Exam 2015-03-19

Solutions

STOCKHOLMS UNIVERSITET
FYSIKUM

Examination in Condensed Matter Physics I, FK7042, 7.5 hp
Thursday, March 19, 2015, 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 and define any introduced variables.

Good luck! / A.R.

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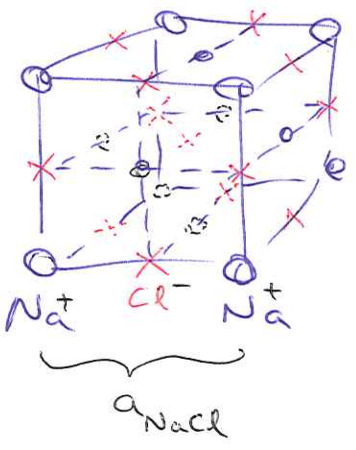
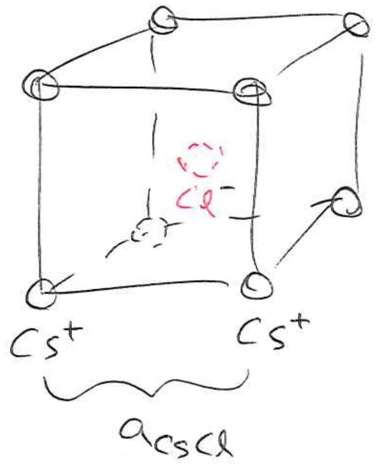
1. Consider two different ionic crystals, sodium chloride (NaCl) and caesium chloride (CsCl). Their lattice parameters are a_{NaCl} = 5.65 Å and a_{CsCl} = 4.12 Å, respectively. In the structures, the Na^+ ions arrange in an *fcc* lattice, while the Cs^+ ions arrange in a simple cubic (*sc*) lattice. 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)





Equations:

$$(1) \quad r_{Cs^+} = 1.6 \cdot r_{Na^+}$$

$$(2) \quad r_{Na^+} + r_{Cl^-} = \frac{1}{2} a_{NaCl}$$

$$(3) \quad r_{Cs^+} + r_{Cl^-} = \frac{1}{2} \cdot \sqrt{3} \cdot a_{CsCl}$$

$$\Longrightarrow \begin{cases} r_{Na^+} = 1.24 \text{ Å} \\ r_{Cl^-} = 1.59 \text{ Å} \\ r_{Cs^+} = 1.98 \text{ Å} \end{cases}$$

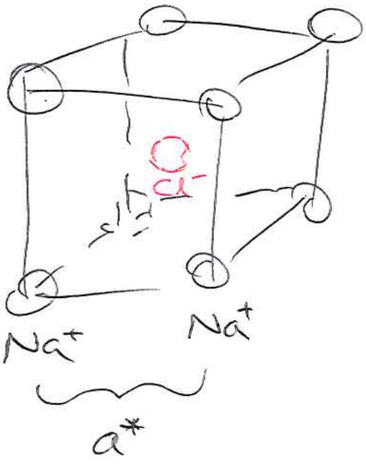
Assuming $2 \cdot r_{Cs^+} < a_{CsCl}$

verify → ok!

1b) Wanted: Density change if NaCl had CsCl structure

Solution: Assume fixed ionic radii according to a)

Imagined structure:



We want to determine a^* and then calculate

$$\frac{\rho_{new}}{\rho_{old}} = \frac{a_{old}^3}{(a^*)^3} \cdot \frac{1\ \text{NaCl/cell}}{4\ \text{NaCl/cell}}$$

Equation: $r_{Na^+} + r_{Cl^-} = \frac{1}{2}\sqrt{3} \cdot a^*$

$$\Rightarrow \quad a^* = \frac{2}{\sqrt{3}}(1.24 + 1.59)\ \text{Å} = 3.27\ \text{Å}$$

Check: $2 r_{Na^+} < a^*$

$$\frac{\rho_{new}}{\rho_{old}} = \left(\frac{5.65\ \text{Å}}{3.27\ \text{Å}}\right)^3 \cdot \frac{1}{4} = 1.29 \iff$$ Density would increase by 29%

2. a) The relaxation time τ for electrons in the Drude model is defined to give a probability dt/τ for an electron to collide during a short time dt. Use this definition to find an expression for the probability of the electron not colliding during a time t. Interpret the result. (2p)
b) How does this relaxation time affect the thermal conductivity of a metal? (0.5p)
c) The electronic specific heat is linear in temperature, $c_{v,\mathrm{el}} = \gamma T$. Use the Lorenz number $L = \pi^2 k_B^2/3e^2$ and Wiedemann-Franz law to express γ in terms of the Fermi energy ε_F. Describe used relations. (1.5p)

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a) Given: $\frac{dt}{\tau}$ = probability for collision during dt

Wanted: $P(t)$ = probability for not colliding during time t

Solution: $P(0)=1$; $P(t_1)\cdot P(t_2) = P(t_1+t_2)$

$$P(t+dt) = P(t)\cdot P(dt) = P(t)\cdot\left(1-\frac{dt}{\tau}\right)$$

$$\Rightarrow \quad \frac{P(t+dt)-P(t)}{dt} = -\frac{P(t)}{\tau}$$

$$\frac{dP}{dt} = -\frac{P}{\tau} \quad \Rightarrow \quad \boxed{P(t) = e^{-t/\tau}}$$

Interpretation: τ is average time between collisions for an electron

2b) The electronic thermal conductivity $K_{el} = \frac{1}{3} C_{el}\cdot v_F \cdot l = \frac{1}{3} C_{el} v_F^2 \cdot \tau$

$\Rightarrow$ Longer τ gives higher thermal conductivity

2c) Given: $C_{v,el} = \gamma T$

Lorenz number $L = \frac{\pi^2 k_B^2}{3e^2}$

Wanted: γ in terms of Fermi energy ε_F

Solution: Wiedemann-Franz law: $\frac{K}{\sigma T} = L$

where $K = \frac{1}{3} C_{v,el} \cdot l \cdot v_F$ thermal conductivity

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

n: el concentration $l = v_F\tau$ mean-free path

$$\gamma = \frac{C_{v,el}}{T} = \left\{\begin{matrix}\text{using}\\ \text{assumed}\\ \text{relations}\end{matrix}\right\} = \frac{3K}{v_F^2\tau \cdot T} = \frac{3 \cdot L \cdot \sigma \cdot T}{v_F^2\tau \cdot T} =$$

$$= \frac{3 \cdot L \cdot ne^2\tau}{m v_F^2 \cdot \tau} = \left(\frac{\pi k_B}{e}\right)^2 \cdot \frac{ne^2}{m v_F^2} =$$

$$= \frac{\pi^2}{2} \cdot n k_B \cdot \frac{k_B}{\frac{1}{2} m v_F^2} = \underline{\underline{\frac{\pi^2}{2} \cdot n k_B \cdot \frac{k_B}{\varepsilon_F}}}$$

3. Transversal, optical lattice vibrations in germanium have a frequency $f \approx 9 \cdot 10^{12}$ Hz, which can be assumed independent of wavelength and propagation direction. Germanium has diamond structure and lattice parameter $a = 5.66$ Å.

a) Calculate the average number of transversal, optical phonons in a 1 cm^3 Ge-crystal at room temperature. Hint: the number of allowed wave vectors in the 1st Brillouin zone equals the number of primitive cells. (2p)

b) Calculate the thermal energy associated with these lattice vibrations for the given crystal. (1p)

c) Estimate the contribution from these lattice vibration to the heat capacity of the crystal at room temperature. (1p)

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a) Solution: Each vibration mode contains a number of phonons given by

$$n(\omega) = \frac{1}{e^{\hbar\omega/k_BT} - 1}$$

The total # transversal, optical phonons in $V = 1\,cm^3$ then is

$$n(\omega) \cdot \underbrace{\#\text{prim, cells}}_{=\#\text{ allowed } k\text{-vectors}} \cdot \#\text{ transverse branches}$$

Diamond structure: "fcc with basis of 2 atoms"

$\Longrightarrow$ primitive cell with volume $V_c = \frac{a^3}{4}$, containing 2 atoms

$N_{\text{prim cell}} = \frac{V}{V_c}$; with 2 at/cell: 3 acoustic branches

3 optical —"—

↳ 1 longitudinal

2 transverse

$$\frac{\hbar\omega}{k_BT} = \underbrace{\boxed{\frac{\hbar}{k_B}}}_{7.64\cdot 10^{12}\,K\cdot s} \cdot \frac{2\pi \cdot 9 \cdot 10^{12}\,Hz}{300\,K} = \underline{1.44}$$

$$\Longrightarrow n(\omega) = \underline{0.31}$$

$$\Longrightarrow \#\text{ transversal, optical phonons} = 0.31 \cdot \frac{V}{V_c} \cdot 2 =$$

$$= 0.31 \cdot \frac{(1\,cm)^3}{(5.66\,\text{Å})^3} \cdot 4 \cdot 2 = 1.37 \cdot 10^{22} \text{ phonons}$$

3b) Wanted: Thermal energy associated with these phonons

Solution:
$$\langle \varepsilon \rangle = \underbrace{\hbar\omega}_{=h\cdot f} \cdot \langle n \rangle = 6.63\cdot 10^{-34}\,\text{J}\cdot\text{s} \cdot 9\cdot 10^{12}\,\text{s}^{-1} \cdot 1{,}37\cdot 10^{22}\,\text{cm}^{-3}$$
$$\approx \underline{\underline{82\ \text{J}/\text{cm}^3}}$$

3c) Wanted: Estimated contribution from these phonons to specific heat at room temperature

Solution:
$$C = \frac{dU}{dT} = \frac{dn(\omega)}{dT} \cdot \underbrace{\frac{(1\ \text{cm})^3}{(5.66\,\text{Å})^3}}_{4.42\cdot 10^{22}} \cdot 4.2 \cdot \underbrace{\hbar\omega}_{5.97\cdot 10^{-21}\,\text{J}}$$

$$\frac{dn(\omega)}{dT} = \frac{1}{\left(e^{\hbar\omega/k_BT}-1\right)^2} \cdot e^{\hbar\omega/k_BT} \cdot \frac{\hbar\omega}{k_BT^2} =$$

$$= (0.31)^2 \cdot e^{1.44} \cdot 1.44 \cdot \frac{1}{300\ \text{K}} = \underline{\underline{1.95\cdot 10^{-3}\ \text{K}^{-1}}}$$

$$\Rightarrow \quad C = \underline{\underline{0.51\ \text{J}/\text{K}}}$$

4. The following three expressions can be found in the formula collection:

$$g_c(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\varepsilon - \varepsilon_c)^{1/2}$$

$$n_c(T) = \int_{\varepsilon_c}^{\infty} \frac{1}{e^{(\varepsilon-\mu)/k_BT} + 1} g_c(\varepsilon)\mathrm{d}\varepsilon$$

$$N_c(T) \approx \frac{1}{4}\left(\frac{2m_e k_B T}{\pi\hbar^2}\right)^{3/2}$$

Explain what they describe and and under what conditions/assumptions they apply. Also explain variables etc. in the expressions. (4p)

Solution: $g_c(\varepsilon)$ is the density of states for the conduction band in a semiconductor.

The energy ε is measured relative to the conduction band edge ε_c.

m_e is the effective electron mass, including the effect of the number of conduction band edges.

Assumptions: Parabolic bands, spherical energy surfaces

$n_c(T)$ is the electron concentration for the conduction band. $g_c(\varepsilon)$ is the density of states of the band. μ is the chemical potential. (Fermi level)

$$f_{FD} = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$$ is the probability that a certain state is occupied.

If $|\varepsilon-\mu| \gg k_BT$, the expression for $n_c(T)$ can be simplified to

$$n_c(T) = e^{-(\varepsilon_c-\mu)/k_BT} \cdot \underbrace{\int_0^\infty e^{-(\varepsilon-\varepsilon_c)/k_BT} \cdot g_c(\varepsilon)\, d(\varepsilon-\varepsilon_c)}_{\text{integrate function of } x = \varepsilon-\varepsilon_c}$$

$$\Longrightarrow N_c(T)$$

5. a) In an experiment, x-rays with a wave length $\lambda = 3.1$ Å are diffracted on a crystal with monoatomic simple cubic (*sc*) structure. The lattice parameter is $a = 3.50$ Å. Find all the possible diffraction angles of the experiment. (2.5p)

b) Suppose that the structure in a) would be modified by adding a light atom with a relatively small atomic form factor to the center of the *sc* cell. This would cause the diffraction intensity of all the diffraction peaks to change slightly. However, the relative change would be different for one of the peaks. Which one, and how would it change? (1.5p)

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a) Solution : $\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2) \le 1$

$$\Rightarrow h^2+k^2+l^2 \le \frac{4a^2}{\lambda^2} = 5.10$$

(h k l)	$h^2+k^2+l^2$	θ (°)
1 0 0	1	26.3
1 1 0	2	38.8
1 1 1	3	50.1
2 0 0	4	62.3
2 1 0	5	82.0
2 1 1	6	

possible

$h^2+k^2+l^2 > 5.1$

b) The intensity would be given by $S_{\bar G} = \sum_j f_j e^{i\bar G \cdot \bar r_j}$

with $\bar r_j = \bar 0$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ $\Rightarrow S_{\bar G} = f_0 + f_1 e^{i\pi(h+k+l)}$

h+k+l odd: $f_0 - f_1$

— " — even: $f_0 + f_1$

(h k l)	S_G
1 0 0	$f_0 - f_1$
1 1 0	$f_0 + f_1$
1 1 1	$f_0 - f_1$
2 0 0	$f_0 + f_1$
2 1 0	$f_0 - f_1$

We see that there are actually two peaks that will increase intensity while the others will decrease

6. a) Pauli paramagnetism and free spin paramagnetism are two types of paramagnetism of quite different origin. Compare the two by explaining their origin, what main physical property they depend on, and their resulting temperature dependence of magnetic susceptibility. (2p)
b) State two formulations of the Bloch theorem and explain with words. (2p)

a)

	Pauli para	Free spin para
Origin	Conduction electron states with spin $\uparrow$ and spin $\downarrow$ will get different energy in magnetic field. $\Rightarrow n(\uparrow) \neq n(\downarrow)$	Localized atomic moments from partially filled shells $(J \neq 0)$
Depends on	Density of states at fermi level	Concentration of moments; J
Temp. dependence of χ	Temp. independent	$\frac{1}{T}$ (curie law)

b) Formulation 1: $\psi_{n\bar{k}}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} \cdot u_{n\bar{k}}(\bar{r})$

where $u_{n\bar{k}}(\bar{r}) = u_{n\bar{k}}(\bar{r}+\bar{R})$

The eigenstate solutions to the Schrödinger equation for electrons in a periodic potential can be described in the form of a plane wave times a function that is periodic in the Bravais lattice.

Formulation 2: $\psi(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}} \cdot \psi(\bar{r})$

Bloch waves are not periodic in $\bar{R}$, but assumes a phase factor $e^{i\bar{k}\cdot\bar{R}}$ when going from $\bar{r}$ to $\bar{r}+\bar{R}$.