

STOCKHOLMS UNIVERSITET
FYSIKUM

Examination in Condensed Matter Physics I, FK7042, 7.5 hp
Tuesday, March 29, 2016, 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.

1. Explain the following concepts through clear examples, including small sketches, simple calculations etc. as needed:

- a) Bravais lattice and coordination number (1p)
- b) Wigner-Seitz cell and Brillouin zone (1p)
- c) Close packing and packing density (1p)
- d) Geometric structure factor (1p)

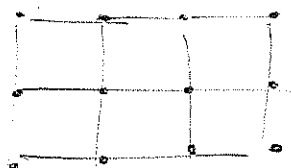
a) Bravais lattice: Infinite periodic array of discrete points appearing exactly the same from any point.

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

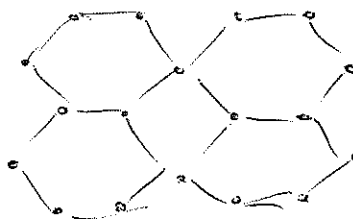
n_i : integers

$\vec{a}_i$: primitive vectors

$\vec{R}$: gives the Bravais lattice



B.L.

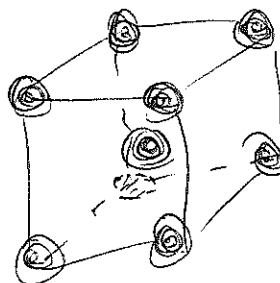


Not a B.L.

Coordination number: Number of nearest neighbors

ex. bcc:

coordination number = 8

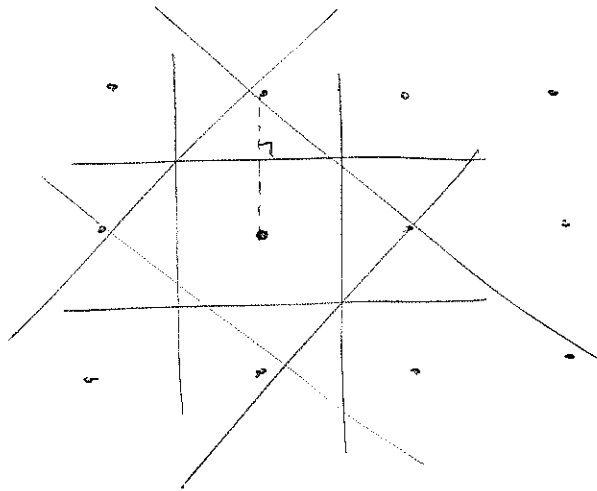


cont.

1b) Wigner-Seitz cell

Primitive unit cell
containing space closest
to the center of the cell

Construction :



Bisect all lines to
neighboring points.
(by planes in 3D)

Any space not crossing any
line/plane belongs to
the WS-cell of that
B.L. point

Brillouin zone : the Wigner-Seitz cell in
reciprocal lattice.

Higher order zones cross 1, 2, 3, ... planes.

1c) Close packing

Structures that pack spheres with
highest possible density : fcc, hcp

Packing density

Assume equal-size spheres at each
lattice point, as large as possible.

Packing density = filled volume / total vol.

1d) Geometric structure factor

X-ray diffraction intensity
will depend on $|S_{\vec{G}}|^2$

$$S_{\vec{G}} = \sum_{j=1}^N f_j e^{i\vec{G} \cdot \vec{r}_j}$$

$\vec{G}$: reciprocal lattice vector
 f_j : atomic form factor
 $\vec{r}_j$: position of atom in basis

$S_{\vec{G}} = 0 \Rightarrow$ destructive interference.

2. Use the information of Figure 1 below to answer the following questions:

- What does the figure describe in general terms? (0.5p)
- What is the crystal structure of the material? (1p)
- Is it a metal, an insulator, or a semimetal? Motivate! (0.5p)
- Making suitable assumptions and approximations, what further information could you get from the figure? Do not perform any calculations, just motivate what could be done. (2.0p)

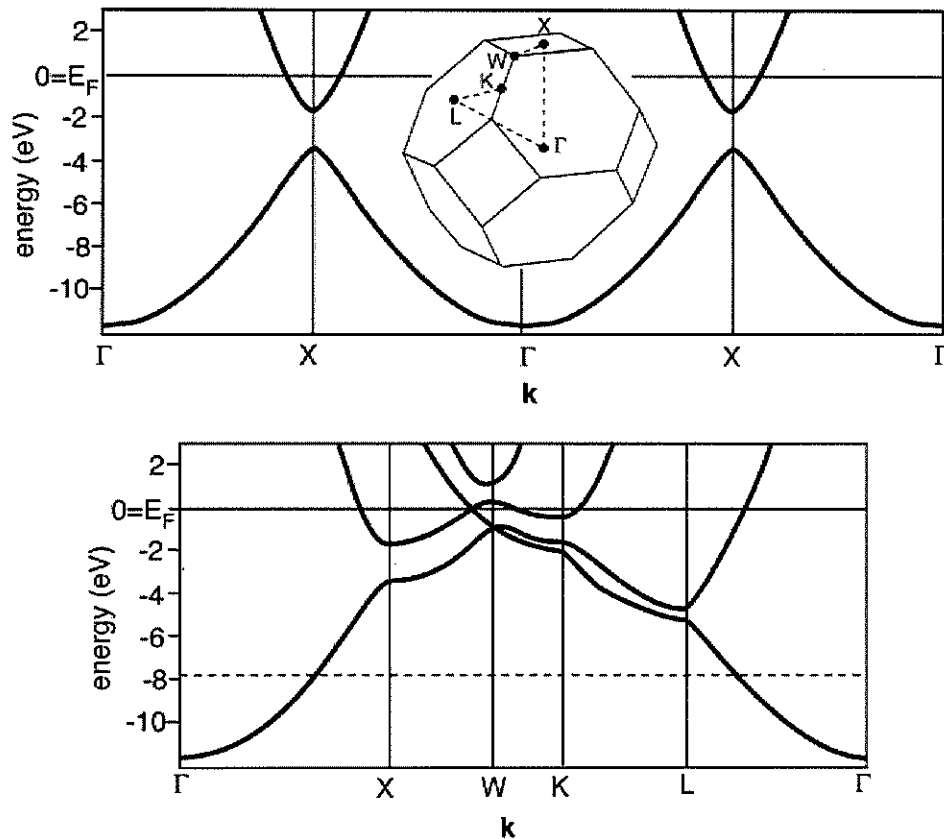


Figure 1: Figure for Problem 2. Top panel and bottom panel belong together.

- The figure describes the electronic band structure, i.e. energy as a function of $\vec{k}$ -vector, for select paths of $\vec{k}$, between points of high symmetry in 1st Brillouin zone.
- The Brillouin zone is a Wigner-Seitz cell of a bcc lattice, so the crystal structure is fcc.
- It is a metal. The Fermi level cuts the band structure. Even if E_F would have been within the gap at X, it would be a metal, since there would be some $\vec{k}$ -vector without a gap.

2d) The $E(k)$ looks free-electron like around Γ .

At X , there is a gap opening of about 1.5 eV.

The 1st B.Z. is completely filled, the 2nd is partially filled, as well as parts of 3rd zone (see between W and K). If it is an element, the valence is thus higher than 2, but probably not 4. Aluminium?

Assuming free electron model between Γ and X and $E(\Gamma) = -11.7 \text{ eV}$, $E(X) = -3 \text{ eV}$ (no gap)

we would get $\Delta E = 8.7 \text{ eV} = \frac{\hbar^2 k_{\Gamma X}^2}{2m_e}$

where $|k_{\Gamma X}| = \frac{2\pi}{a}$ and a is the fcc lattice param.

$$\Delta E = \frac{\hbar^2 \cdot \left(\frac{2\pi}{a}\right)^2}{2m_e} \Rightarrow a = \frac{\hbar}{\sqrt{2m_e \Delta E}} = \frac{6.63 \cdot 10^{-34}}{\sqrt{2 \cdot 9.11 \cdot 10^{-31} \cdot 8.7}} = 1.602 \cdot 10^{-10} \text{ m}$$

$$\Rightarrow a = 4.16 \text{ \AA}$$

Compare Al: $a = 4.05 \text{ \AA}$) quite close!

Other info : Group velocities, effective masses,
Fermi energy $\approx 11.7 \text{ eV}$

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. (1.5p)

b) In an x-ray diffraction experiment on iron powder, the first observed diffraction peak was located at $2\theta = 44.60^\circ$. Determine the maximum number of diffraction peaks that could possibly be observed in this experiment and give their expected locations. (2.0p)

c) If the wavelength λ could be increased, at what λ would it no longer be possible to see any diffraction peaks? (0.5p)

a)

$$v_c = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) \quad \text{where } \bar{a}_i \text{ are the lattice params.}$$

$$v_g = \bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3) \quad \text{--- " --- } \bar{b}_i \text{ --- " --- reciprocal lattice ---}$$

$$\text{Use } \bar{b}_3 = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{v_c}$$

$$v_g = \bar{b}_1 \cdot (\bar{b}_2 \times [2\pi \frac{\bar{a}_1 \times \bar{a}_2}{v_c}]) = \frac{2\pi}{v_c} \bar{b}_1 \cdot (\bar{b}_2 \times [\bar{a}_1 \times \bar{a}_2])$$

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

$$\text{and } \bar{a}_i \cdot \bar{b}_j = 2\pi \delta_{ij}$$

$$v_g = \frac{2\pi}{v_c} \bar{b}_1 \cdot (\underbrace{[\bar{a}_2 \cdot \bar{b}_2]}_{2\pi} \bar{a}_1 - \underbrace{[\bar{a}_1 \cdot \bar{b}_2]}_0 \bar{a}_2) = \frac{(2\pi)^2}{v_c} \cdot 2\pi = \frac{(2\pi)^3}{v_c}$$

b) Iron: bcc with $a = 2.87 \text{ \AA}$ (periodic table)

bcc: reflections when Miller indices $h+k+l = \text{even}$

$$\text{(calculate } S_g = \sum_j e^{i\vec{G} \cdot \vec{r}_j} \text{ with } \vec{r}_j = \vec{0} \text{ and } \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \\ = \frac{1}{2}(\bar{a}_1 + \bar{a}_2 + \bar{a}_3))$$

First diffraction peak for (110)

$$\text{at } \theta = \frac{44.60^\circ}{2} = 22.30^\circ \Rightarrow \sin^2(22.30^\circ) = \frac{\lambda^2}{4 \cdot a^2} \cdot 2$$

$$\Rightarrow \lambda = \sqrt{2} a \cdot \sin(22.30^\circ) = \underline{\underline{1.540 \text{ \AA}}}$$

$$\text{Max } \sin^2 \theta = 1 \Rightarrow (h^2 + k^2 + l^2)_{\max} = \frac{4a^2}{\lambda^2} = \frac{4a^2}{2a^2 \sin^2(22.30^\circ)} = \frac{2}{\sin^2(\theta)}$$

$$(h^2 + k^2 + l^2) \Big|_{\max} = 13.89 \Leftrightarrow 13 : \text{list and count these}$$

cont. 3b)

$(h \ k \ l)$	$h^2+k^2+l^2$	$\sin^2\theta$	$\theta(^{\circ})$	
1 1 0	2	0.144	22.30	} Peaks to be observed
2 0 0	4	0.288	32.45	
2 1 1	6	0.432	41.09	
2 2 0	8	0.576	49.36	
3 1 0	10	0.720	58.04	
2 2 2	12	0.864	68.34	
3 2 1	14			

c) $\sin^2\theta = 1$ for (110) reflection ($h^2+k^2+l^2=2$)

$$\text{when } \lambda = \frac{2a}{\sqrt{2}} = \sqrt{2} \cdot a \approx 4.06 \text{ \AA}$$

$$\underline{\underline{\lambda_{\max} = 4.06 \text{ \AA}}}$$

4. a.) Explain briefly the following concepts related to lattice vibrations: Phonon, dispersion relation, optical branch, Debye model, Umklapp process. (2p)

b.) Copper has a sound velocity $v_s = 3560$ m/s and a lattice parameter $a = 3.61$ Å. Estimate the highest vibration frequency of phonons in Cu and discuss the probability that a mode of this frequency is excited at room temperature. (2p)

a) Phonon: Energy quantum of elastic wave.

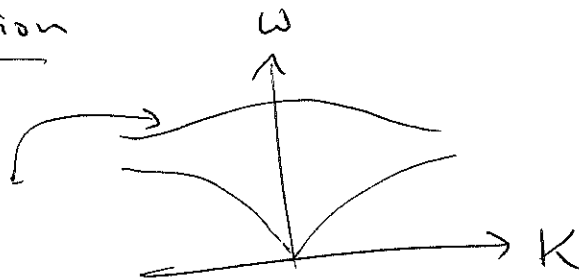
Properties: $\left\{ \begin{array}{l} \text{Frequency } \omega, \text{ energy } \hbar\omega \\ \text{Wave vector, } |\vec{K}| = \frac{2\pi}{\lambda} \\ \text{Polarization direction (1 L, 2 T)} \end{array} \right.$

Dispersion relation

$\omega(\vec{K})$ or $\hbar\omega(\vec{K})$

Optical branch

has $\omega(\vec{K}) \neq 0$
for $\vec{K} \rightarrow 0$



Debye model

Model for dispersion relation:

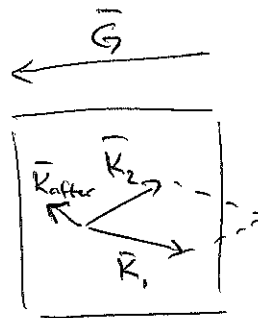
$$1) \omega = v_s \cdot |\vec{K}|$$

$$2) \text{ cut-off } \omega_D: 3N = \int_0^{\omega_D} D(\omega) d\omega$$

Umklapp process

Phonon collision where

$$\vec{K}_{\text{after}} = \vec{K}_1 + \vec{K}_2 + \vec{G}; \quad \vec{G} \neq 0$$



1st B.Z.

Cont. 4)

4b) Given : Cu, $v_s = 3560 \text{ m/s}$, $a = 3.61 \text{ \AA}$

Wanted : * Highest vib. freq. of phonons in Cu

* Probability that a mode of highest freq. is excited at room temp.

Solution : Assume Debye model, $\omega_D = v_s \cdot K_D$

$$3N = \int_0^{K_D} D(K) dK = \int_0^{K_D} 3 \cdot \left(\frac{L}{2\pi}\right)^3 4\pi K^2 dK = \frac{V}{(2\pi)^3} 4\pi K_D^3$$

$$\Rightarrow K_D = \left(6\pi^2 \frac{N}{V}\right)^{1/3}$$

Cu: $\frac{N}{V} = \frac{4}{a^3}$ since fcc has 4 at/cell, valence 1 for Cu assumed

$$\Rightarrow K_D = \frac{(24\pi^2)^{1/3}}{a}; \quad \omega_D = \frac{v_s}{a} \cdot (24\pi^2)^{1/3} = 6.1 \cdot 10^{13} \text{ s}^{-1} \quad (f_{\max} \sim 10 \text{ THz})$$

Probability for excitation :

Assume that "a mode" means a particular mode.

Such a mode would have occupancy

$$\langle n \rangle = \frac{1}{e^{\hbar\omega/4k_B T} - 1} \quad \text{with } \omega = \omega_D$$

$$\langle n \rangle = \left\{ \frac{\hbar\omega_D}{4k_B T_{RT}} = 7.64 \cdot 10^{-12} \text{ K} \cdot \text{s} \cdot \frac{6.1 \cdot 10^{13} \text{ s}^{-1}}{300 \text{ K}} = 1.55 \right\} =$$

$$= 0.27$$

Conclusion: Probability rather high, about 25% occupancy of one phonon, but not a lot of phonons in each mode.

5. a) Discuss the experimental observation and interpretation of the de Haas – van Alphen effect. (2p)
 b) Suppose that you are studying an unknown material. You are carrying out the following measurements:
 A. Resistivity as a function of temperature.
 B. Hall effect.
 C. Optical absorption.
 D. X-ray diffraction.

Explain how you would use the results of each of these measurements to improve your understanding of what kind of material you have. (2p)

a) de Haas – van Alphen effect can be used as a Fermi surface probe. The effect gives oscillations in magnetization/susceptibility as a function of applied magnetic field. The oscillations have periodicities in $\frac{1}{B}$ given by extremal (maxima, minima) Fermi surface cross-sections perpendicular to the field.

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{h} \cdot \frac{1}{A_e} \quad \text{extremal area of F.S. in plane } \perp \vec{B}$$

b) Resistivity $R(T)$: Gives metal/insulator/semiconductor/supercond. possible phase transitions, disorder

Hall effect: Sign and concentration of charge carriers

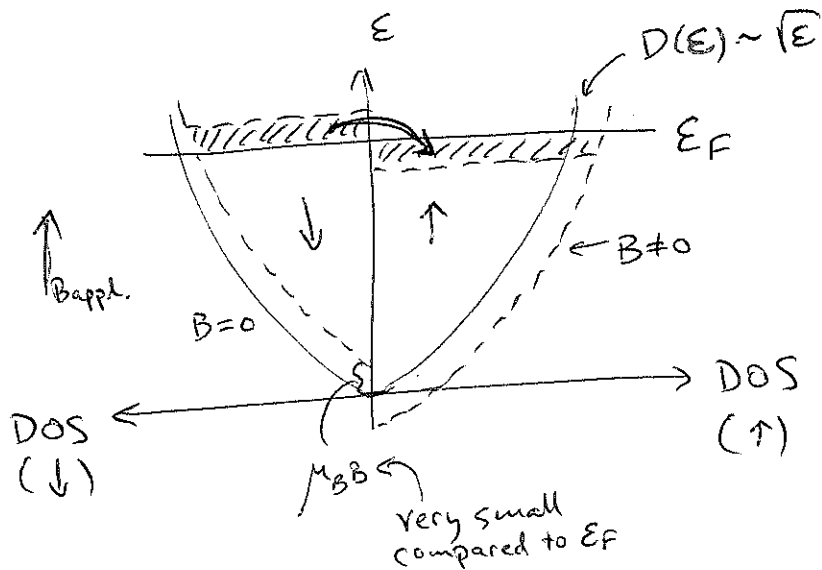
Optical absorption: Band gap, defects

X-ray diffraction: Structure, lattice parameters

6. a) Pauli paramagnetism is a weak form of paramagnetism, involving itinerant (as opposed to localized) electrons. Make suitable assumptions and deduce an expression for the susceptibility of a Pauli paramagnet. (2p)
 b) Discuss the concept of low-angle grain boundaries and how they can be studied. (2p)

a) Given: Itinerant electrons - assume that we can use free electron model

Wanted: Susceptibility $\chi = \frac{\partial M}{\partial H} \approx \frac{M}{H} = \frac{\mu_0 M}{B_{\text{applied}}}$



$$M = \mu_B [n(\uparrow) - n(\downarrow)]$$

Applied field

↓
Lower energy for electrons with spin along field.

$$\Rightarrow n(\uparrow) \neq n(\downarrow)$$

$$M = \mu_B (n_{\uparrow} - n_{\downarrow}) = \frac{\mu_B}{V} \int_0^{\infty} \left[f_{FD}(\epsilon) \cdot \frac{1}{2} D(\epsilon + \mu_B B) - f_{FD}(\epsilon) \cdot \frac{1}{2} D(\epsilon - \mu_B B) \right] d\epsilon =$$

$$= \frac{\mu_B}{V} \int_0^{\infty} f_{FD} \cdot \frac{1}{2} \left\{ D(\epsilon) + \mu_B B \cdot \frac{dD(\epsilon)}{d\epsilon} - (D(\epsilon) - \mu_B B \cdot \frac{dD(\epsilon)}{d\epsilon}) \right\} d\epsilon =$$

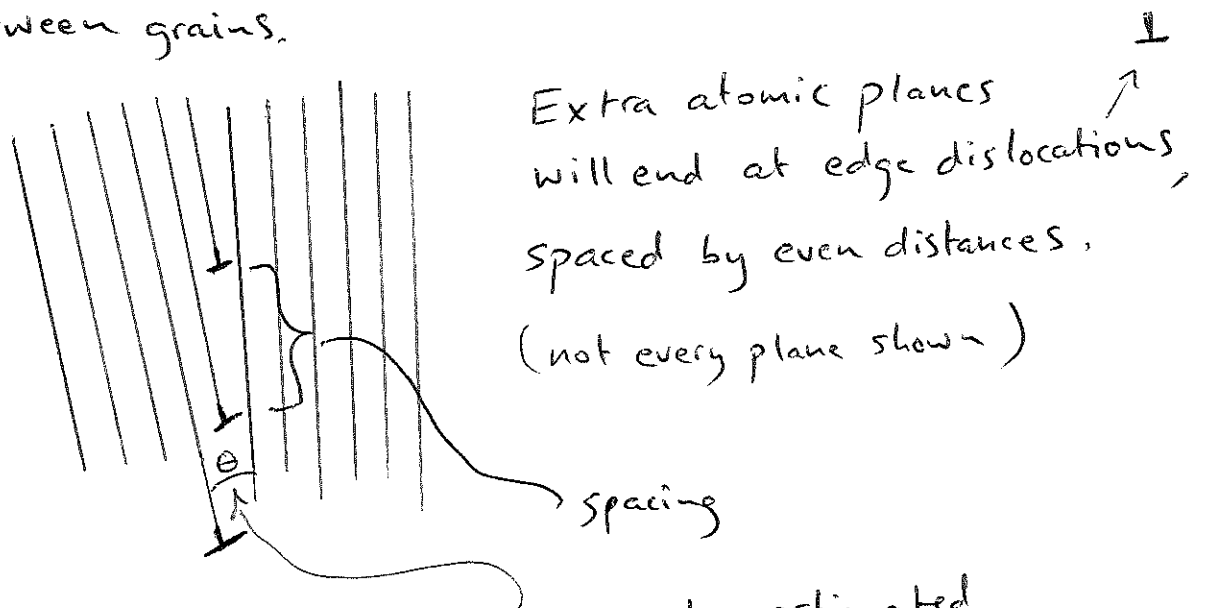
$$= \frac{\mu_B^2 B}{V} \int_0^{\infty} f_{FD}(\epsilon) \cdot \frac{dD(\epsilon)}{d\epsilon} d\epsilon = \left\{ \text{part. integration} \right\} =$$

$$= \frac{\mu_B^2 B}{V} \cdot \left\{ \underbrace{\left[f_{FD}(\epsilon) D(\epsilon) \right]_0^{\infty}}_{\substack{f_{FD}(\epsilon) \rightarrow 0 \text{ at } \infty \\ D(\epsilon) \rightarrow 0 \text{ at } 0}} - \int_0^{\infty} \underbrace{f'_{FD}(\epsilon)}_{\substack{\text{negative} \\ \delta\text{-spike at } E_F}} D(\epsilon) d\epsilon \right\} = + \frac{\mu_B^2 B}{V} \cdot D(E_F)$$

$$\chi = \frac{\mu_0 \mu_B^2 B}{V} \cdot D(E_F)$$

6b) Low-angle grain boundaries

Grain boundary with small misalignment angle between grains.



The misalignment angle can be estimated from the dislocation spacing.

The dislocations can be seen through etching of the surface $\rightarrow$ higher energy at dislocation gives faster etch $\rightarrow$ etch pit.

