Exam 2014-03-20 Solutions

STOCKHOLMS UNIVERSITET
FYSIKUM

Examination in Condensed Matter Physics I, FK7042 / FK3004, 7.5 hp
Thursday, March 20, 2014, 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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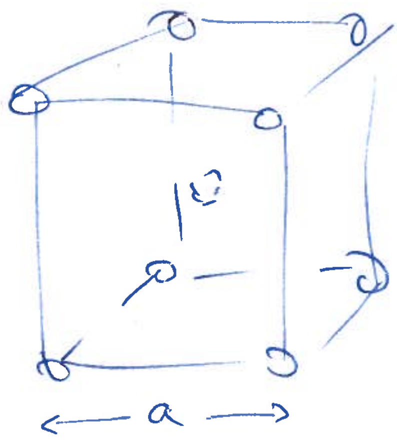
1. The *bcc* structure can be described as a simple cubic (*sc*) Bravais lattice with a 2-point basis of $\mathbf{0}$ and $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$, where a is the lattice parameter of the cubic Bravais lattice.
a) Can the *bcc* structure be described as a Bravais lattice with a single-point basis? If so, specify the primitive lattice vectors (in cartesian coordinates). If not, motivate why the structure would not be a Bravais lattice. (2p)
b) Suppose that we keep the nearest neighbor distance constant. Find the ratio of the two structural densities, ρ_{bcc}/ρ_{sc}, under this condition. (2p)

Solution

a) The bcc lattice is a Bravais lattice, since every lattice point sees the same surrounding. Primitive lattice vectors can be chosen in many ways.



Find 3 vectors that span a volume $\frac{a^3}{2} = \frac{V^{conv.}_{c,bcc}}{2}$

$$\left.\begin{aligned}\bar{a}_1 &= \left(-\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)a\\ \bar{a}_2 &= \left(\tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{2}\right)a\\ \bar{a}_3 &= \left(\tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\right)a\end{aligned}\right\} V_c = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) =$$

$$= \left(-\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)\cdot\left(0, \tfrac{1}{2}, \tfrac{1}{2}\right)a^3$$

$$= \left(\tfrac{1}{4} + \tfrac{1}{4}\right)a^3 = \frac{a^3}{2}$$

b)

$$\frac{\rho_{bcc}}{\rho_{sc}} = \frac{\left(\frac{2}{a^3_{bcc}}\right)}{\left(\frac{1}{a^3_{sc}}\right)} = \left\{ a_{sc} = \frac{\sqrt{3}}{2} a_{bcc} \right\} = 2\left(\frac{a_{sc}}{a_{bcc}}\right)^3 = 2\left(\frac{\sqrt{3}}{2}\right)^3 = \frac{3\sqrt{3}}{4} \approx 1.30$$

if n.n the same

2. The free electron model in 2D is important not only for two-dimensional systems, but also for materials with nearly cylindrical Fermi surfaces.

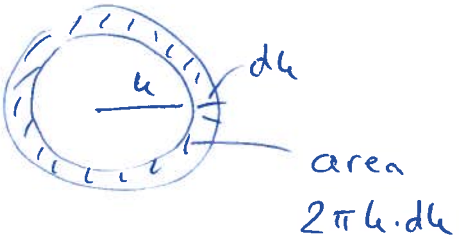
a) Derive an expression for the density of states $g(\varepsilon)$ for free electrons in two dimensions. (1p)

b) Find a corresponding expression for the Fermi energy ε_F in 2D. Express the answer in terms of the electron density n. (1p)

c) Assume a square lattice with 1 electron per atom and a lattice parameter $a = 2.4$ Å. Calculate the average energy (in eV) of free electrons in 2D. (2p)

Solution a) $g(\varepsilon)d\varepsilon = g(k)dk$

$$g(k)dk = \underset{\text{spin}}{2} \cdot \frac{2\pi k\, dk}{\left(\frac{2\pi}{L}\right)^2}$$



Free el:

$$\varepsilon = \frac{\hbar^2 k^2}{2m}$$

$$d\varepsilon = \frac{\hbar^2 k}{m} dk$$

$$g(\varepsilon) = g(k)\cdot\frac{dk}{d\varepsilon} = \frac{L^2\cdot k}{\pi}\cdot\frac{m}{\hbar^2 k}$$

$$\boxed{g(\varepsilon) = \frac{L^2\cdot m}{\pi\hbar^2}}$$

b) With electron density $n = \frac{N}{L^2}$ the Fermi energy becomes:

$$N = \int_0^{\varepsilon_F} g(\varepsilon)d\varepsilon = \frac{L^2\cdot m}{\pi\hbar^2}\cdot\varepsilon_F \implies \boxed{\varepsilon_F = \frac{\pi\hbar^2}{m}\cdot n}$$

c)

$$\langle\varepsilon\rangle = \frac{\int_0^{\varepsilon_F}\varepsilon\cdot g(\varepsilon)\,d\varepsilon}{\int_0^{\varepsilon_F} g(\varepsilon)\,d\varepsilon} = \frac{\left(\varepsilon_F^2/2\right)}{\varepsilon_F} = \frac{\varepsilon_F}{2}$$

$$n = \frac{N}{L^2} = \frac{1}{a^2} \implies \langle\varepsilon\rangle = \frac{\varepsilon_F}{2} = \frac{\pi\hbar^2}{2\cdot m}\cdot\frac{1}{a^2}$$

with numbers: $\langle\varepsilon\rangle = \pi\cdot\left(\frac{a_0}{a}\right)^2 Ry$, where $a_0 = 0.529$ Å and $1\ Ry = 13.6$ eV

$$\implies \langle\varepsilon\rangle = \pi\cdot\left(\frac{0.529}{2.4}\right)^2\cdot 13.6\,\text{eV} \approx \underline{2.08\,\text{eV}}$$

3. A polycrystalline sample with bodycentered tetragonal structure was studied with monochromatic x-ray, λ = 1.5405 Å. The four lowest Bragg angles were measured to θ = 21.00°, 22.06°, 28.78°, and 32.09°.

a) Give an expression for a general reciprocal lattice vector **G**(*hkl*) for the tetragonal lattice, which has lattice vectors $a\hat{x}$, $a\hat{y}$, and $c\hat{z}$. (0.5p)

b) Start with the diffraction condition $\Delta\mathbf{k} = \mathbf{G}$ and deduce the quadratic form for a tetragonal lattice. (1.5p)

c) For *bcc* structures, the allowed reflexes have $h + k + l = 2n$, where n is an integer. Motivate that this is also the case for the bodycentered tetragonal structure. (0.5p)

d) Index the structure and determine the lattice parameters a and c. (1.5p)

Solution : See exam 2009-06-17, problem 3 for detailed solution

a) $\bar{G}(hkl) = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$, where $\bar{b}_1 = \frac{2\pi}{a}\hat{x}$, $\bar{b}_2 = \frac{2\pi}{a}\hat{y}$, $\bar{b}_3 = \frac{2\pi}{c}\hat{z}$

b) $\sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2\right)$

c) Calculate $S = \sum_j f_j e^{i\bar{G}\cdot\bar{r}_j} = \left\{ \begin{matrix} \text{basis } \bar{0} \text{ and} \\ \left(\frac{a}{2}, \frac{a}{2}, \frac{c}{2}\right) \end{matrix} \right\} = \ldots = \begin{cases} 2f & \text{even sum} \\ 0 & \text{odd sum} \end{cases}$

d)

θ (deg)	(h k l)
21.00	(011), (101)
22.06	(110)
28.78	(002)
32.09	(200), (020)

$a = 2.900$ Å

$c = 3.200$ Å

4. A measurement of the heat capacity C_v of silver resulted in the following data:

T (K)	C_v (mJ/mol K)
1.32	1.28
1.62	1.85
2.26	3.40
3.12	6.92

a) Explain what information you could obtain from the data. (1p)

b) Analyze the data to draw as many conclusions as possible! Make suitable assumptions. (3p)

Solution

a) Low-temperature heat capacity $C_v = \underbrace{\gamma T}_{\text{electronic contribution}} + \underbrace{AT^3}_{\text{contribution from phonons}}$

$$\gamma = \frac{\pi^2}{3} k_B^2 \cdot \underbrace{g(\varepsilon_F)}_{\text{density of states at } \varepsilon_F}$$

$$g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F} \quad \text{for free el.}$$

may apply for Ag

$$\varepsilon_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m}$$

$$A = 234 \cdot \frac{1}{\underbrace{\Theta_D^3}_{\text{Debye temperature}}} \cdot n k_B$$

$$\hbar\omega_D = k_B \Theta_D$$

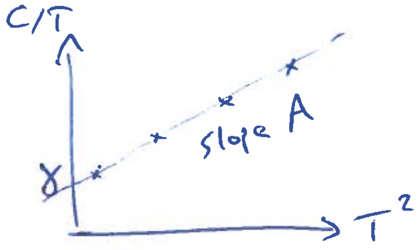
$$(\omega_D = v_s \cdot K_D, \quad K_D = (6\pi^2 n)^{1/3}$$

: Phonons

Main information: Electronic density of states at ε_F / Fermi energy

Sound velocity / Debye temperature

b) Plot C/T vs T^2



$\gamma \approx 0.72$ mJ/mol·K^2

$A \approx 0.154$ mJ/mol·K^4

(Cont. #4b)

Note that $C\left[\frac{J}{mol.K}\right] = C\cdot\left[\frac{J}{m^3 K}\right]\cdot\frac{M}{\rho}$ $\begin{matrix}[g/mo \\ [g/m^3\end{matrix}$

$$n = \frac{N}{V} = \frac{N_A\cdot\rho}{M}$$

$\Longrightarrow$ Replace n by N_A when C in $J/mol.K$
(i.e. $nk_B \rightarrow N_A\cdot k_B$)

$$\Longrightarrow \gamma = \frac{\pi^2}{2} N_A k_B^2 \cdot \frac{1}{\varepsilon_F} = \left\{N_A\cdot k_B = R\right\} = \frac{\pi^2}{2}\cdot \underset{8.314\ J/mol.K}{R}\cdot \underset{8.62\cdot 10^{-5}\ eV/K}{k_B}\cdot\frac{1}{\varepsilon_F}$$

This gives $\underline{\underline{\varepsilon_F = 4.91\,eV}}$

$$A = 234\cdot\frac{1}{\Theta_D^3}\cdot nk_B \Longrightarrow A = \underbrace{234\cdot R}_{\substack{1943.7\\ J/mol\cdot K}}\cdot\frac{1}{\Theta_D^3}$$

$$\Longrightarrow \underline{\underline{\Theta_D \approx 233\ K}}$$

$$K_D = (6\pi^2 n)^{1/3}, \quad n = \frac{N_A\cdot\rho}{M} = \frac{6.022\cdot 10^{23}\cdot 10.3}{107.87}\ \frac{at}{cm^3}$$

from periodic table

$$\Longrightarrow K_D = 1.50\cdot 10^{10}\ m^{-1}$$

$$v_s = \frac{\omega_D}{K_D} = \frac{\boxed{k_B}\,\Theta_D}{\boxed{\hbar}\,K_D} = \frac{233\ [K]}{7.64\cdot 10^{-12}\,[K\cdot s]\cdot 1.50\cdot 10^{10}\,[m^{-1}]}$$

$$\underline{\underline{v_s = 2026\ m/s}}$$

5. a) For direct optical absorption in a semiconductor, the excitation of an electron is assumed to occur vertically in the band structure (ε vs. k). Estimate if this is a reasonable model. (2p)
b) Explain the following concepts: Bloch function, localized states. (2p)

Solution

a) The band gap of a semiconductor has $\mathcal{E}_g \sim 1\,\text{eV}$

For absorption of a photon, the change in k of the electron will be of the order of k_{photon}:

$$k_{photon} = \frac{p_{photon}}{\hbar} = \frac{\mathcal{E}_{photon}}{\hbar c} \sim \frac{1\,[\text{eV}]}{6.58\cdot 10^{-16}\,[\text{eV}\cdot\text{s}]\cdot 3\cdot 10^{8}\,[\text{m/s}]}$$

$$\underline{\underline{k_{photon} \sim 5\cdot 10^{6}\ \text{m}^{-1}}}$$

But scale of band structure $k \sim 10^{10}\ \text{m}^{-1} \gg k_{photon}$

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

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

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

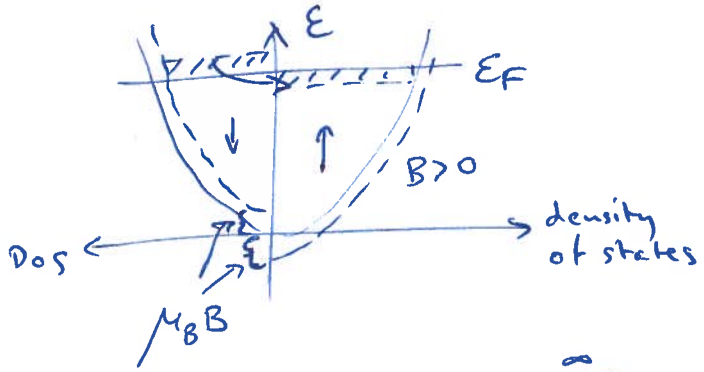
Example: States introduced by electron/hole-doping in semiconductors

The states do not need to be occupied.

6. a) Show that the magnetic susceptibility of free conduction electrons is proportional to the density of states at the Fermi energy. (2.5p)
b) Discuss the classification of insulators. (1.5p)

a) $\chi = \frac{\mu_0 M}{B_a}$, where $M = \mu_B \left[n(\uparrow) - n(\downarrow) \right]$

spin up   spin down



$D(\varepsilon) \sim \sqrt{\varepsilon}$

$$M = \mu_B (n_\uparrow - n_\downarrow) = \mu_B \cdot \int_{-\infty}^{\infty} \left[f_{FD}(\varepsilon) \cdot \frac{1}{2} D(\varepsilon + \mu_B B) - f_{FD} \cdot \frac{1}{2} D(\varepsilon - \mu_B B) \right] d\varepsilon =$$

$$= \mu_B \cdot \int_{-\infty}^{\infty} f_{FD} \cdot \frac{1}{2} \left\{ D(\varepsilon) + \mu_B B \cdot \frac{dD(\varepsilon)}{d\varepsilon} - \left(D(\varepsilon) - \mu_B B \cdot \frac{dD(\varepsilon)}{d\varepsilon} \right) \right\} d\varepsilon =$$

$$= \mu_B^2 B \cdot \int_{-\infty}^{\infty} f_{FD}(\varepsilon) \cdot \frac{dD(\varepsilon)}{d\varepsilon} d\varepsilon = \left\{ \begin{matrix} \text{part.} \\ \text{integration} \end{matrix} \right\} =$$

$$= \underbrace{\mu_B^2 B \cdot \left[f_{FD}(\varepsilon) \cdot D(\varepsilon) \right]_{-\infty}^{\infty}}_{=0} - \mu_B^2 B \cdot \int_{-\infty}^{\infty} f'(\varepsilon) D(\varepsilon) d\varepsilon \qquad = +\mu_B^2 B \cdot D(\varepsilon$$

delta-spike at ε_F

$$\Rightarrow \chi = \mu_0 \mu_B^2 D(\varepsilon_F)$$

b) Insulators can be categorized by looking at local electron density. Crystalline insulators can be covalent crystals, molecular crystals, and ionic crystals.

Cont. #6b)

Covalent crystals	have bonds in preferred directions sharing electrons between atoms
Molecular crystals	Have filled shells and crystallize using dipole or fluctuating dipole forces
Ionic crystals	Are similar to molecular crystals, but with ions ⟹ Electrostatic forces determine properties