. Thermal expansion
2. Thermal resistivity (or finite thermal conductivity)

Thermal expansion

In a 1-D lattice where each atom experiences the same potential energy function U(x), we can calculate the average displacement of an atom from its T=0 equilibrium position:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-U(x)/kT} dx}{\int_{-\infty}^{+\infty} e^{-U(x)/kT} dx}$$

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Thermal Expansion in 1-D

Evaluating this for the harmonic potential energy function U(x) = cx^2 gives:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-cx^2/kT} dx}{\int_{-\infty}^{+\infty} e^{-cx^2/kT} dx}$$

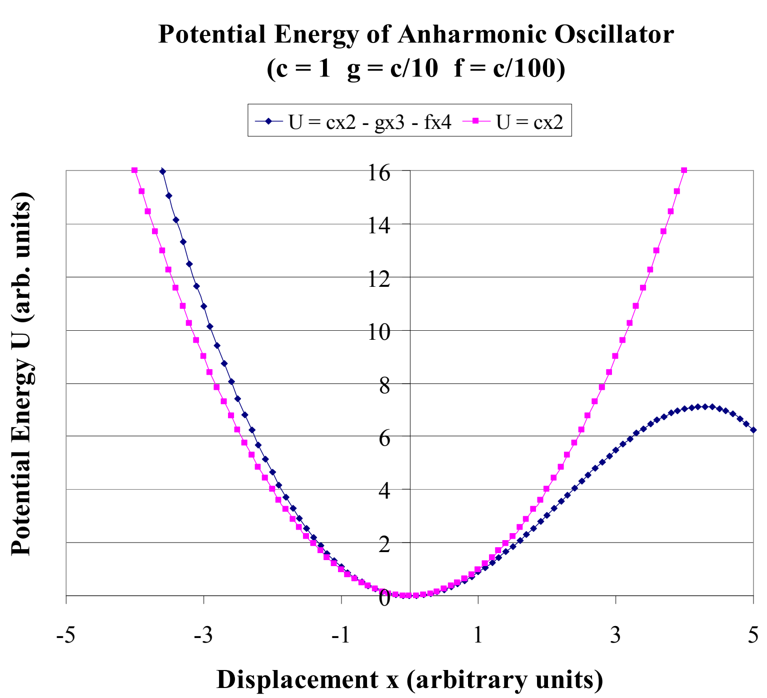
Now examine the numerator carefully…what can you conclude?

$\langle x \rangle = 0\,!$ independent of T !

Thus any nonzero <x> must come from terms in U(x) that go beyond x^2. For HW you will evaluate the approximate value of <x> for the model function

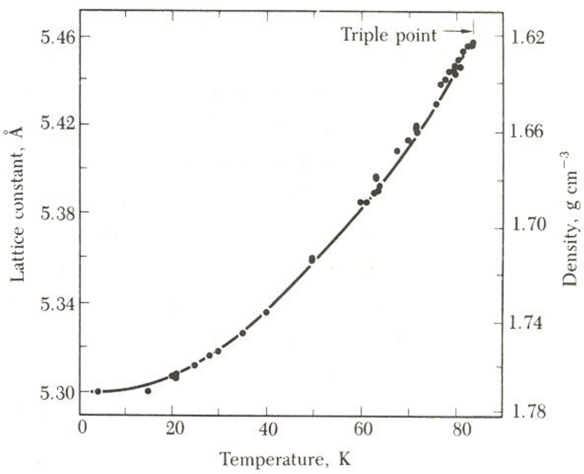
$$U(x) = cx^2 - gx^3 - fx^4 \qquad (c,\, g,\, f > 0 \quad and \quad gx^3,\, fx^4 << kT)$$

Why this form? On the next slide you can see that this function is a reasonable model for the kind of U(r) we have discussed for molecules and solids.



Do you know what form to expect for <x> based on experiment?

Lattice Constant of Ar Crystal vs. Temperature



Above about 40 K, we see: $a(T) - a(0) \propto \langle x \rangle \propto T$

Usually we write: $L = L_0\left(1 + \alpha\left[T - T_0\right]\right)$ α = thermal expansion coefficient

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Phenomenological description of thermal conductivity

When thermal energy propagates through a solid, it is carried by lattice waves or phonons. If the atomic potential energy function is harmonic, lattice waves obey the superposition principle; that is, they can pass through each other without affecting each other. In such a case, propagating lattice waves would never decay, and thermal energy would be carried with no resistance (infinite conductivity!). So…thermal resistance has its origins in an anharmonic potential energy.

low T

high T

Thermal energy flux (J/m^{2}s)

$$J = -\kappa \frac{dT}{dx}$$

Classical definition of thermal conductivity

$$\kappa = \frac{1}{3} C_V v \Lambda$$

C_V heat capacity per unit volume

v wave velocity

Λ mean free path of scattering (would be ∞ if no anharmonicity)

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Temperature dependence of thermal conductivity as a cause of phonon scattering

There are three basic mechanisms to consider:

1. Impurities or grain boundaries in polycrystalline sample
2. Sample boundaries (surfaces)
3. Other phonons (deviation from harmonic behavior)

} deviation from perfect crystalline order

To understand the experimental dependence $\kappa(T)$, consider limiting values of C_V and Λ (since v does not vary much with T).

$$C_V \begin{cases} \propto T^3 & low\,T \\ 3R & high\,T \end{cases}$$

$$\Lambda \propto \frac{1}{n_{ph}} = e^{\hbar\omega/kT} - 1 \begin{cases} \to \infty & low\,T \\ \frac{\hbar\omega}{kT} & high\,T \end{cases}$$

Temperature dependence of thermal conductivity as a cause of phonon scattering

The low and high T limits are summarized in this table:

	C_V	Λ	κ
low T	$\propto T^3$	$n_{ph} \to 0$, so $\Lambda \to \infty$, but then $\Lambda \to D$ (size)	$\propto T^3$
high T	3R	$\propto 1/T$	$\propto 1/T$

How well does this match experimental results?

Temperature dependence of thermal conductivity as a cause of phonon scattering

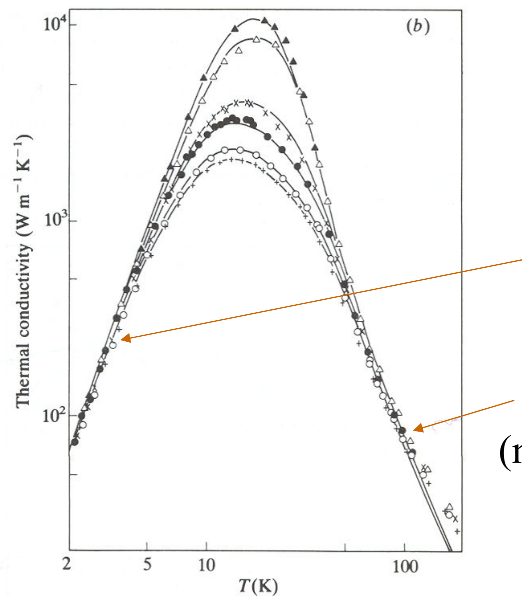

Figure 5.27 (a) The principal form for the variation of thermal conductivity. (b) Experimental data for LiF crystals containing different amounts of the isotope ^{6}Li: ▲, 0.02% ^{6}Li; △, 0.01%; ×, 4.6%; ●, 9.4%; ○, 25.4%; +, 50.1%. (After Berman and Brock 1965.)

Experimental $\kappa(T)$

$\propto T^3$

$\propto T^{-1}$?

(not quite)

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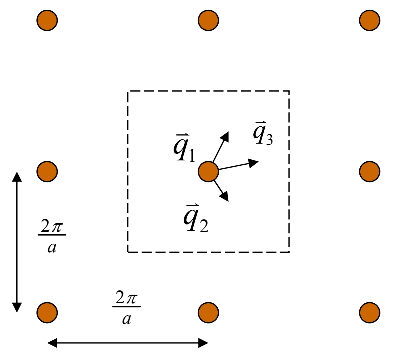
Phonon collisions: N and U processes

How exactly do phonon collisions limit the flow of heat?

2-D lattice → 1st BZ in k-space:



$$\hbar\vec{q}_1 + \hbar\vec{q}_2 = \hbar\vec{q}_3$$

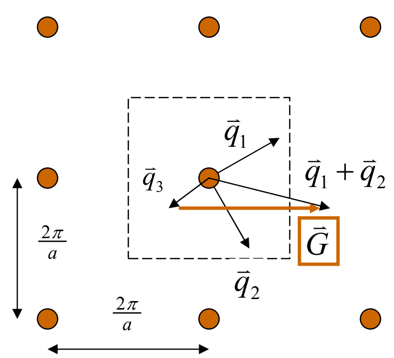
No resistance to heat flow
(N process; phonon momentum conserved)

→ Predominates at low T << θ_D since ω and q will be small

Phonon collisions: N and U processes

What if the phonon wavevectors are a bit larger?

2-D lattice → 1st BZ in k-space:



$$\hbar\vec{q}_1 + \hbar\vec{q}_2 = \hbar\vec{q}_3 + \hbar\vec{G}$$

Two phonons combine to give a net phonon with an opposite momentum! This causes resistance to heat flow.
(U process; phonon momentum "lost" in units of ħG.)

→ More likely at high T >> θ_D since ω and q will be larger

Umklapp = "flipping over" of wavevector!