Solid state physics 2018 Final Exam

20th April 2018

Good luck!

You may not use textbooks, notes, or calculators.

Fill out your student number, your name, and your family name below. Only provide answers inside the answer boxes.

Student number:

1 2 3 4 5 6 7 8 9 0

First name:

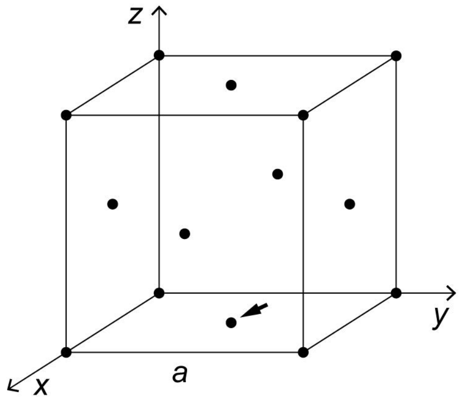
Last name:

1. **Crystal structure**

   (a) Write down definitions of: a primitive unit cell, a conventional unit cell, and a Wigner-Seitz unit cell. *(5 points)*

Primitive unit cell: minimally possible volume that covers the complete space upon translations by the lattice vectors.
Conventional unit cell: a unit cell "comfortable" to work with (often cubic).
WS unit cell: all points in space closer to a specific lattice point than to any other.

(b) Consider the FCC lattice shown below with lattice constant a. Write down the basis using the conventional unit cell. Compute the structure factor and determine the selection rules of (h, k, l) which give both constructive and destructive interference. *(5 points)*



Basis: $(0, 0, 0)$, $(1/2, 1/2, 0)$, $(1/2, 0, 1/2)$, $(0, 1/2, 1/2)$.

$$S = f \times (1 + e^{i\pi(h+l)} + e^{i\pi(h+k)} + e^{i\pi(k+l)})$$

Constructive interference: h, k, l all even or all odd. Destructive interference: all the other options.

(c) **Distorting Crystal structure**

We now displace the atom marked by an arrow in the image above in the positive z-direction by a distance δ as well as all the atoms equivalent to that one by the translations of the conventional unit cell.

Write the *primitive* lattice vectors for the cases $\delta = 0$ and $0 < \delta < a$. *(10 points)*

$\delta = 0$: $(a/2, a/2, 0)$, $(a/2, 0, a/2)$, $(0, a/2, a/2)$.
$\delta \neq 0$: $(a, 0, 0)$, $(0, a, 0)$, $(0, 0, a)$.

(d) Compute the structure factor for the scattering vector (h, k, l) as a function of δ. Then use this expression to determine the scattering amplitudes for scattering vectors $(1, 1, 1)$, $(1, 1, 0)$ and $(0, 0, 1)$. *(10 points)*

$$S = f \times (1 + e^{i\pi(h+l)} + e^{2i\pi l\delta/a} e^{i\pi(h+k)} + e^{i\pi(k+l)})$$

$(1, 1, 1)$: $S = f(3 + e^{2\pi i\delta/a})$
$(1, 1, 0)$: $S = 0$
$(0, 0, 1)$: $S = f(3 + e^{2\pi i\delta/a})$

(e) Which additional diffraction peaks appear when $\delta \neq 0$, compared to $\delta = 0$? Which peaks stay absent when $\delta \neq 0$? *(10 points)*

h, k odd, $l = 0$ are still absent from the interference pattern, all the other peaks appear.

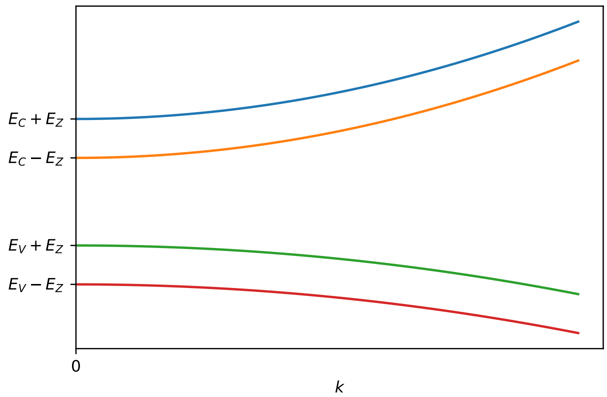
(f) Compute the intensity of the new peaks that appear for $\delta > 0$ when $l \ll a/\delta$. Explain how the intensities of these diffraction peaks may be used to determine δ in an X-ray experiment. *(10 points)*

Expanding S in Taylor series we get $S \approx f \times 2\pi i l\delta/a$, and the intensity is proportional to $|S^2|$. Therefore comparing the brightness of these peaks with the peaks corresponding to constructive interference allows to determine δ.

2. **Magnetic semiconductor**
An undoped semiconductor with electron and hole effective masses m_e and m_h is placed in an external magnetic field, so that all electrons experience a Zeeman splitting $g\mu_B B$. This makes the dispersion relation of electrons with spin up differ from that of electrons with spin down (in both the conduction and the valence band). We consider a sufficiently weak magnetic field, so that $g\mu_B B \ll E_G$, with E_G the semiconductor band gap. *In this problem if you do not know how to deal with Zeeman splitting, disregard spin-related phenomena to get partial points in any subquestion except for the last one.*

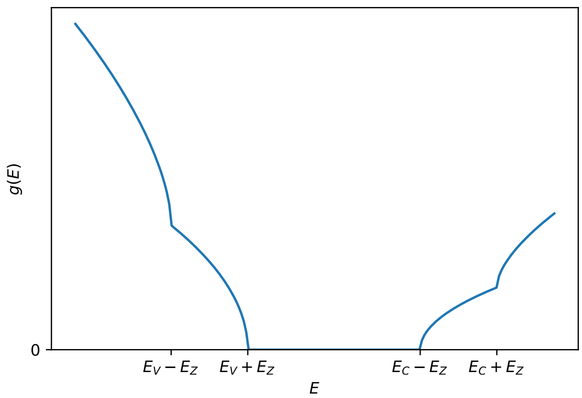
   (a) Draw the band structure of such a semiconductor, showing both the bands of spin up electrons and spin down electrons. *Hint: check that when $B = 0$ your answer coincides with band structure of a semiconductor. (10 points)*

Zeeman splitting moves spin up electrons and holes up by $E_Z \equiv g\mu_B B$ and spin down bands down by the same amount. Therefore the dispersion consists of 4 parabolas:



   (b) Draw the density of states $g(E)$ of this semiconductor and indicate the relevant energy scales. *Hint: once again check that when $B = 0$ your answer coincides with density of states of a regular semiconductor. (10 points)*

Each of the four different bands contributes a square root-shaped density of states starting at the energy of that band at $k = 0$. Summing up all 4 contributions we get



Note: not summing up the contributions of different spins only resulted in a minor penalty

(c) Compute the number of electrons and holes with spin up and spin down as a function of E_F. Write down the charge neutrality condition for this material. Use that you may approximate Fermi-Dirac distribution as Boltzmann distribution when $E_G \gg k_B T$. *Hint: once again your answer should agree with a regular semiconductor when* $B = 0$. *(10 points)*

While repeating the full derivation of the semiconductor number of particles would be a correct solution, we do not need to redo all the work. Instead we can observe that the situation is the same as in the regular semiconductor, except for two changes:

i. The number of particles in each band is half of that in the original sermiconductor
ii. The bands are displaced in energy by $\pm E_Z$

Therefore we get

$$
\begin{aligned}
n_{e\uparrow} &= \frac{N_C}{2} e^{-\beta(E_C + E_Z - E_F)} \\
n_{e\downarrow} &= \frac{N_C}{2} e^{-\beta(E_C - E_Z - E_F)} \\
n_{h\uparrow} &= \frac{N_V}{2} e^{-\beta(-E_V - E_Z + E_F)} \\
n_{h\downarrow} &= \frac{N_V}{2} e^{-\beta(-E_V + E_Z + E_F)},
\end{aligned}
$$

with $\beta = 1/k_B T$. The charge balance condition requires that $n_{e\uparrow} + n_{e\downarrow} = n_{h\uparrow} + n_{h\downarrow}$

(d) Using the charge neutrality condition determine the concentrations of electrons and holes with spin up and spin down when magnetic field is large $g\mu_B B \gg k_B T$. **Hint: two of the four concentrations will be small.** *(10 points)*

Substituting the expressions for the particle concentrations into the charge balance equation we get

$$N_C e^{-\beta(E_C - E_F)} \cosh \beta E_Z = N_V e^{-\beta(E_F - E_V)} \cosh \beta E_Z$$

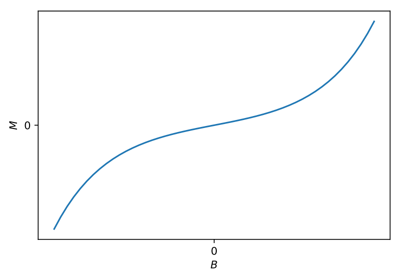
This is the same as the charge balance condition in a regular seminconductor, except for the extra factor of $\cosh \beta E_Z$ in front of N_C and N_V. To solve this equation we can express E_F through the rest of the problem parameters ans substitute it back into the answer for the previous problem. Alternatively we may once again adjust the answer for the regular intrinsic semiconductor by observing that the spin down electron band shifts towards E_F by the same amount as the spin up hole band, and therefore E_F does not change with magnetic field. This means that the concentrations of the bands closer to E_F are increased: $n_{e\downarrow} = n_{h\uparrow} = n_i e^{\beta E_Z}/2$, while the other two concentrations are decreased by the same amount: $n_{e\uparrow} = n_{h\downarrow} = n_i e^{-\beta E_Z}/2$.
Here we did not use $E_Z \gg k_B T$, which simplifies the math a bit, but does not change the answer.

(e) Using the answer of the previous subproblem, compute the total magnetization M of this semiconductor due to spins when $g\mu_B B \gg k_b T$. Sketch $M(B)$, the dependence of magnetization on B. *(10 points)*

$M = -\mu_B(n_{e\uparrow} - n_{e\downarrow} - n_{h\uparrow} + n_{h\downarrow})$. Note that:

- The contribution of holes to magnetization is the opposite of that of electrons because we are *removing* particles with a certain spin.
- The signs are such that we obtain a paramagnet, just like we would if having free spins.

Substituting the expressions for concentrations we get $M = 2\mu_B n_i \sinh \beta E_Z$. In the limit $E_Z \gg k_B T$, M is given by the concentration of majority spin carriers, and equals $\mu_B n_i e^{\beta E_Z}$. If we only derived that limit, we could understand the behavior of magnetization at small fields by observing that at $B = 0$ the magnetization should vanish. We then arrive to the following sketch of magnetization:



3. **Extra answer space**