

# 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
<b>27-28/5/2010:</b>	<b>Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Aarhus University, Denmark, <a href="http://person.au.dk/en/ani@phys.au.dk">http://person.au.dk/en/ani@phys.au.dk</a>)</b>	

## Lecture 12: Phonon density of states and Debye model

- **Repetition: Einstein model for lattice heat capacity decrease - breakthroughs and limitations**
- **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**

## Lecture 12: Phonon density of states and Debye model

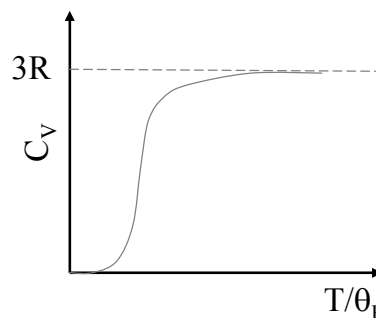
- **Repetition: Einstein model for lattice heat capacity decrease - breakthroughs and limitations**
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### Einstein model for lattice heat capacity decrease - breakthroughs and limitations

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

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

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



## Einstein model for lattice heat capacity decrease - breakthroughs and limitations

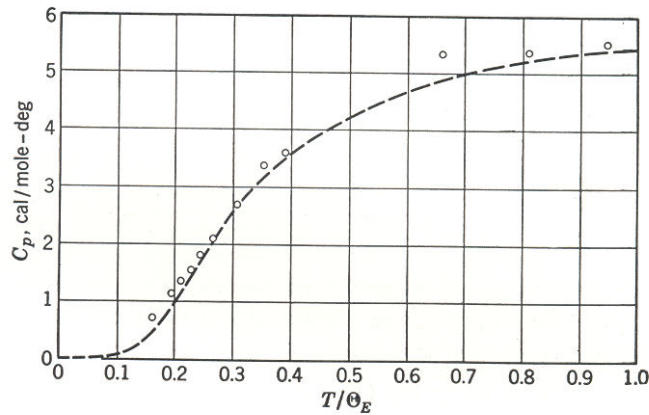


Fig. 6.2. Comparison of experimental values of the heat capacity of diamond and values calculated on the Einstein model, using  $\Theta_E = 1320^\circ\text{K}$ . [After A. Einstein, Ann. Physik **22**, 180 (1907).]

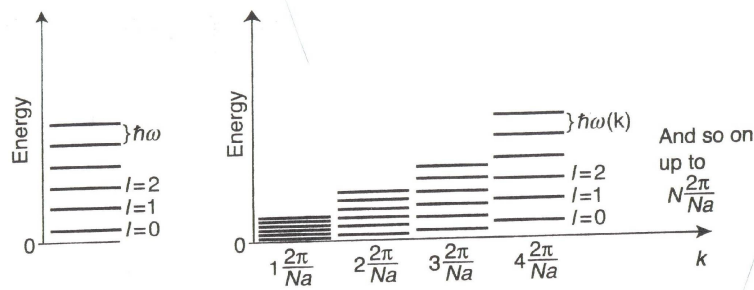
High T behavior:  
Reasonable  
agreement with  
experiment

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

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## Calculating phonon density of states – DOS – in 1-, 2- and 3-D



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

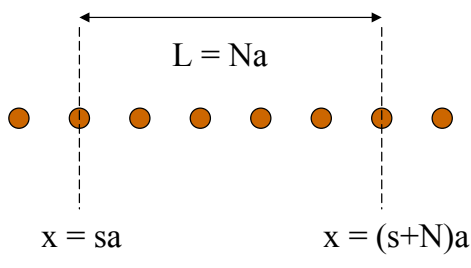
## Calculating phonon density of states – DOS – in 1-D

A vibrational mode is a vibration of a given wave vector  $\vec{k}$  (and thus  $\lambda$ ), frequency  $\omega$ , and energy  $E = \hbar\omega$ . How many modes are found in the interval between  $(\omega, E, \vec{k})$  and  $(\omega + d\omega, E + dE, \vec{k} + d\vec{k})$ ?

$$\# \text{ modes} \quad dN = N(\omega)d\omega = N(E)dE = N(k)d^3\vec{k}$$

We will first find  $N(k)$  by examining allowed values of  $k$ . Then we will be able to calculate  $N(\omega)$  and evaluate  $C_V$  in the Debye model.

First step: simplify problem by using periodic boundary conditions for the linear chain of atoms:



We assume atoms  $s$  and  $s+N$  have the same displacement—the lattice has periodic behavior, where  $N$  is very large.

## 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:

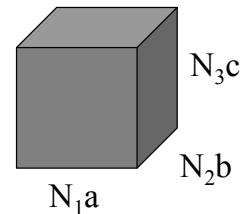
$$\Delta k = \frac{2\pi}{Na} \quad \Delta n = \frac{2\pi}{Na} \quad \text{independent of } k, \text{ so the density of modes in } k\text{-space is uniform}$$

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  $\omega$  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  $\omega(\mathbf{k})$ .

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

### Lecture 12: Phonon density of states and Debye model

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## Debye model

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

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

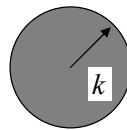
If the dispersion relation is known, the upper limit will be the maximum  $\omega$  value. But Debye made several simple assumptions, consistent with a uniform, isotropic, elastic solid:

- 3 independent polarizations (L, T<sub>1</sub>, T<sub>2</sub>) with equal propagation speeds  $v_g$
- continuous, elastic solid:  $\omega = v_g k$
- $\omega_{\max}$  given by the value that gives the correct number of modes per polarization (N)

## Debye model

First we can evaluate the density of modes:  $v_g = \frac{d\omega}{dk} \longrightarrow N(\omega) = \frac{V}{8\pi^3} \int dS_{\omega} \frac{1}{v_g} = \frac{V}{8\pi^3 v_g} \int dS_{\omega}$

Since the solid is isotropic, all directions in k-space are the same, so the constant  $\omega$  surface is a sphere of radius  $k$ , and the integral reduces to:



$$\int dS_{\omega} = 4\pi k^2$$

Giving:  $N(\omega) = \frac{V}{8\pi^3 v_g} 4\pi k^2 = \frac{V\omega^2}{2\pi^2 v_g^3}$  for one polarization

Next we need to find the upper limit for the integral over the allowed range of frequencies.



## Debye model

Since there are  $N$  atoms in the solid, there are  $N$  unique modes of vibration for each polarization. This requires:

$$\int_{\omega=0}^{\omega_{\max}} N(\omega) d\omega = N$$

$$\text{Giving: } \frac{V}{2\pi^2 v_g^3} \int_{\omega=0}^{\omega_{\max}} \omega^2 d\omega = \frac{V \omega_{\max}^3}{6\pi^2 v_g^3} = N \longrightarrow \omega_{\max} = v_g \left( \frac{6\pi^2 N}{V} \right)^{1/3} \equiv \omega_D$$

The Debye cutoff frequency

Now the pieces are in place to evaluate the heat capacity using the Debye model! This is the subject of problem 5.2 in Myers' book. Remember that there are three polarizations, so you should add a factor of 3 in the expression for  $C_V$ . If you follow the instructions in the problem, you should obtain:

$$C_V(T) = 9Nk_B \left( \frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{z^4 e^z dz}{(e^z - 1)^2}$$

And you should evaluate this expression in the limits of low  $T$  ( $T \ll \theta_D$ ) and high  $T$  ( $T \gg \theta_D$ ).

## 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

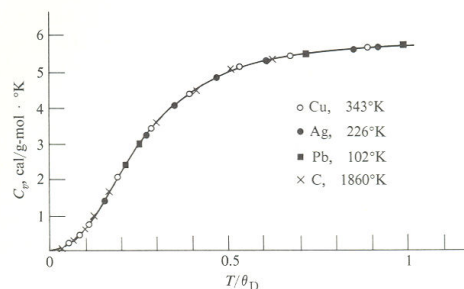


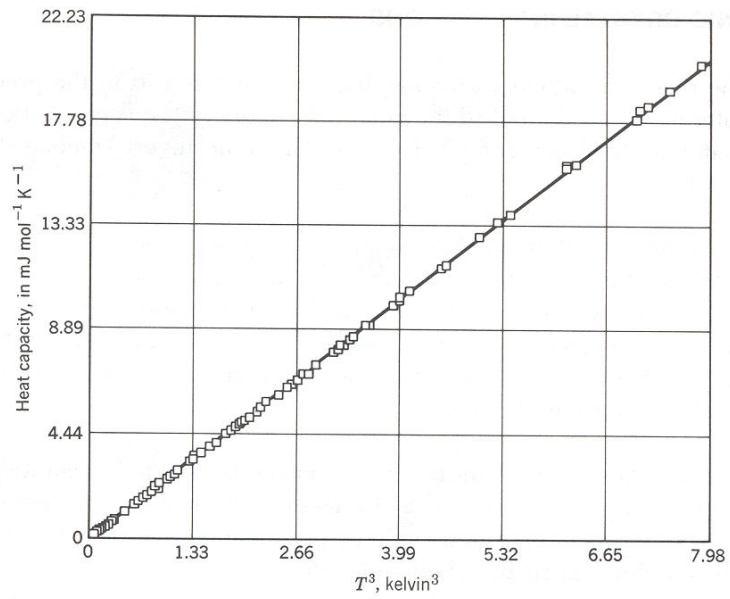
Fig. 3.13 Specific heats versus reduced temperature for four substances. Numbers refer to Debye temperatures. Note the high Debye temperature for diamond.

Table 3.1  
Debye Temperatures

Element	$\theta_D$ , °K	Compound	$\theta_D$ , °K
Li	335	NaCl	280
Na	156	KCl	230
K	91.1	CaF <sub>2</sub>	470
Cu	343	LiF	680
Ag	226	SiO <sub>2</sub> (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.)