

FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

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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/ani@phys.au.dk)	

Lecture 13: Debye model, general results for DOS, anharmonic interactions

- **Repetition: Calculating phonon density of states – DOS – in 1-, 2- and 3-dimensions**
- **Debye model: explaining approximations and derivation of T^3 temperature dependence for heat capacity**
- **Anharmonic crystal interactions**

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Calculating phonon density of states – DOS – in 1-D

Since atoms s and $s+N$ have the same displacement, we can write:

$$u_s = u_{s+N} \longrightarrow ue^{i(ksa-\omega t)} = ue^{i(k(s+N)a-\omega t)} \longrightarrow 1 = e^{ikNa}$$

This sets a condition on
allowed k values:

$$kNa = 2\pi n \rightarrow k = \frac{2\pi n}{Na} \quad n = 1, 2, 3, \dots$$

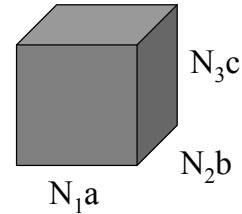
So the separation between
allowed solutions (k values) is:

$$\Delta k = \frac{2\pi}{Na} \quad \Delta n = \frac{2\pi}{Na} \quad \text{independent of } k, \text{ so the density of modes in } k\text{-space is uniform}$$

$$\text{Thus, in 1-D: } \frac{\# \text{ of modes}}{\text{interval of } k\text{-space}} = \frac{1}{\Delta k} = \frac{Na}{2\pi} = \frac{L}{2\pi}$$

Calculating phonon density of states – DOS – in 3-D

Now for a 3-D lattice we can apply periodic boundary conditions to a sample of $N_1 \times N_2 \times N_3$ atoms:



$$\frac{\# \text{ of modes}}{\text{volume of } k\text{-space}} = \frac{N_1 a}{2\pi} \frac{N_2 b}{2\pi} \frac{N_3 c}{2\pi} = \frac{V}{8\pi^3} = N(k)$$

Now we know from before that we can write the differential # of modes as:

$$dN = N(\omega)d\omega = N(k)d^3\vec{k} = \frac{V}{8\pi^3} d^3\vec{k}$$

We carry out the integration in k -space by using a “volume” element made up of a constant ω surface with thickness dk :

$$d^3\vec{k} = (\text{surface area}) dk = \left[\int dS_\omega \right] dk$$

Calculating phonon density of states – DOS – in 3-D

Rewriting the differential number of modes in an interval:

$$dN = N(\omega)d\omega = \frac{V}{8\pi^3} \int dS_\omega dk$$

We get the result:

$$N(\omega) = \frac{V}{8\pi^3} \int dS_\omega \frac{dk}{d\omega} = \frac{V}{8\pi^3} \int dS_\omega \frac{1}{\frac{\partial \omega}{\partial k}}$$

A very similar result holds for $N(E)$ using constant energy surfaces for the density of electron states in a periodic lattice!

This equation gives the prescription for calculating the density of modes $N(\omega)$ if we know the dispersion relation $\omega(k)$.

We can now set up the Debye’s calculation of the heat capacity of a solid.

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Debye model

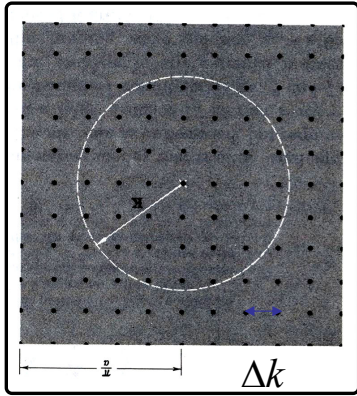
We know that we need to evaluate an upper limit for the heat capacity integral:

$$C_V(T) = \int_{\omega=0}^{\omega_{\max}} N(\omega) C_E(\omega, T) d\omega$$

If the dispersion relation is known, the upper limit will be the maximum ω value. But Debye made several simple assumptions, consistent with a uniform, isotropic, elastic solid:

- 3 independent polarizations (L, T_1 , T_2) with equal propagation speeds v_g
- continuous, elastic solid: $\omega = v_g k$
- ω_{\max} given by the value that gives the correct number of modes per polarization (N)

Lattice heat capacity: Debye model



$$\Delta k = \frac{2\pi}{L}$$

N_k : Allowed number of k points in a sphere with a radius k

$$N_k = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k^3 = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi\omega^3}{3v^3} = \frac{V\omega^3}{6\pi^2v^3}$$

$$D(\omega) = \frac{dN_k}{d\omega} = \frac{V\omega^2}{2\pi^2v^3} \quad \text{Density of states of acoustic phonons for 1 polarization}$$

$$\omega(k) = vk \quad \text{phonon dispersion relation}$$

Debye temperature θ

$$N = \frac{V\omega_D^3}{6\pi^2v^3}$$

$$\hbar\omega_D = k_B\theta$$

$$\theta = \frac{\hbar v}{k_B} \left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}}$$

N : number of unit cell

Thermal energy U and lattice heat capacity C_V : Debye model

3 polarizations for acoustic modes



$$U = 3 \int d\omega D(\omega) n(\omega) \hbar\omega = 3 \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2v^3} \frac{\hbar\omega}{\exp(\hbar\omega/k_B T) - 1}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{3V\hbar^2}{2\pi^2v^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 \exp(\hbar\omega/k_B T)}{[\exp(\hbar\omega/k_B T) - 1]^2}$$

$$C_V = 9Nk_B \left(\frac{T}{\theta}\right)^3 \int_0^{x_D} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

Debye model

Better agreement than Einstein model at low T

Universal behavior for all solids!

Debye temperature is related to “stiffness” of solid, as expected

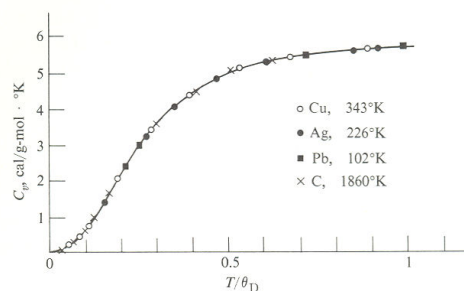


Fig. 3.13 Specific heats versus reduced temperature for four substances. Numbers refer to Debye temperatures. Note the high Debye temperature for diamond.

Table 3.1
Debye Temperatures

Element	$\theta_D, ^\circ\text{K}$	Compound	$\theta_D, ^\circ\text{K}$
Li	335	NaCl	280
Na	156	KCl	230
K	91.1	CaF ₂	470
Cu	343	LiF	680
Ag	226	SiO ₂ (quartz)	255
Au	162		
Al	428		
Ga	325		
Pb	102		
Ge	378		
Si	647		
C	1860		

Debye model

Quite impressive agreement with predicted $C_V \propto T^3$ dependence for Ar! (noble gas solid)

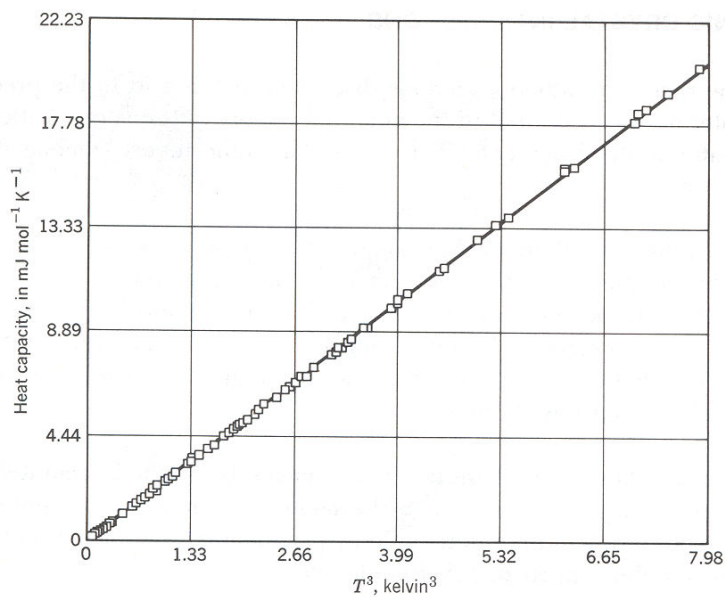


Figure 11 Low temperature heat capacity of solid argon, plotted against T^3 . In this temperature region the experimental results are in excellent agreement with the Debye T^3 law with $\theta_0 = 92.0$ K. (Courtesy of L. Finegold and N. E. Phillips.)

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I 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:

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

I Thermal Expansion in 1-D

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

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

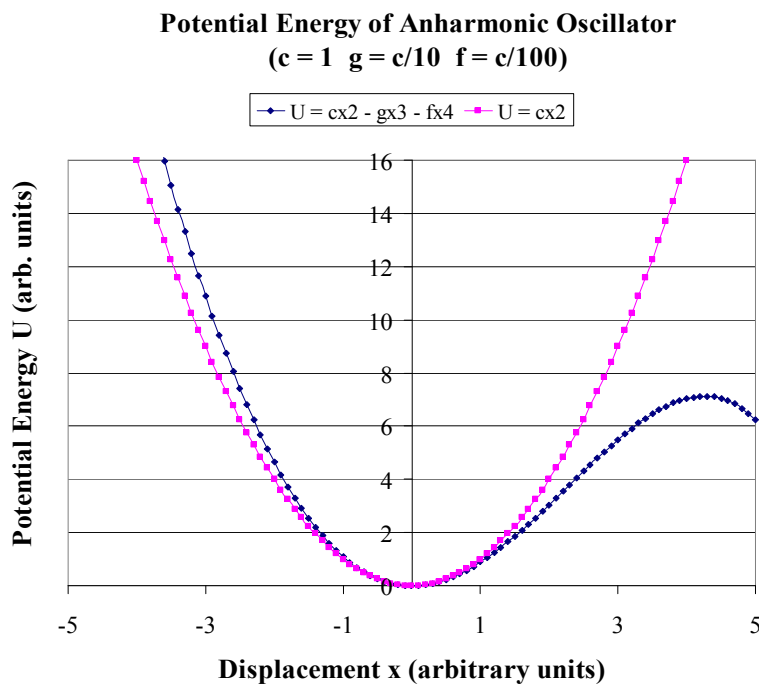
Now examine the numerator carefully... what can you conclude?

$$\langle x \rangle = 0! \quad \text{independent of } T!$$

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

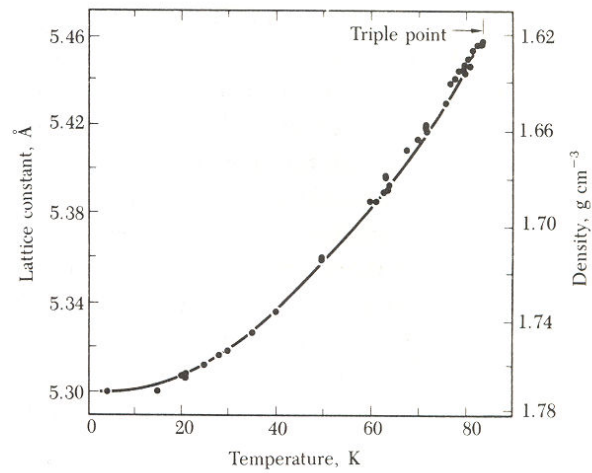
$$U(x) = cx^2 - gx^3 - fx^4 \quad (c, g, f > 0 \text{ and } gx^3, fx^4 \ll kT)$$

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 $\langle x \rangle$ 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: $L = L_0(1 + \alpha[T - T_0])$ α = thermal expansion coefficient