Exam 2012-03-15 Solutions

STOCKHOLMS UNIVERSITET
FYSIKUM

Examination in Condensed Matter Physics I, FK7042/FK3004, 7.5 hp
Thursday, March 15, 2012, 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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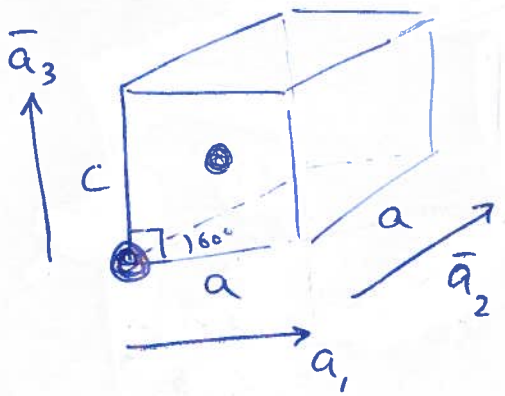
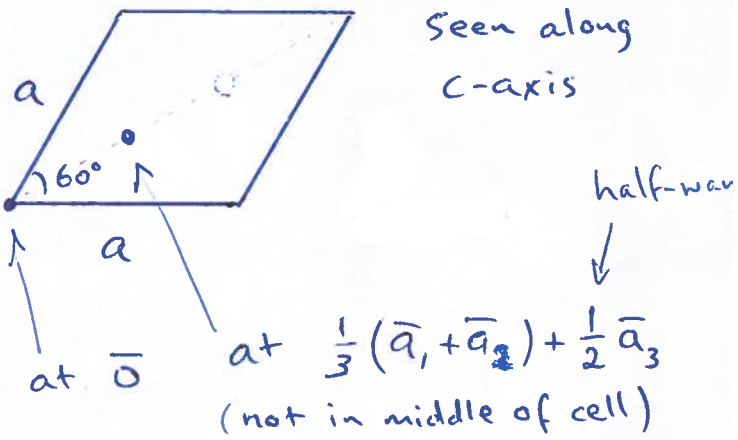
1. Metallic Zinc has a molar mass $M = 65.38$ g/mol and density 7.14 g/cm^3. The crystal structure is *hcp* (hexagonal close-packed).
a) Describe the *hcp* structure in terms of a Bravais lattice and specify the basis. (1.5p)
b) According to the periodic table, the *hcp* structure of Zn is not ideal. Instead $c/a \approx 1.856 > \sqrt{8/3}$, where a and c are the conventional lattice parameters. Use this information to determine a and c. (2.5p)

a) The primitive cell of hcp contains 2 atoms.

Its Bravaislattice is simple hexagonal (sh)

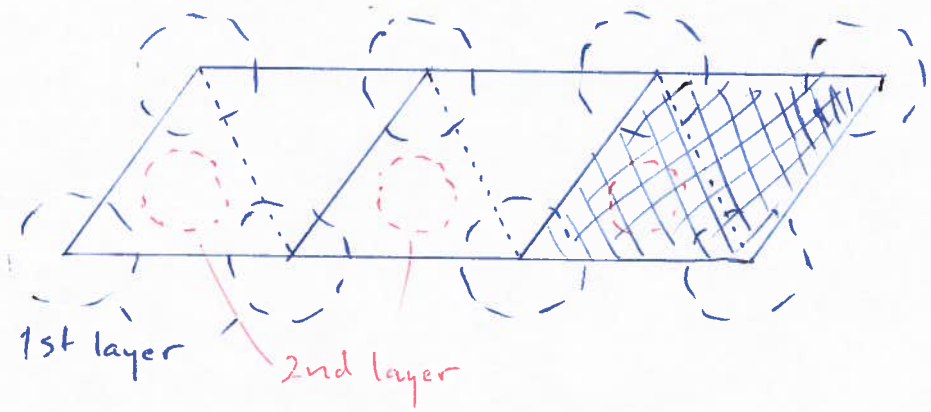




The Bravaislattice has lattice vectors

$$\bar{a}_1 = a\hat{x} \; ; \; \bar{a}_2 = a\cdot\underbrace{\cos 60^\circ}_{1/2}\cdot\hat{x} + a\cdot\underbrace{\sin 60^\circ}_{\sqrt{3}/2}\cdot\hat{y} \; ; \; \bar{a}_3 = c\hat{z}$$

cont. 1a)



Note that the 2nd layer has two possible locations for close-packing.

The basal area is $a \cdot \frac{\sqrt{3}}{2} a$

$\Rightarrow$ cell volume $c \cdot a^2 \cdot \frac{\sqrt{3}}{2}$

b) Given: $\frac{c}{a} \approx 1.856$, density $\rho = 7.14\ g/cm^3$, molar mass $M = 65.38\ g/mol$

Wanted: a, c

Solution: The cell with volume $\frac{\sqrt{3}}{2} a^2 c \approx \frac{\sqrt{3}}{2} \cdot 1.856 \cdot a^3$ contains 2 atoms

Eq: $\frac{2}{V} = \frac{\#at}{vol} = \frac{\rho \cdot N_A}{M}$; $N_A = 6.022 \cdot 10^{23}\ \frac{at}{mol}$

$$\frac{2}{\frac{\sqrt{3}}{2} \cdot 1.856 \cdot a^3} = \frac{\rho \cdot N_A}{M}$$

$$a^3 = \frac{4}{\sqrt{3}} \cdot \frac{M}{1.856 \cdot \rho \cdot N_A} = \frac{4^{at} \cdot 65.38\ g/mol}{\sqrt{3} \cdot 1.856 \cdot 7.14\ g/cm^3 \cdot 6.022 \cdot 10^{23}\ at/mol}$$

$a = 2.66 \cdot 10^{-8}\ cm = 2.66\ \text{Å}$; $c = 4.95\ \text{Å}$

(agrees with periodic system)

2. The Drude model is a simple model of the metallic state that treats electrons as independent, classical particles.
a) Define and interpret the relaxation time τ in the Drude model, and find the probability for an electron not to collide during a time t. (2p)
b) Show how the introduction of τ together with the Drude assumption of scattering in random directions leads to Ohm's law. (2p)

a) The relaxation time τ is defined to give a probability for collision during a short time dt to be equal to $\frac{dt}{\tau}$.

Now, let $P(t)$ be the probability for an electron not to collide during a (possibly long) time t.

$$P(0) = 1 \qquad P(t_1) \cdot P(t_2) = P(t_1 + t_2)$$

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

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

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

Interpretation: τ is the average time between collisions for an electron

2b) Given: Drude assumption of scattering in random directions, introduced τ

Wanted: Ohm law

Solution:

$$\bar{j} = -n \cdot e \cdot \langle \bar{v} \rangle$$

($\langle \bar{v} \rangle$: average velocity)

$$\bar{v}(t) = \bar{v}_0 - \frac{e\bar{E}}{m} \cdot t$$

effect of el. field on velocity of an electron

Random directions: $\langle \bar{v}_0 \rangle = 0$

Effect of $\bar{E}$ works on average time τ

$$\Rightarrow \quad \langle \bar{v}(t) \rangle = -\frac{e\bar{E}}{m} \cdot \tau$$

$$j = -ne \cdot \left(-\frac{eE}{m}\tau\right) = \underbrace{\frac{ne^2\tau}{m}}_{\text{identify } \sigma} \cdot E$$

$$j = \sigma \cdot E \quad \text{ohms law}$$

or $\quad E = \rho \cdot j \qquad \rho = \frac{1}{\sigma}$

3. Aluminium (Al) has *fcc* structure with a lattice parameter $a = 4.05$ Å.
a) Express the k-volume of the 1:st Brillouin zone for Al in terms of a. (1.5p)
b) From de Haas – van Alphen data one can conclude that there are no fourth-zone electron pockets in Al. From a table of high-field Hall measurements one can find that $-1/(R_H ne) = -0.3$ for Al. According to theory, one should expect the high-field Hall coefficient to be $R_H = -1/(n_e - n_h)e$. Assume that Al has 3 valence electrons per atom. Discuss how well the experimental Hall data agrees with theory. (2.5p)

a) The 1:st B.Z. is the Wigner-Seitz cell of the reciprocal lattice. It is a primitive cell with 1 pt.

The reciprocal lattice of fcc is a bcc lattice with lattice parameter $\frac{4\pi}{a}$

The bcc lattice has 2 pts/cell $\Rightarrow$ volume for primitive cell is $\frac{1}{2}\cdot\left(\frac{4\pi}{a}\right)^3$ in k-space, i.e,

$V_g = \frac{32\pi^3}{a^3}$. Alternatively $V_g = \frac{(2\pi)^3}{V_c} = \frac{(2\pi)^3}{a^3/4} = \frac{32\pi^3}{a^3}$

↳ primitive cell vol.

b) Given: $-\frac{1}{R_H \cdot ne} = -0.3$; no fourth-zone el. pockets.
Al : 3 val.el/at.

Solution: We identify $n = 3$ so that experiments give $R_H = +\frac{1}{0.9\cdot e}$

Theory says $R_H = -\frac{1}{(n_e - n_h)e}$, so what is n_e and n_h?

It is easy to see that 1:st B.Z. is completely filled, using 2el/at.

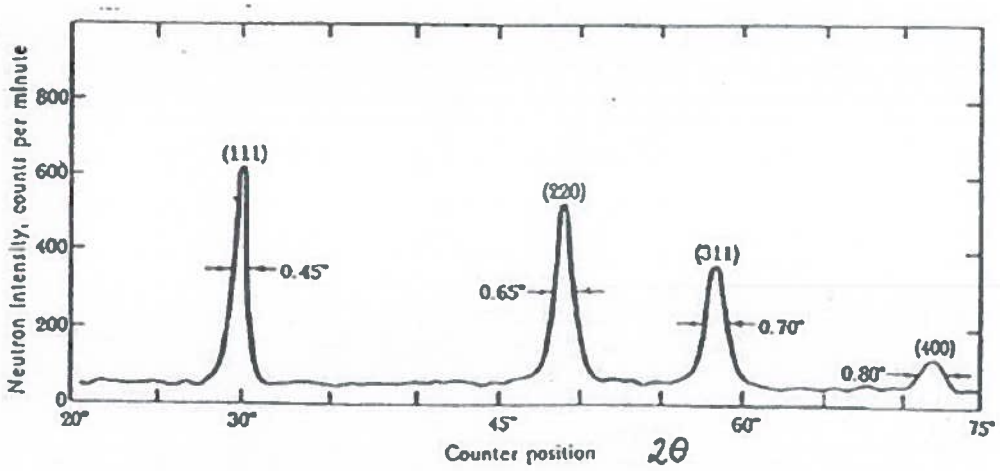
$\Rightarrow$ 1 el/at left for 2:nd and 3:rd zone:

$n_e^{II} + n_e^{III} = 1$ But $n_e^{II} + n_h^{II} = 2$ (each zone can fit 2 el/at)

$\Rightarrow n_h^{II} = 2 - n_e^{II} = 2 - \left(1 - n_e^{III}\right) = 1 + n_e^{III}$

$R_H = -\frac{1}{n_e - (1+n_e)e} = \frac{1}{e} = +\frac{1}{1.0\cdot e}$ Quite good agreement!

4. The figure shows a diffraction pattern obtained from a neutron beam scattered against powdered diamond.
a) It is seen that the Miller indices (h k l) are all even or all odd. However, some peaks, such as (2 2 2), are missing. Motivate why this is expected. (1p)
b) Calculate the wavelength and kinetic energy of the neutrons. Hint: Use the de Broglie relation $p = h/\lambda$. (3p)



Neutron diffraction pattern for powdered diamond. (After C. Bacon.)

a) The diamond structure can be described as an fcc-lattice with a basis of 2 atoms.
For an fcc lattice, diffraction occurs if Miller indices (h k l) are all even or all odd, using conv. cubic Bravais lattice.
Additional basis ⟹ more peaks will disappear.
(8 at/cell instead of 4 for fcc)

b) From graph:

2θ	(h k l)	$\sin^2\theta$	$h^2+k^2+l^2$
30	111	0.067	3
49	220	0.172	8
58	311	0.235	11
72	400	0.345	16

From periodic table:
$a_{diamond} = 3.57\ \text{Å}$

$\Rightarrow \lambda \approx 1.049\ \text{Å}$

$p = \frac{h}{\lambda}$; $\varepsilon = \frac{p^2}{2m}$

$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2) \Rightarrow \varepsilon = \frac{h^2}{2m_n\lambda^2}$

$$\varepsilon = \frac{(6.63\cdot10^{-34})^2}{2\cdot1.67\cdot10^{-27}\cdot(1.049\cdot10^{-10})^2} \approx 70\ \text{meV}$$

5. a) An intrinsic semiconductor has a temperature independent energy gap $\varepsilon_G = 0.8$ eV. Assume that the mean free path for electrons and holes are the same at 250 K and 300 K. Estimate the resistivity ratio $\rho(300\text{ K})/\rho(250\text{ K})$. State your assumptions. (2p)
b) Explain the following concepts: Bloch function, localized states. (2p)

a) See exam 2011-03-25, problem 4a

$\sigma = ne\mu_e + pe\mu_h$; intrinsic $n = p = n_i$

Assume weak temp. dep. (=110) of mobility $\mu = \frac{e\tau}{m} = \frac{e v_F}{m \cdot l}$

band-structure properties are norm. temp.-indep.

constant according to given conditions

$n_i = \sqrt{n \cdot p} = \sqrt{N_c P_v}\, e^{-E_g/2k_BT}$

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

$\rho = \frac{1}{\sigma} = \frac{1}{n_i e(\mu_e + \mu_h)} \sim \frac{1}{T^{3/2}\, e^{-E_g/2k_BT}}$

$$\frac{\rho(300)}{\rho(250)} = \frac{250^{3/2} \cdot e^{-0.8/(2 \cdot 8.62 \cdot 10^{-5} \cdot 250)}}{300^{3/2} \cdot e^{-0.8/(2 \cdot 8.62 \cdot 10^{-5} \cdot 300)}} = \left(\frac{250}{300}\right)^{3/2} e^{\underbrace{\frac{0.8}{2 \cdot 8.62 \cdot 10^{-5}} \cdot \left(\frac{1}{250} - \frac{1}{300}\right)}_{3.09}}$$

$= 0.034$

b) **Bloch function:** Electron wave function appearing as the solution of the Schrödinger equation with a periodic potential.

$\psi_{nk}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} \cdot u_{nk}(\bar{r})$; $u_{nk}(\bar{r}+\bar{R}) = u_{nk}(\bar{r}$

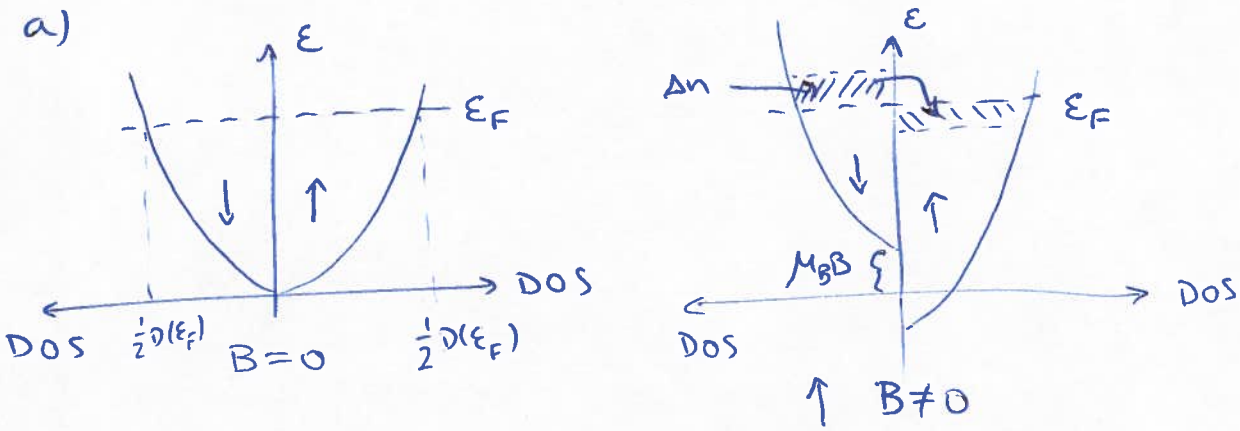
Localized states: States that are spatially confined, i.e, not itinerant.

Example: states introduced by electron/hole-doping in semiconductors

(the state does not need to be occupied)

6. a) Find an expression for the Pauli paramagnetic susceptibility due to conduction electrons. A strict derivation is not needed, but motivate and explain how you obtain the expression. (2p)
b) Sketch the magnetic susceptibility as a function of applied magnetic field for type-I and type-II superconductors. (1p)
c) For conventional superconductors that are described by the BCS theory the critical temperature is proportional to the Debye temperature. Discuss how this gives rise to the isotope effect.(1p)

a)



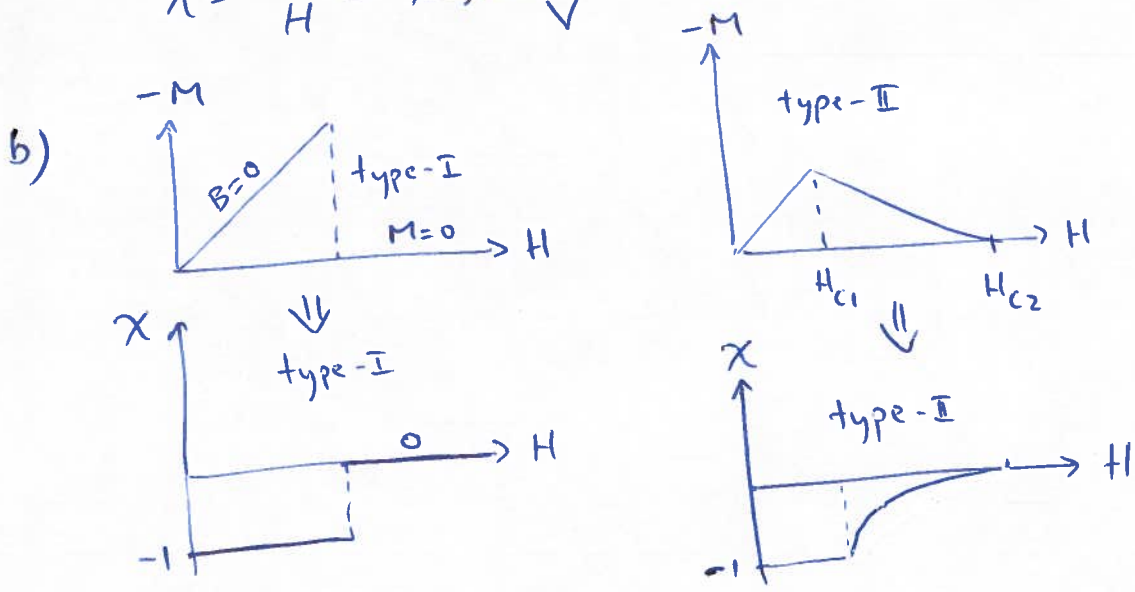
$$M = \mu_B \cdot (n_\uparrow - n_\downarrow) = \mu_B \cdot \left(\frac{1}{2} \cdot (n_{tot} + \Delta n) - \frac{1}{2}(n_{tot} - \Delta n) \right) =$$

$$= \frac{1}{2}\mu_B \cdot 2\Delta n = \mu_B \cdot \Delta n = \mu_B \cdot \frac{D(\varepsilon_F) \cdot \mu_B B}{V}$$

$$B \approx \mu_0 H$$

$$\chi = \frac{M}{H} = \frac{\mu_0 \mu_B^2 D(\varepsilon_F)}{V}$$

b)



c) $T_c \propto \Theta_D \propto \omega_D \sim \omega_{max} \sim \frac{\sqrt{C}}{M} \sim \frac{1}{M^{1/2}}$ $\quad T_c \sim M^{-1/2}$ isotope effect