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/anl@phys.au.dk)**	

Lecture 11: Lattice heat capacity: Dulong-Petit and Einstein models

- **Repetition for introduction of phonons and phonon dispersion in real crystals**
- **Classical (Dulong-Petit) theory for heat capacity of solids treating atoms as classical harmonic oscillators**
- **Contribution of electrons in metals and temperature dependence of experimentally measured heat capacitance**
- **Einstein model for heat capacity considering quantum properties of oscillators constituting a solid**
- **Problem of Einstein model to reproduce the rate of heat capacitance decrease at low temperatures and more careful consideration of phonon occupancy modes as a way to improve the agreement with experiment**

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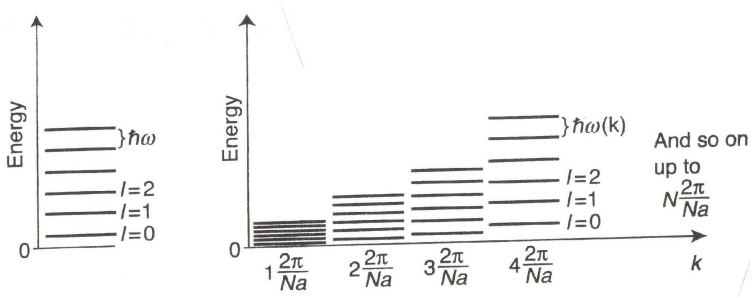
Energy level diagram for one harmonic oscillator

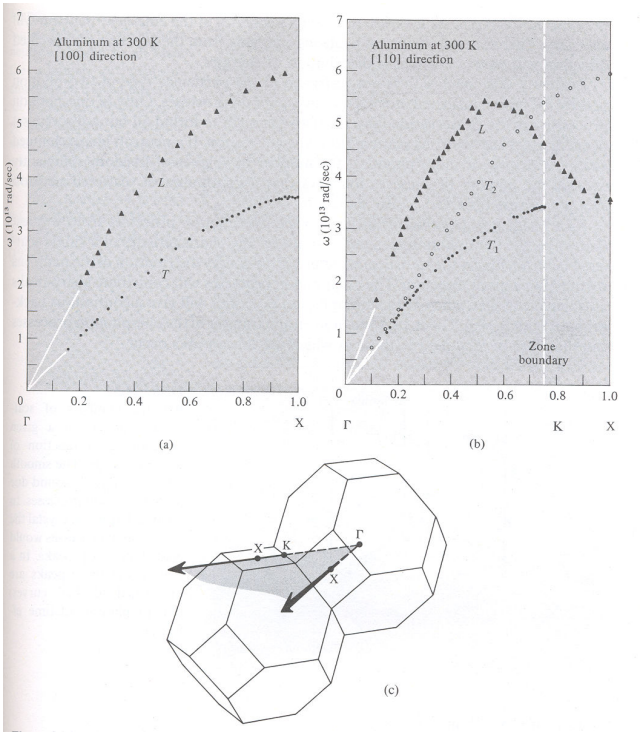


Energy level diagram for a chain of atoms with one atom per unit cell and a lengt of N unit cells

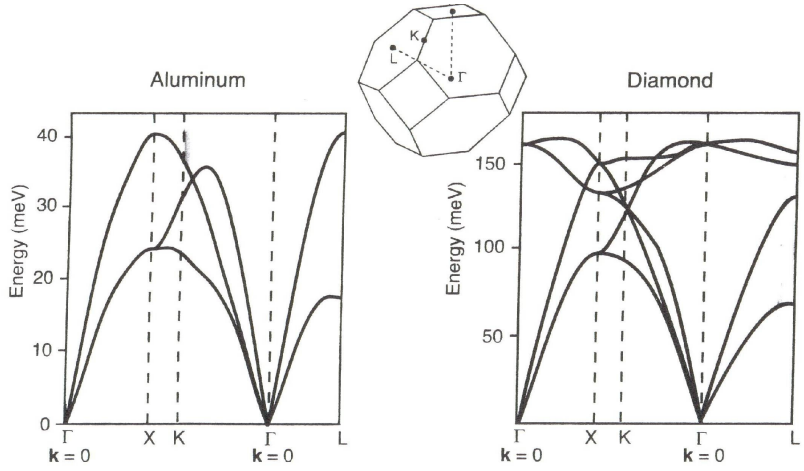
Phonon dispersion in real crystals: aluminium FCC lattice with 1 atom in the basis

In a 3-D atomic lattice we expect to observe 3 different branches of the dispersion relation, since there are two mutually perpendicular transverse wave patterns in addition to the longitudinal pattern we have considered.

Along different directions in the reciprocal lattice the shape of the dispersion relation is different. But note the resemblance to the simple 1-D result we found.



Phonon dispersion in real crystals: FCC lattice with 1 (Al) and 2 (Diamond) atoms in the basis



Characteristic points of the reciprocal space – Γ, X, K, and L points are introduced at the center and bounduries of the first Brillouin zone

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Classical (Dulong-Petit) theory for heat capacity

For a solid composed of N such atomic oscillators: $\overline{E} = N\overline{E}_1 = 3Nk_BT$

Giving a total energy per mole of sample: $\frac{\overline{E}}{n} = \frac{3Nk_BT}{n} = 3N_Ak_BT = 3RT$

So the heat capacity at constant volume per mole is: $C_V = \frac{d}{dT}\left(\frac{\overline{E}}{n}\right)_V = 3R \approx 25 \frac{J}{mol\ K}$

This law of Dulong and Petit (1819) is approximately obeyed by most solids at high T (> 300 K).

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Temperature dependence of experimentally measured heat capacity

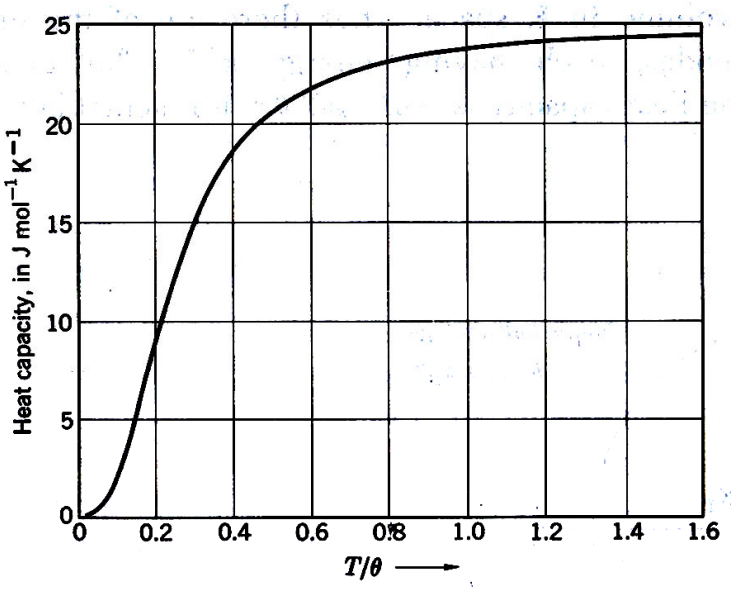

Figure 9a. Heat capacity C_V of a solid, according to the Debye approximation. The vertical scale is in J mol^{-1} K^{-1}. The horizontal scale is the temperature normalized to the Debye temperature θ. The region of the T^3 law is below 0.1θ. The asymptotic value at high values of T/θ is 24.943 J mol^{-1} deg^{-1}.

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Einstein model for heat capacity accounting for quantum properties of oscillators constituting a solid

Planck (1900): vibrating oscillators (atoms) in a solid have quantized energies $E_n = n\hbar\omega \quad n = 0, 1, 2, \ldots$

[later showed $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ actually correct]

Einstein (1907): model a solid as a collection of 3N independent 1-D oscillators, all with constant ω, and use Planck's equation for energy levels

occupation of energy level n: (probability of oscillator being in level n)

$$f(E_n) = \frac{e^{-E_n/kT}}{\sum_{n=0}^{\infty} e^{-E_n/kT}}$$

classical physics (Boltzmann factor)

Average total energy of solid:

$$E = U = 3N\sum_{n=0}^{\infty} f(E_n)E_n = 3N\frac{\sum_{n=0}^{\infty} E_n e^{-E_n/kT}}{\sum_{n=0}^{\infty} e^{-E_n/kT}}$$

Boltzmann factor determines Planck distribution

$$e^{-E_i / kT}$$

Boltzmann factor is a weighting factor that determines the relative probability of a state *i* in a multi-state system in thermodynamic equilibrium at tempetarure *T*.

Where k_B is Boltzmann's constant and E_i is the energy of state *i*. The ratio of the probabilities of two states is given by the ratio of their Boltzmann factors.

Einstein model for heat capacity accounting for quantum properties of oscillators constituting a solid

Using Planck's equation: $U = 3N \dfrac{\sum_{n=0}^{\infty} n\hbar\omega\, e^{-n\hbar\omega/kT}}{\sum_{n=0}^{\infty} e^{-n\hbar\omega/kT}}$ Now let $x \equiv \dfrac{\hbar\omega}{kT}$

$U = 3N\hbar\omega \dfrac{\sum_{n=0}^{\infty} n\, e^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}}$ Which can be rewritten: $U = 3N\hbar\omega \dfrac{-\frac{d}{dx}\sum_{n=0}^{\infty} e^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}} = 3N\hbar\omega \dfrac{-\frac{d}{dx}\sum_{n=0}^{\infty}\left(e^{-x}\right)^n}{\sum_{n=0}^{\infty}\left(e^{-x}\right)^n}$

Now we can use the infinite sum: $\sum_{n=0}^{\infty} x^n = \dfrac{1}{1-x} \quad for \ |x| < 1$ To give: $\sum_{n=0}^{\infty}\left(e^{-x}\right)^n = \dfrac{1}{1-e^{-x}} = \dfrac{e^x}{e^x - 1}$

So we obtain: $U = 3N\hbar\omega \dfrac{-\frac{d}{dx}\left(\frac{e^x}{e^x-1}\right)}{\left(\frac{e^x}{e^x-1}\right)} = \dfrac{3N\hbar\omega}{e^x - 1} = \dfrac{3N\hbar\omega}{e^{\hbar\omega/kT} - 1}$

Einstein model for heat capacity accounting for quantum properties of oscillators constituting solids

Using our previous definition: $$C_V = \frac{d}{dT}\left(\frac{U}{n}\right)_V = \frac{d}{dT}\left(\frac{3N_A\hbar\omega}{e^{\hbar\omega/kT}-1}\right)$$

Differentiating: $$C_V = \frac{-3N_A\hbar\omega\left[e^{\hbar\omega/kT}\left(\frac{-\hbar\omega}{kT^2}\right)\right]}{\left(e^{\hbar\omega/kT}-1\right)^2} = \frac{3R\left(\frac{\hbar\omega}{kT}\right)^2 e^{\hbar\omega/kT}}{\left(e^{\hbar\omega/kT}-1\right)^2}$$

Now it is traditional to define an "Einstein temperature": $$\theta_E \equiv \frac{\hbar\omega}{k}$$

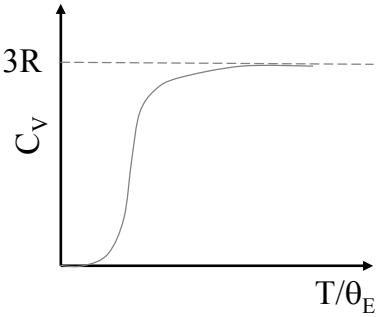
So we obtain the prediction: $$C_V(T) = \frac{3R\left(\frac{\theta_E}{T}\right)^2 e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2}$$

Einstein model for heat capacity accounting for quantum properties of oscillators constituting solids

High T limit: $\frac{\theta_E}{T} << 1$ $$C_V(T) \approx \frac{3R\left(\frac{\theta_E}{T}\right)^2\left(1+\frac{\theta_E}{T}\right)}{\left(1+\frac{\theta_E}{T}-1\right)^2} \approx 3R$$

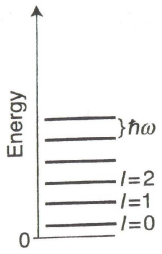
Low T limit: $\frac{\theta_E}{T} >> 1$ $$C_V(T) \approx \frac{3R\left(\frac{\theta_E}{T}\right)^2 e^{\theta_E/T}}{\left(e^{\theta_E/T}\right)^2} \approx 3R\left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}$$

These predictions are qualitatively correct: $C_V \to 3R$ for large T and $C_V \to 0$ as $T \to 0$:



Correlation with energy level diagram for a harmonic oscillator

Energy level diagram for one harmonic oscillator



High T limit: $\frac{\theta_E}{T} << 1$

Low T limit: $\frac{\theta_E}{T} >> 1$

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Problem of Einstein model to reproduce the rate of heat capacity decrease at low temperatures

High T behavior: Reasonable agreement with experiment

Low T behavior: $C_V \rightarrow 0$ too quickly as $T \rightarrow 0$!

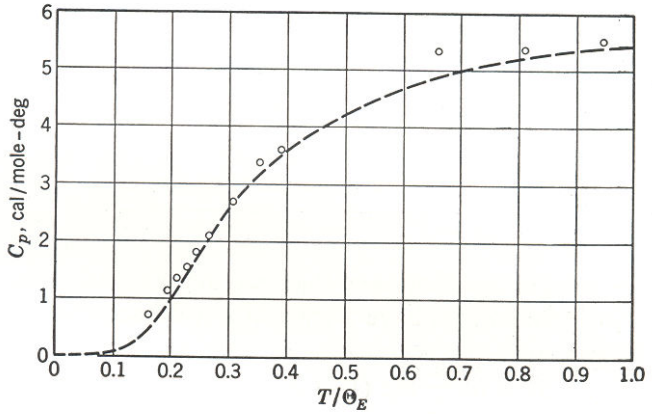
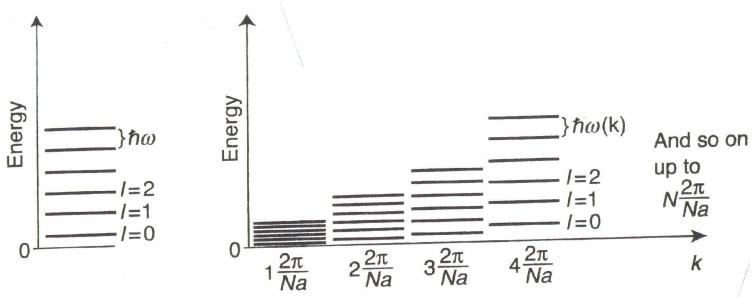


Fig. 6.2. Comparison of experimental values of the heat capacity of diamond and values calculated on the Einstein model, using $\Theta_E = 1320°K$. [After A. Einstein, Ann. Physik **22,** 180 (1907).]

More careful consideration of phonon occupancy modes as a way to improve the agreement with experiment



Energy level diagram for a chain of atoms with one atom per unit cell and a lengt of N unit cells

More careful consideration of phonon occupancy modes as a way to improve the agreement with experiment

Debye's model of a solid:

- 3N normal modes (patterns) of oscillations
- Spectrum of frequencies from $\omega = 0$ to ω_{max}
- Treat solid as continuous elastic medium (ignore details of atomic structure)

This changes the expression for C_V because each mode of oscillation contributes a frequency-dependent heat capacity and we now have to integrate over all ω:

$$C_V(T) = \int_{\omega=0}^{\omega_{max}} \underbrace{D(\omega)}_{\text{\# of oscillators per unit } \omega} \underbrace{C_E(\omega, T)}_{\text{Einstein function for one oscillator}} d\omega$$