

Allowed help:

- periodic table and fundamental constants (distributed)
- formula sheet (distributed)
- pocket calculator, BETA / mathematics handbook or similar

Instructions:

All solutions should be easy to read and have enough details to be followed. The use of nontrivial formulas from the formula sheet should be explained. *Summarize each problem* before its solution, so that the solution becomes self-explained. State any assumptions or interpretation of a problem formulation.

Good luck! / A.R.

1. The atoms in a lattice can be modelled as hard spheres.

a) Calculate the filling fraction of such atoms arranged in *bcc* and *diamond* structure, respectively. (2p)

b) What are the coordination numbers for the atoms in these structures? (0.5p)

c) The *hcp* structure is close-packed. Should this correspond to a lower or higher coordination number? Motivate! (0.5p)

d) The diamond structure does not itself correspond to a Bravais lattice, but can be described as a cubic Bravais lattice with a basis of 8 atoms. However, another Bravais lattice exists that could be used together with a smaller cell / basis to generate the diamond structure. Find the cell volume for this smallest possible cell expressed in the conventional (cubic) lattice parameter a . Motivate clearly. (1p)

See exam 2007-06-20 problem 1

a) $f \approx 0.68$ (bcc)

$f \approx 0.34$ (diamond)

b) 8 (bcc)

4 (diamond)

c) Higher at. density $\longleftrightarrow$ higher coordination #
Close-packed $\longleftrightarrow$ highest ——— (12)

d) Diamond structure = fcc + basis of 2 atoms

Primitive cell of fcc contains 1 atom

$\Rightarrow$ primitive cell of diamond contains 2 atoms

$\Rightarrow$ volume $\frac{2}{8} a^3 = \frac{a^3}{4}$

2. a) Find expressions for the density of states $g(\epsilon)$ for electrons in one, two, and three dimensions. Verify that $g(\epsilon)$ becomes constant in the two-dimensional case. Use the free electron model. (1.5p)
 b) Find corresponding expressions for the Fermi energy ϵ_F in 2D and 3D. (1p)
 c) The electronic specific heat is linear in temperature, $c_{v,el} = \gamma T$. Use the Lorenz number $L = \pi^2 k_B^2 / 3e^2$ and Wiedemann-Franz law to express γ in terms of ϵ_F . Describe used relations. (1.5p)

a, b See Exam 2007-06-20 problem 2a, b

$$a) \quad 1D: \quad g(\epsilon) = \frac{L}{\pi \hbar} \frac{\sqrt{2m}}{\sqrt{\epsilon}}$$

$$2D: \quad g(\epsilon) = \frac{L^2 \cdot m}{2\pi \hbar^2}$$

$$3D: \quad g(\epsilon) = \frac{L^3 (2m)^{3/2}}{4\pi^2 \hbar^3} \sqrt{\epsilon}$$

$$b) \quad \epsilon_F^{2D} = \frac{\pi \hbar^2}{m} \cdot \frac{N}{L^2}$$

$$\epsilon_F^{3D} = \frac{\hbar^2}{2m} \left(3\pi^2 n \right)^{2/3} ; \quad n = \frac{N}{L^3}$$

c) See Exam 2008-06-05 problem 2c

$$c_{el} = \gamma T$$

$$\text{Wiedemann-Franz law: } \frac{\kappa}{\sigma T} = L = \frac{\pi^2 k_B^2}{3e^2}$$

$$\kappa = \frac{1}{3} c \lambda v_F$$

$$\sigma = \frac{ne^2 \tau}{m}$$

$$\Rightarrow \gamma = \frac{\pi^2}{2} n k_B \cdot \frac{k_B}{\epsilon_F}$$

After this, b) above could be used to obtain $\gamma(\epsilon_F)$ without n -dependence

$$\gamma \sim n^{1/3} \sim \sqrt{\epsilon_F} \sim g(\epsilon_F)$$

3. a) Show that the volume v_g of the reciprocal lattice primitive cell is $v_g = (2\pi)^3/v_c$, where v_c is the volume of the direct lattice primitive cell. Hint: $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$. (1.5p)
- b) Describe what a Brillouin zone is. (1p)
- c) Iron (Fe) at room temperature has bcc structure with a lattice parameter $a = 2.87 \text{ \AA}$. Find the maximum k value of the first Brillouin zone in the $\langle 110 \rangle$ direction for iron. (1.5p)

See Exam 2011-03-25, problem #3

a) Use $\bar{\mathbf{a}}_i \cdot \bar{\mathbf{b}}_j = 2\pi\delta_{ij}$ with $\bar{\mathbf{b}}_3 = 2\pi \frac{\bar{\mathbf{a}}_1 \times \bar{\mathbf{a}}_2}{v_c}$

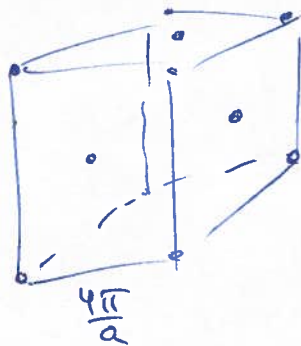
$$v_c = \bar{\mathbf{a}}_1 \cdot (\bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3)$$

$$v_g = \bar{\mathbf{b}}_1 \cdot (\bar{\mathbf{b}}_2 \times \bar{\mathbf{b}}_3)$$

$$\bar{\mathbf{B}} \times (\bar{\mathbf{C}} \times \bar{\mathbf{D}}) = (\bar{\mathbf{B}} \cdot \bar{\mathbf{D}})\bar{\mathbf{C}} - (\bar{\mathbf{B}} \cdot \bar{\mathbf{C}})\bar{\mathbf{D}}$$

b) The B.Z. is a Wigner-Seitz cell in the reciprocal lattice

c) R.L. of bcc is a fcc lattice with side $\frac{4\pi}{a_{\text{bcc}}}$



In $\langle 110 \rangle$ direction, the max k is given by the bisected distance between surface diagonal points,

$$\text{i.e., } \frac{1}{4} \cdot \left(\sqrt{2} \cdot \frac{4\pi}{a} \right) = \frac{\sqrt{2}\pi}{a}$$

4. a) Define what a phonon is and explain the properties that are needed to describe it. (1p)
 b) Discuss the difference between the Debye model and the Einstein model. (1p)
 c) Show how the Bose-Einstein distribution can be obtained starting from the Maxwell-Boltzmann distribution and a harmonic oscillator. (2p)
 Hint: The allowed energies of an oscillator with frequency ν are given by

$$\epsilon_n = \left(n + \frac{1}{2}\right) h\nu, \quad n = 0, 1, 2, \dots \quad (h\nu = \hbar\omega).$$

a) See lecture 12, 13

The phonon is the energy quantum of the elastic wave.

It is completely described by

ω	$E = \hbar\omega$
$\vec{K}$	$\lambda = \frac{2\pi}{ \vec{K} }$
pol. direction	1 L + 2 T in 3D

b) The Einstein model

assumes that all oscillators have the same $\omega = \omega_E$, while the Debye model assumes a linear dispersion, $\omega = v_s |\vec{K}|$

This makes the Einstein model suitable for optical phonons, while Debye is better for acoustic phonons.

c) Use $P_n = \frac{e^{-E_n/k_B T}}{\sum_n e^{-E_n/k_B T}}$ with $E_n = \left(n + \frac{1}{2}\right) \hbar\omega$

$$\langle n \rangle = \sum_{n=0}^{\infty} n \cdot P_n = \left\{ \text{put } x = e^{-\hbar\omega/k_B T} \right\} = \frac{\sum n \cdot x^n}{\sum x^n}$$

Use $\left\{ \begin{array}{l} \sum x^n = \frac{1}{1-x} \\ \sum n \cdot x^n = x \cdot \frac{d}{dx} \sum x^n = x \cdot \frac{d}{dx} \left(\frac{1}{1-x} \right) = \frac{x}{(1-x)^2} \end{array} \right.$

$$\Rightarrow \langle n \rangle = \frac{x}{1-x} = \frac{1}{\frac{1}{x} - 1} = \frac{1}{e^{\hbar\omega/k_B T} - 1} = f_{BE}$$

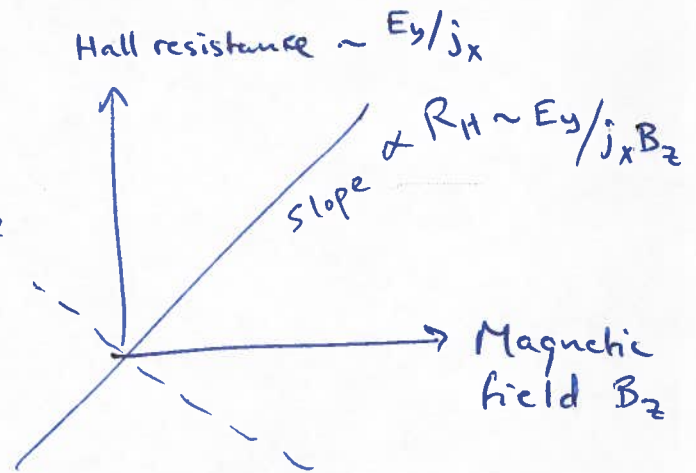
5. Suppose that you have two differently doped semiconductors that you want to investigate. You plan to study Hall effect and Seebeck effect at room temperature, and the temperature dependence of resistivity, thermal conductivity, and specific heat. Discuss what you would expect to see in the measurements by sketching graphs (with labels on the axes) of anticipated behavior. Motivate and explain the graphs! (4p)

Solution:

Hall effect:

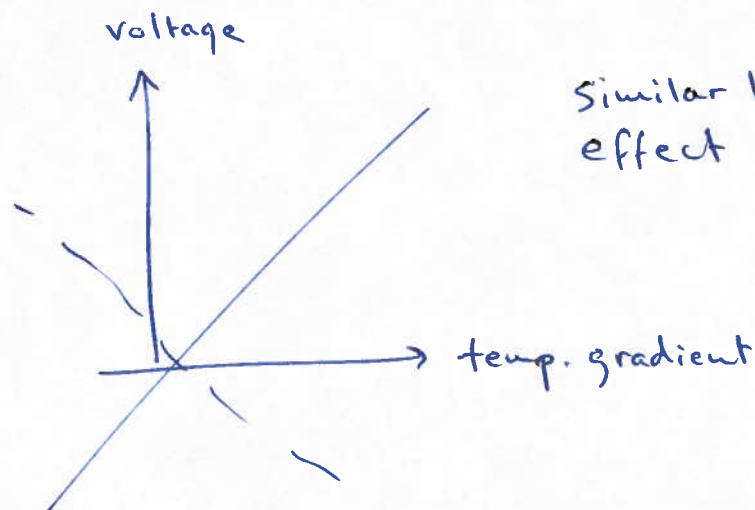
$$R_H = \frac{p - nb^2}{e(p + nb)^2}$$

where $n \cdot p = n_i^2$
and $b = \mu_e / \mu_h$



Complicated, but sign of R_H will give dominant carriers

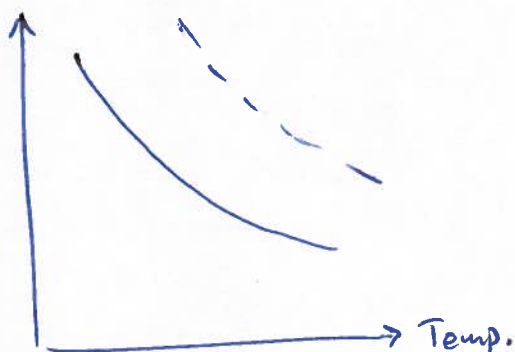
Seebeck effect:



Similar to Hall effect

Resistivity:

Resistivity (Ωm)

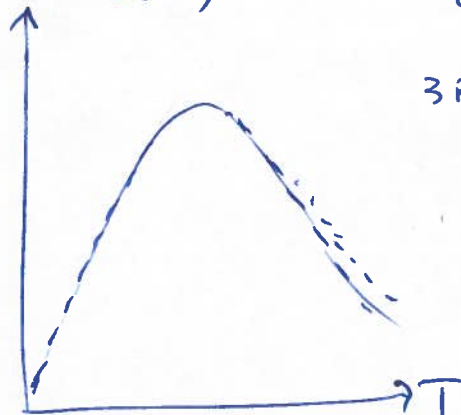


$$\rho \sim \frac{1}{\sigma} \sim \frac{1}{\left(\frac{ne^2\tau}{m}\right)}$$

n thermally activated

Thermal conductivity:

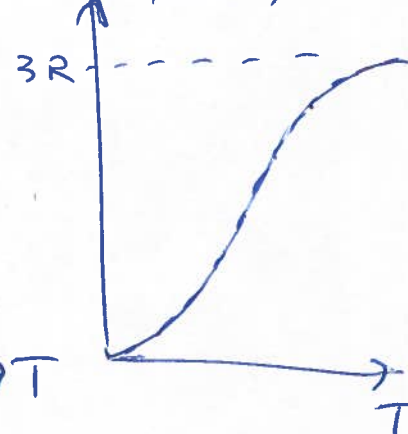
K ($W/m \cdot K$)



Mainly phonons,
since rather low
electron conc.

Specific heat:

C ($J/mol \cdot K$)



Mainly
phonons

6. a) Derive an expression for the Curie temperature in the mean field approximation. Assume an exchange field $B_E = \mu_0 \lambda M$. Describe your starting point. (1.5p)
 b) Discuss how magnetic ions interact. (1p)
 c) Describe the Meissner effect. (1.5p)

a) See Exam 2008-06-05 problem 5b

Start with $M = \frac{\mu_B N}{V} \tanh\left(\frac{\mu_B B}{k_B T}\right)$

If $B = B_E$ (no applied field) $\Rightarrow M = \frac{\mu_B N}{V} \tanh\left(\frac{\mu_0 \mu_B \lambda M}{k_B T}\right)$

set $m = \frac{M \cdot V}{\mu_B N}$

$\Rightarrow m = \tanh\left(\frac{m}{t}\right)$ where $t = \frac{V \cdot k_B T}{\mu_0 \mu_B^2 \lambda N}$

Equation with non-zero m solution

for $t < 1$, i.e., $t = 1 \Leftrightarrow T = T_C$

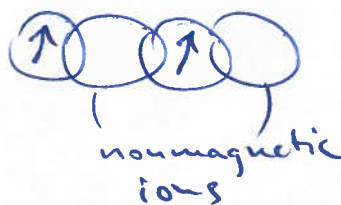
$$T_C = \frac{\mu_0 \mu_B^2 \lambda n}{k_B}$$

b) Main source of interaction between magnetic ions is electrostatic electron-electron interaction.

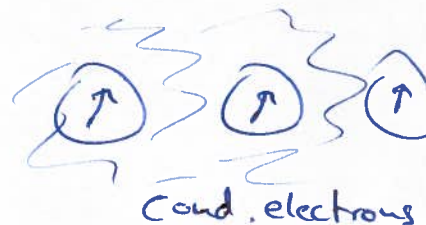
Direct exchange



Superexchange



Indirect exchange



c) See Exam 2007-03-30
#65

Meissner effect: Expulsion of magnetic field
if superconductor cooled below T_C