Exam 2013-03-21
Solutions

STOCKHOLMS UNIVERSITET
FYSIKUM

Examination in Condensed Matter Physics I, FK7042/FK3004, 7.5 hp
Thursday, March 21, 2013, 09.00-14.00.

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.

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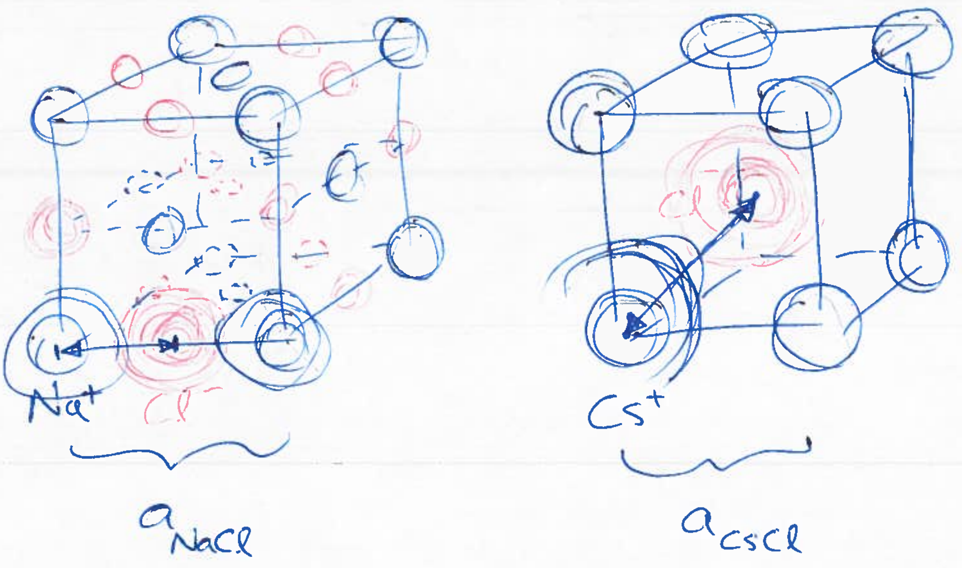
1. Consider two different ionic crystals, sodium chloride (NaCl) and caesium chloride (CsCl). Their lattice parameters are $a_{NaCl} = 5.65$ Å and $a_{CsCl} = 4.12$ Å, respectively. In the structures, the Na^+ ions arrange in an *fcc* lattice, while the Cs^+ ions arrange in a simple cubic (*sc*) lattice. The Cs^+ ion is about 60% larger than the Na^+ ion.
a) Use this information to make a crude estimate of the ionic radii for Na^+, Cs^+, and Cl^-. (2p)
b) Find how much the density of NaCl would change if NaCl had the CsCl structure. (2p)

a)



$r_{Cs} = 1.6\, r_{Na}$

⟷ Nearest neighbors touching

$$r_{Na} + r_{Cl} = \frac{1}{2} a_{NaCl} \qquad r_{Cs} + r_{Cl} = \frac{\sqrt{3}}{2} a_{CsCl}$$

if touch along diagonal

$$\Rightarrow 0.6 \cdot r_{Na} = \underbrace{\frac{\sqrt{3}}{2} a_{CsCl}}_{3.568 \text{ Å}} - \underbrace{\frac{1}{2} a_{NaCl}}_{2.825 \text{ Å}} \Rightarrow r_{Na} \approx 1.24 \text{ Å}$$

$r_{Cl} \approx 1.59$ Å

$r_{Cs} \approx 1.98$ Å

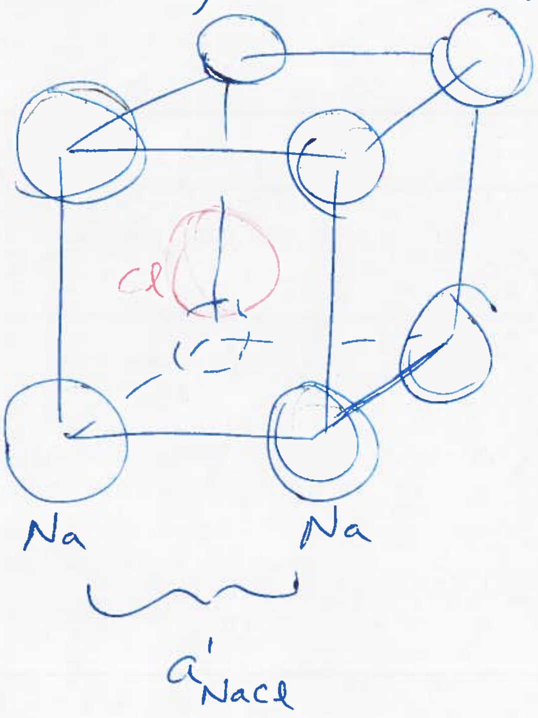
Check: $2 \cdot r_{Cs} < a_{CsCl}$

1b)

Problem: to find how ~~much~~ density would change if NaCl had CsCl structure.

Solution Assume that the ion radii do not change.

That would give this imagined structure:



Eq: $r_{Na} + r_{Cl} = \frac{\sqrt{3}}{2} a'_{NaCl}$

$$\Longrightarrow a'_{NaCl} = \frac{2}{\sqrt{3}}(1.24+1.59)\ \text{Å} = \underline{\underline{3.27\ \text{Å}}}$$

Initial density $= \dfrac{4 \cdot (NaCl)}{(a_{NaCl})^3}$

Final density $= \dfrac{1 \cdot (NaCl)}{(a'_{NaCl})^3}$

Relative change $= \dfrac{\rho_{final} - \rho_{initial}}{\rho_{initial}} = \dfrac{1}{4}\left(\dfrac{a_{NaCl}}{a'_{NaCl}}\right)^3 - 1$

$$= \frac{1}{4}\left(\frac{5{,}65}{3{,}27}\right)^3 - 1 = 0{,}29$$

Answer: The density would increase by 29 %

2. Silver (Ag) is a monovalent metal with a Fermi surface that can be approximated with a sphere. The resistivity of Ag is 3.8 nΩcm at 20 K, its density is 10.5 g/cm^3, and its molar mass is 107.9 g/mol.

a) Calculate the Fermi energy ε_F (in eV), the Fermi velocity v_F (in m/s) and Fermi temperature T_F (in K) for Ag. (1.5p)

b) Calculate the electron density n (in cm^{-3}), the electronic relaxation time τ at low temperatures (20 K), and the corresponding mean free path l for Ag. (1.5p)

c) Discuss the feasibility of performing de Haas–van Alphen experiments on Ag in moderate magnetic fields (B = 1 T) by studying the product $\omega_c\tau$, where ω_c is the cyclotron frequency. (1p)

a) $\varepsilon_F = \{\text{spherical}\} = \dfrac{\hbar^2 k_F^2}{2m}$ where $k_F = (3\pi^2 n)^{1/3}$

Ag is fcc with $a = 4.09$ Å (from periodic system)

The lattice parameter can also be obtained as

$$\frac{4}{a^3} = \text{at. density} = \frac{10.5\ \mathrm{g/cm^3}}{107.9\ \mathrm{g/mol}} \cdot 6.022 \cdot 10^{23}\ \mathrm{at/mol} = 5.86 \cdot 10^{22}\ \mathrm{cm}^{-}$$

$$\Longrightarrow a \approx 4.09\ \text{Å} \iff n = \frac{4}{a^3} = \underline{\underline{5.86 \cdot 10^{22}\ \mathrm{cm^{-3}}}}$$

$$\varepsilon_F = \frac{(1.055 \cdot 10^{-34}\ \mathrm{J\,s})^2 \cdot (3\pi^2 \cdot 5.86 \cdot 10^{28}\ \mathrm{m^{-3}})^{2/3}}{2 \cdot 9.11 \cdot 10^{-31}\ \mathrm{kg}} =$$

$$= \frac{(1.055)^2 \cdot (10^{-34})^2 \cdot (1.73 \cdot 10^{30})^{2/3}}{2 \cdot 9.11 \cdot 10^{-31}}\ \mathrm{J} \cdot \frac{1}{1.602 \cdot 10^{-19}\ \mathrm{J/eV}} =$$

$$= 55 \cdot 10^{-3} \cdot 10^{-68+20+31+19}\ \mathrm{eV} = \underline{\underline{5.5\ \mathrm{eV}}}$$

$$v_F: \quad \varepsilon_F = \frac{m v_F^2}{2} \iff v_F = \frac{\hbar k_F}{m} = \frac{1.055 \cdot 10^{-34}\ \mathrm{Js}}{9.11 \cdot 10^{-31}\ \mathrm{kg}} \cdot (\overbrace{1.73 \cdot 10^{24}}^{3\pi^2 n})^{1/3}\ \mathrm{cm}^{-}$$

$$v_F = 0.139 \cdot 10^{5}\ \frac{\mathrm{kg\,(m/s)^2 \cdot s}}{\mathrm{kg \cdot cm}} = \underline{\underline{1.39 \cdot 10^{6}\ \mathrm{m/s}}}$$

$$\varepsilon_F = k_B T_F \Longrightarrow T_F = \frac{5.5\ \mathrm{eV}}{8.617 \cdot 10^{-5}\ \mathrm{eV/K}} = \underline{\underline{63.8 \cdot 10^{3}\ \mathrm{K}}}$$

Check: Orders of magnitude; reasonable numbers

2b)

$n = 5.86 \cdot 10^{22}\ cm^{-3}$ (see a))

Given : $\rho_{Ag} = 3.8\ n\Omega cm$ @ 20 K el. resistivity

Wanted : τ and l

Solution : $\sigma_{Ag} = \frac{ne^2\tau}{m} = \frac{1}{\rho_{Ag}} \Rightarrow \tau = \frac{m}{ne^2 \cdot \rho_{Ag}}$

$$\tau = \frac{9.11 \cdot 10^{-31}\ kg}{5.86 \cdot 10^{22} (cm)^{-3} \cdot (1.602 \cdot 10^{-19}\ C)^2 \cdot 3.8 \cdot 10^{-9}\ \Omega \cdot cm}$$

$$\tau = 0.159 \cdot 10^{-4} \cdot 10^{-31-22+38+9}\ s = \underline{\underline{15.9\ ps}}$$

$$l = v_F \tau = \underline{\underline{22.1\ \mu m}}$$

2c) Wanted : Feasibility of de Haas - van Alphen ?

$B = 1\ T$

Solution : Scattering should be low enough to allow at least a full orbit ; $\omega_c \tau \gtrsim 1$ (order of magnitude)

$$\omega_c = \frac{eB}{m} \Rightarrow B \gtrsim \frac{m}{e\tau} = ne\rho_{Ag}$$

$B \gtrsim 0.36\ T$ 1 T should be barely enough

With $\omega_c \tau > 2\pi$ somewhat higher fields may be needed.

The periodicity in $\left(\frac{1}{B}\right)$ will be very short for the maximum extremal area $A_{e,max} = \pi k_F^2$

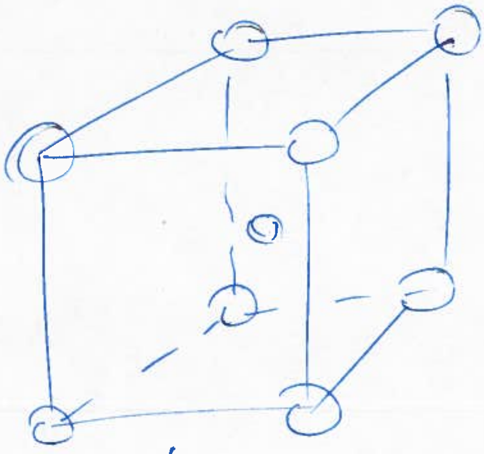
3. A given metal has *fcc* structure with lattice parameter *a* and can be described by the free electron model. Let the number of valence electrons per atom *x* (not necessarily an integer number) be such that the Fermi surface barely touches the surface of the 1:st Brillouin zone.

a) Find the Fermi *k*-vector at which the Brillouin zone is touched. (1.5p)

b) Determine *x*. (2.5p)

a) Solution: The Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice

The reciprocal lattice of an fcc lattice is bcc with conventional unit cell lattice param. $\frac{4\pi}{a}$



$\frac{4\pi}{a}$

To create the Brillouin zone, we bisect the distances to neighboring reciprocal lattice points.

Shortest distance is along the diagonal.

If we bisect $\Rightarrow$ $k_F\big|_{diagonal} = \frac{1}{4}\sqrt{3}\cdot\left(\frac{4\pi}{a}\right) = \frac{\sqrt{3}\,\pi}{a}$

b) With $k_F = (3\pi^2 n)^{1/3} = \frac{\sqrt{3}\cdot\pi}{a}$

$\Longrightarrow \quad n = \left(\frac{\sqrt{3}\cdot\pi}{a}\right)^3\cdot\frac{1}{3\pi^2} = \frac{\sqrt{3}\cdot\pi}{a^3}$

With x el/atom and 4 at/cell for fcc

$\Rightarrow \quad n = \frac{4\cdot x}{a^3}$

$x = \frac{n\cdot a^3}{4} = \frac{\sqrt{3}\cdot\pi}{4} \approx \underline{\underline{1.36}}$

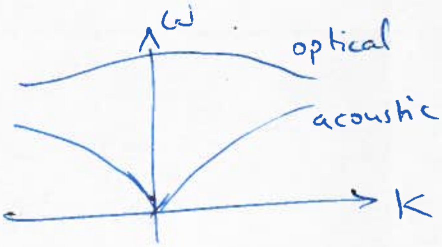
4. **a)** Explain briefly the following concepts related to lattice vibrations: Phonon, dispersion relation, optical branch, Debye model, Umklapp process. (2.5p)
b) Copper has a sound velocity v_s = 3560 m/s and a lattice parameter a = 3.61 Å. Estimate the Debye temperature of Cu. (1.5p)

a) Phonon: Energy quantum of elastic wave with properties

$$\begin{cases} \text{Frequency} & \omega \\ \text{Energy} & \hbar\omega \\ \text{Wave vector} & |K| = \frac{2\pi}{\lambda} \\ \text{Polarization direction} & \text{longitudinal / transverse} \end{cases}$$

Dispersion relation: Relation $\omega(K)$

Optical branch: Branch with $\lim\limits_{K \to 0} \omega(K) \neq 0$

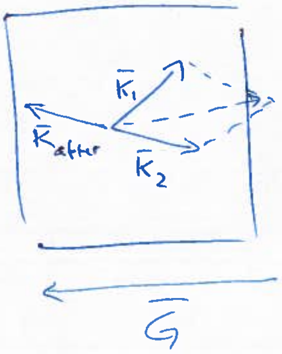


Debye model: Model for the phonon dispersion relation.

Assumes
① $\omega = v_s \cdot |K|$
② ω_D from $3N = \int_0^{\omega_D} D(\omega)\, d\omega$

Umklapp process: Scattering process that involves a resulting wave vector in another Brillouin zone, so that the net phonon $\bar{K}$ is not preserved, i.e. $\bar{K}_{after} = \bar{K}_{initial} + \bar{G}$, $\bar{G} \neq 0$

Example:



$\bar{K}_{initial} = \sum_i \bar{K}_i = \bar{K}_1 + \bar{K}$

$\bar{K}_{after} = \bar{K}_{initial} - \bar{G}$

4b) <u>Given</u> : Cu $v_s = 3560$ m/s

$a = 3.61$ Å

<u>Wanted</u> : Θ_D Debye temperature

<u>Solution</u> : Assume the Debye model, $\hbar\omega_D = k_B\Theta_D$

$$3N = \int_0^{\omega_D} D(\omega)\,d\omega = \int_0^{K_D} D(K)\,dK \quad , \quad \omega = v_s \cdot K$$

$$D(K)\,dK = 3 \cdot \left(\frac{L}{2\pi}\right)^3 \cdot 4\pi K^2 dK = \frac{3 \cdot V}{2\pi^2} \cdot K^2 dK$$

$$3N = \int_0^{K_D} D(K)\,dK = \frac{V}{2\pi^2} K_D^3 \Longrightarrow K_D = \left(6\pi^2 \frac{N}{V}\right)^{1/3}$$

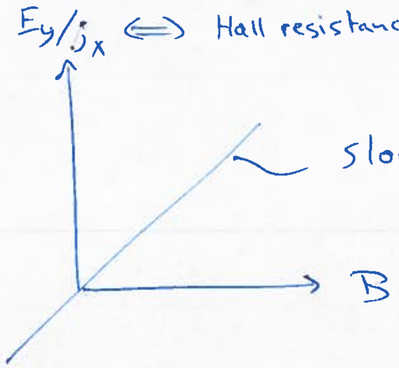
Cu: fcc, 4 at/cell $\Longrightarrow \frac{N}{V} = \frac{4}{a^3}$, $K_D = \frac{(24\pi^2)^{1/3}}{a}$

$$\Theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar v_s K_D}{k_B} = (24\pi^2)^{1/3} \frac{\hbar v_s}{k_B a} =$$

$$= (24\pi^2)^{1/3} \cdot 7.638 \cdot 10^{-12}\,\frac{K}{s} \cdot \frac{3560\ m/s}{3.61 \cdot 10^{-10}\ m} = \underline{\underline{466\ K}}$$

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)

Hall effect:

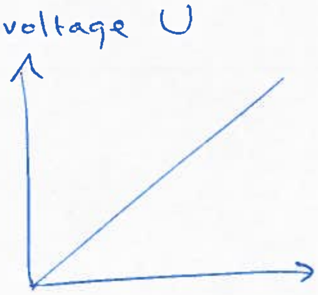


$E_y/j_x \Leftrightarrow$ Hall resistance proportional to field

slope $R_H \sim \frac{E_y}{j_x B_z} \sim -\frac{1}{ne}$ for el-doped

$\sim \frac{1}{pe}$ hole-doped

Seebeck effect:



$U \sim S \cdot \Delta T$

depends on doping

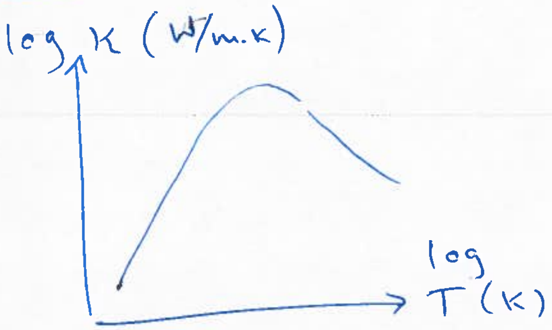
Resistivity:

$\rho \sim \frac{1}{\sigma} \sim \frac{m}{ne^2\tau}$

thermally activated

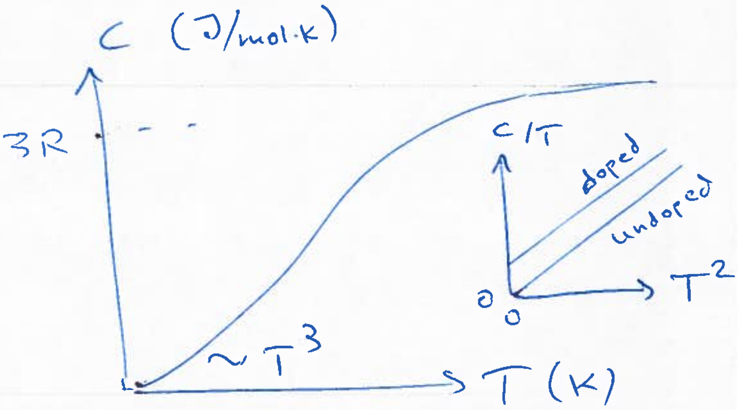
$\Rightarrow \rho$ increases with decreasing T

Thermal conductivity



thermal conductivity mainly from phonons since n low at low T

Specific heat



Electronic contrib. small

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) Discuss the concentration of vacancies in materials. (1.5p)

a) $$M = \frac{\mu_B N}{V} \tanh\left(\frac{\mu_B B}{k_B T}\right) \quad ; \quad B = \underset{\hookrightarrow = 0}{B_a} + B_E = \mu_0 \lambda M$$

$$\Longrightarrow \frac{M \cdot V}{\mu_B N} = \tanh\left(\frac{\mu_0 \mu_B \lambda M}{k_B T}\right) \qquad \text{Set } m = \frac{M \cdot V}{\mu_B N}$$

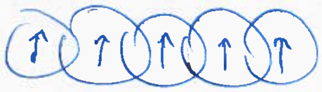
$$\Longrightarrow m = \tanh\left(\frac{m}{t}\right) \quad \text{where} \quad t = \frac{V \cdot k_B T}{\mu_0 \mu_B^2 \lambda N}$$

Solution with non-zero m for $t < 1$ $\quad t = 1 \Longleftrightarrow T = T_c$

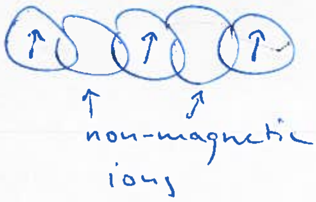
$$T_c = \frac{\mu_0 \mu_B^2 \lambda N}{V \cdot k_B} = \frac{\mu_0 \mu_B^2 \lambda n}{k_B}$$

b) Main source of interaction is electrostatic el-el interaction

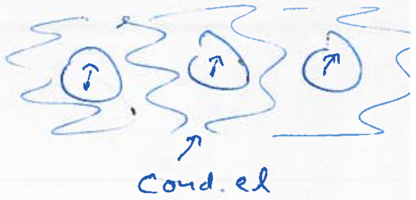
Direct exchange



Superexchange



Indirect exchange



c) Concentration of vacancies

Vacancies are thermally activated : $n_v \sim N_0 e^{-U/k_B T}$

Annealing at high temp. gives equilibrium concentration.

Quick quenching may freeze the vacancies