# Modul 3

Kandidatnummer: 27

25. april 2017

# 1

#### a

The drude model assumes that all the thermal energy be in the form of kinetic energy.

$$\underbrace{\frac{1}{2}mv_t^2}_{\text{kinetic}} = \underbrace{\frac{3}{2}k_bT}_{\text{thermal}}$$

From the velocity of the particle in the electric field on can find the conductivity.

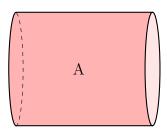
$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}m_e = -e\mathbf{E}$$

$$\int_v \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}m_e \,\mathrm{d}t = \int_t -e\mathbf{E} \,\mathrm{d}t$$

$$\mathbf{v}(t) = \frac{-e\mathbf{E}t}{m_e}$$

Here we define  $\tau$  to be the average time between collisions. Inserting this into the expression gives the average drift speed:

$$\bar{v} = \frac{-e\mathbf{E}\tau}{m_e}$$



The number of electrons passing though the unit per unit time is  $n|\bar{v}|A$ , or  $-en|\bar{v}|A$  for negative charged electrons. The current density is area independent and is equal to  $\mathbf{j} = -n\bar{v}e$ . Figure made in tikz.

Combining the two expressions found above gives:

$$\mathbf{j} = -en\left(\frac{-e\mathbf{E}\tau}{m_e}\right) = \frac{ne^2\tau}{m_e}\mathbf{E}$$

Current density of defined as  $\mathbf{j} = \sigma \mathbf{E}$ . This can further be solved to find an expression for the conductivity.

$$\sigma = \mathbf{j} \cdot \mathbf{E}^{-1}$$

$$\sigma = \frac{ne^2\tau}{m_e} \mathbf{E} \cdot \mathbf{E}^{-1} = \frac{ne^2\tau}{m_e}$$

 $\kappa = \frac{1}{3}v_t^2 \tau c_v$  was found in *Module II*.

 $\kappa$  and  $\sigma$  both contains the mean free path for electrons. Given that the assumtion of the mean free path is in the same order of magnitude as the interatomic distance both these properties are questionable. If however one takes the ratio the dependency of  $\tau$  is removed. So even if this assumtion if wrong the Widemann-Franz coefficient is unaffected.

$$\frac{\kappa}{\sigma} = \frac{\frac{1}{3}v_t^2 \tau c_v}{\frac{ne^2 \tau}{m_e}} = \frac{v_t^2 c_v m_e}{3e^2}$$

this can be written in terms of  $k_b$  instead:

$$L = \frac{\kappa}{\sigma T} = \frac{3}{2} \frac{k_B^2}{e^2}$$

When comparing this to the actual quantum mechanical result taken from *lecture 12* which gives:

$$L = \frac{\kappa}{\sigma T} = \frac{\pi^2}{3} \frac{k_B^2}{e^2}$$

The only difference is a factor of  $\pi^2/3$  versus 3/2 which is very close.

### b

Further one can refine the result by deriving L in terms of the free electron Fermi gas by taking into account that  $C_{el} = \frac{\pi^2 k_B T}{2T_F}$ . This gives:

$$\frac{\kappa}{\sigma T} = \frac{v_F^2 \left(\frac{\pi^2 k_B T}{2T_F}\right) m_e}{3e^2 T}$$

$$\frac{\kappa}{\sigma T} = \frac{v_F^2 \pi^2 k_B m_e}{6e^2 T_F}$$

Isolating the terms that makes up the energy written introductory gives  $\frac{E}{2} = 3k_BT_F = m_ev^2$  gives a further refined expression:

$$\frac{\kappa}{\sigma T} = \frac{\pi^2 k_B}{6e^2 T_F} m_e v_F^2$$

$$\frac{\kappa}{\sigma T} = \frac{\pi^2 k_B}{6e^2 T_F} 3k_B T_F$$

$$\frac{\kappa}{\sigma T} = \frac{\pi^2 k_B^2}{2e^2}$$

Comparing this to the results found in a, and the quantum mechanical answer taken from the lectures, this refinement gives approximation which is closer to the quantum mechanical answer.

# 3

#### a

At  $T=0\,\mathrm{K}$  the Gibbs energy  $G=N\mu$ . This can be compared to G=E+pV. From

From the derivation of FEFG one had to introduce boundary conditions for the wave-function resulting in k being restricted numbers governed by an integer number. This also gave an expression for the energy:

$$E(N) = \frac{\hbar^2}{2m_e} \left(\frac{3\pi^2 N}{V}\right)^{2/3} \tag{1}$$

$$D(E) = \frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} E^{1/2} \tag{2}$$

$$N(E) = \frac{V}{3\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} E^{3/2}$$

Pressure can be expressed as  $p = -\left(\frac{\partial \epsilon(N)}{\partial V}\right)$ . Applying this to the results above gives:

$$p = -\left(\frac{\partial \epsilon(N)}{\partial V}\right) = -\frac{\partial}{\partial V} \left(\frac{\hbar^2}{2m_e} \left(\frac{3\pi^2 N}{V}\right)^{2/3}\right)$$
$$p = \frac{\hbar^2}{2m_e} \left(3\pi^2 N\right)^{2/3} \frac{2}{3} V^{-5/3}$$

Inserting this into the Gibbs energy formula gives:

$$G = E + pV = E + \left(\frac{\hbar^2}{2m_e} (3\pi^2 N)^{2/3} \frac{2}{3} V^{-5/3}\right) V$$

$$G = E + \frac{\hbar^2}{2m_e} (3\pi^2 N)^{2/3} \frac{2}{3} V^{-2/3} = E + \frac{2}{3} \frac{\hbar^2}{2m_e} \left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

The last term is almost the same expression for E(N) that we started with. The expression can therefore be rewritten in terms of E:

$$G = E + \frac{2}{3}E = \frac{5}{3}E$$

The introductory equations now gives:

$$G = E + pV = N\mu$$
$$\mu = \frac{1}{N}(E + pV)$$
$$\mu = \frac{5}{3}\frac{E}{N}$$

E is found by integrating the product of density of states, Fermi-Dirac distribution and the energy at all points:

$$E = \int_0^\infty D(\epsilon)\epsilon \cdot FFD \, \mathrm{d}\epsilon$$

Here one can use the definition of the Fermi-Dirac distribution which gives 1 for all values below a point, here denoted as  $\epsilon_F$  and 0 for all further points. The limits can therefore be shifted.

$$E = \int_0^{\epsilon_F} D(\epsilon) \epsilon \, \mathrm{d}\epsilon$$

Inserting for the expressions above gives:

$$E = \int_0^{\epsilon_F} D(\epsilon) \epsilon \, d\epsilon$$

$$E = \int_0^{\epsilon_F} E \cdot \frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} E^{1/2} \, dE$$

$$E = \left[\frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} \frac{2}{5} E^{5/2}\right]_0^{\epsilon_F}$$

$$E = \frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} \frac{2}{5} \epsilon_F^{5/2}$$

Inserting this into the expression for  $\mu$  gives:

$$\mu = \frac{5}{3} \frac{1}{N} \left( \frac{V}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \frac{2}{5} \epsilon_F^{5/2} \right)$$

$$\mu = \frac{5}{3} \left( \frac{V}{3\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \epsilon_F^{3/2} \right)^{-1} \left( \frac{V}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \frac{2}{5} \epsilon_F^{5/2} \right)$$

$$\mu = \epsilon_F$$

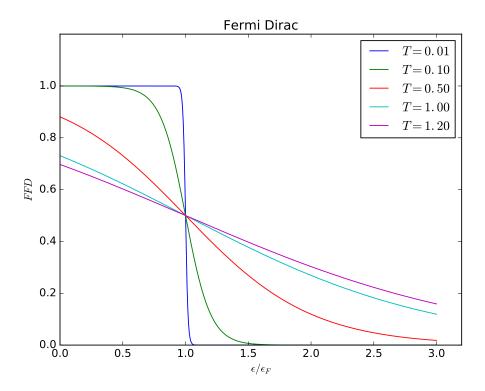
Which was the expected result.

b

Plotting the Fermi-Dirac distribution with unitless variables.  $\epsilon = \epsilon/\epsilon_F, \mu = \mu/\epsilon_F = 1, k_B T = k_B T/\epsilon_F$ .

$$FFD(\epsilon) = \frac{1}{1 + e^{(\epsilon - \mu)/k_B T}}$$
$$FFD(\epsilon) = \frac{1}{1 + e^{(\epsilon - 1)/k_B T}}$$

Code in appendix.



Figur 1: Fermi-Dirac distribution for different temperatures. All temperatures plotted are relative to  $T_F$ .

This approximation is a good one for low temperatures,  $T=0.01,\,T=0.1$  and 0.5. For higher temperatures should the plots be shifted downwards. The plot obtained shows one point in which all the lines meet while the plot in the book does not.

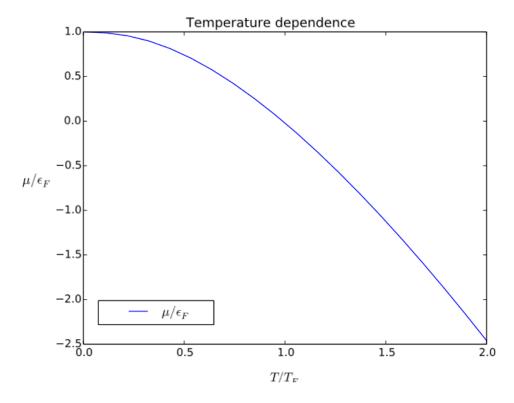
Starting with the equations on page 140 in Kittel,  $N_{T=0} = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar} \epsilon_F\right)^{3/2}$ . When looking at higher temperatures one has to take into account that the electrons will be more spread over the energystates. The density of states is  $D(\epsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar}^{3/2}\right)$ . Integration over the Feri-Dirac distribution multiplied by the density of states gives:

$$N = \int_0^\infty FFD(\epsilon)D(\epsilon) d\epsilon \qquad T > 0$$

The total amount of electrons, the left hand side is the same amount of electrons found at T=0.

$$N(T=0) = N(T>0) = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar} \epsilon_F\right)^{3/2} \frac{V}{3\pi^2} \left(\frac{2m}{\hbar} \epsilon_F\right)^{3/2} = \int_0^\infty FFD(\epsilon)D(\epsilon) \,d\epsilon \quad T>0$$

In the plot there has been introduced unitless variables as in b. A change of variable also has to be done to introduce a unitless integration.

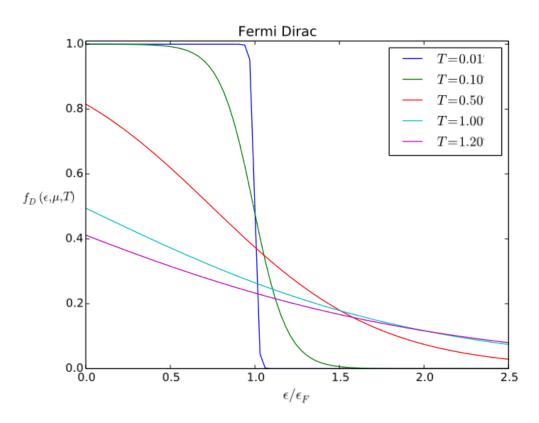


Figur 2: Plot illustrating the temperature dependence of the unitless chemical potential as a function of temperature. All variables in this plot are given unitless.

This plot is consistent with what is expected. From the plot of the Fermi-Dirac in the book compared to the one in b one expects lower values and a lower intersection point with the curve at T=0.001. A lower chemical potential will account for this difference.

### d

Using the values obtained in c the new plot of the Fermie-Dirac becomes:



Figur 3: Plot of unitless Fermi-Dirac distribution taking into account a changing chemical potential. All temperatures plotted are relative to  $T_F$ .

#### $\mathbf{e}$

Due to Pauli exclusion principle one cannot assign equal energy to every electron. So when heating a sample from absolute zero only the electrons with energy in the range of  $k_bT$  of the Fermie level will be excited thermally. An alternative way to explain this phenomenon is by looking at the change in the Fermie-Dirac distribution. A change in temperature will lead to a much

larger difference near  $\epsilon_F$  than any other place. This gives an estimate of which energy range electrons are influenced. Assuming the system starts with N electrons. Only electrons within  $k_bT$  are affected, so only the fraction  $T/T_F$ . The number of electrons affected are therefore  $N_{aff} = NT/T_F$ . Each of there electrons has, as stated above, energy in the range  $k_BT$ . The total electronic thermal kinetic energy is roughly in the order of  $U \simeq (NT/T_F)k_BT$ . Using that  $C_{el} = \frac{\partial U}{\partial T}$  the electronic heat capacity becomes  $C_{el} = Nk_B(T/T_F)$ .

4

a

 $D_2(k)$  will in this case be given by the x and y directions. From the derivation of FEFG one had to introduce boundary conditions for the wave-function resulting in k being restricted numbers governed by an integer number:

$$\mathbf{k} = (k_x, k_y) = \left(\frac{2n_x \pi}{L}, \frac{2n_x \pi}{L}\right)$$
$$\epsilon(k) = \frac{\hbar^2}{2m_e} (k_x^2 + k_y^2) = \frac{\hbar^2}{2m_e} (k^2)$$

From these results there are one distinct wavevector per duplet of wavenumbers  $k_x, k_y$ , in the ground state, which takes up a "volume" (area) element of  $V = \pi r^2$ . The uppermost k is at ground state at the Fermi-level, and is therefore denoted  $k_F$ . Thus the total number of states are:

$$N = \underbrace{2}_{\text{from spinn}} \cdot \frac{\pi k_F^2}{\left(\frac{2\pi}{L}\right)^2} = \frac{V}{2\pi} k_F^2$$

This can now be solved for  $k_F$ :

$$k_F^2 = N\left(\frac{2\pi}{V}\right)$$
$$k_F = \left(\frac{2\pi N}{V}\right)^{1/2}$$

This depends only on the particle concentration. This result can be inserted into the energy expression above to find the total energy.

$$\epsilon_F = \frac{\hbar^2}{2m_e} \left(\frac{2\pi N}{V}\right)^{2\cdot 1/2}$$

$$\epsilon_F = \frac{\hbar^2}{m_e} \frac{\pi N}{V}$$

The density of states is defined as the change in states per energy,  $D(\epsilon) = \frac{dN}{d\epsilon}$ . This can be derived from the expression above up until the Fermi-level.

$$N = \frac{m_e V \epsilon}{\hbar^2 \pi}$$

$$D(\epsilon) = \frac{m_e V}{\hbar^2 \pi}$$

$$\epsilon \le \epsilon_F$$

Which is not dependent on energy. Note here that i have used the same variable for the volume area as done in three dimensions. This could also be named A for the area but to ease the comparison between the three cases i have chosen to use the same variable.

#### b

In one dimension the system has the same introductory expressions as in a, with the only difference being that the system now are restricted in two dimensions.

$$\mathbf{k} = (k_x) = \left(\frac{2n_x\pi}{L}\right)$$
$$\epsilon(k) = \frac{\hbar^2}{2m_e}k^2$$

There are one distinct wavevector per wavenumber in k, in ground state, which takes up a "volume" (line) element. The uppermost k is now that at the Fermi-level. From this the total number of states are:

$$N = \underbrace{2}_{\text{from spinn}} \cdot \frac{k_F}{\left(\frac{2\pi}{L}\right)} = \frac{V}{\pi} k_F$$

Solving for k gives:

$$k_F = \frac{N\pi}{V}$$

This depends only on the particle concentration. This result can be inserted into the energy expression above to find the total energy.

$$\epsilon_F = \frac{\hbar^2}{2m_e} \left(\frac{\pi N}{V}\right)^2$$
 
$$\epsilon_F = \frac{\hbar^2}{2m_e} \frac{\pi^2 N^2}{V^2}$$

The density of states is defined as the change in states per energy,  $D(\epsilon) = \frac{dN}{d\epsilon}$ . This can be derived from the expression above up until the Fermi-level.

$$N = \frac{\sqrt{2m_e}V}{\hbar\pi}\sqrt{\epsilon}$$

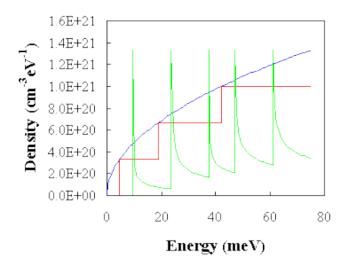
$$\epsilon \leq \epsilon_F$$

$$D(\epsilon) = \frac{V}{\hbar\pi} \left(\frac{2m_e}{\epsilon}\right)^{1/2}$$

$$\epsilon \leq \epsilon_F$$

 $\mathbf{c}$ 

If one considers a somewhat realistic example where there exists no zero-dimensional directions one has to consider that the wavevector has to have a komponent in the  $k_z$  direction. One now assumes that there exists a third dimension but that this is very thin. This results in few allowed states for the third direction. These allowed states will be quantized with a significant difference in energy from  $n_z = 1$  to  $n_z = 2$ . For each of these states the x and y directions are infinite and thus there are an infinite amount of states in these directions. When the total energy of the k vector exceeds a new value for  $n_z$  there are equally many states there. This leads to DOS having a step like form, where each step reflects a increase in  $n_z$ . The function will only access new states(have an increase in DOS) when a new  $n_z$  is possible to fill. This



Figur 4: Figure showing the dependency of a three dimensional block, in blue. A two dimensional block, in red and a one dimensional block in green. Illustration taken from the lecture slides.

was shown in 4 a where it was shown that DOS was independent of energy in 2D.

Similarly for the one dimentional case. Now there are restrictions in two dimensions. This leads to a jump every time it is possible to access a new state in the either of the two constricted dimensions. Between the jumps the DOS will diminish proportional to  $E^{-1/2}$  as shown in  $4\ b$ .

### $\mathbf{d}$

For a realistic model in one dimension there are two restricted directions. A jump in  $n_y$  is the same as a jump in  $n_z$ . So for one jump more than one combination gives the same energy and wavenumber. This results on more possible states for the system than if each of these restricted directions where unique.

### 6

### $\mathbf{a}$

We know from Chapter 2 that the first Brillouin zone in a simple cubic lattice is defined as  $B_{1\text{BZ}} = \frac{1}{2}G[100]$ . Derived from the condition  $\mathbf{k} \cdot (\frac{1}{2}\mathbf{G}) = (\frac{1}{2}\mathbf{G})^2$ .

The komponents of the wavevector  $\mathbf{k}$  satisfies  $k_x = \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \ldots$ , and similarly for  $k_y$  and  $k_z$ . In the ground state of a system with N can be represented by a vector in the  $\mathbf{k}$ -space. The total amount of states is given by the total volume of the sphere divided by the volume per state. One state will in this case take up  $\frac{2\pi}{L_x} \cdot \frac{2\pi}{L_y} \cdot \frac{2\pi}{L_z}$ . Assuming that Lx, y, z are the same length the volume of one state becomes  $\left(\frac{2\pi}{L}\right)^3$ .

The total volume of the sphere is given from the outermost state  $k_F$ ,  $\frac{4\pi k_F^3}{3}$ . The expression then becomes:

$$N = 2 \cdot \frac{\frac{4\pi k_F^3}{3}}{\left(\frac{2\pi}{L}\right)^3}$$

Here the factor of two comes from the spinn nature of electrons. Solving for  $k_F$  gives:

$$k_F = \left(\frac{3\pi^2 N}{L^3}\right)^{1/3}$$

The edge of the first Brillouin zone is from the initial conditions  $k_{BZ,1} = \frac{1}{2} \frac{2\pi}{L} = \frac{\pi}{L}$ .

Assuming a block of equal length in all directions, the amount of atoms in one direction will be:

$$N = (L_x L_y L_z) \frac{1}{a} = \frac{L^3}{a}$$
$$L = aN^{1/3}$$

Applying this to both k vectors found above will make it possible to calculate the ratio, and compare the two:

$$\frac{k_F}{k_{BZ,1}} = \frac{\left(\frac{3\pi^2 N}{L^3}\right)^{1/3}}{\frac{\pi}{L}}$$

$$= \frac{\left(\frac{3\pi^2 N}{(aN^{1/3})^3}\right)^{1/3}}{\frac{\pi}{aN^{1/3}}}$$

$$\frac{k_F}{k_{BZ,1}} = \left(\frac{3}{\pi}\right)^{1/3} = 98.5\%$$

This makes  $K_F$  98.5 percent of the  $k_{BZ,1}$ .

### b

There are two ways of calculating this. Numerically and algebraically. Starting with the assumption that one has to swap out monovalent atoms with divalent. Assume that x is the amount of atoms, and thus for only monovalent atoms also the amount of electrons. The volume has to stay constant, so the amount of electrons has to be constant. The only parameter one has to work with now is the amount of divalent atoms. The total amount of electrons can be represented as N(x-1) + 2xN = N(x+1). This formula represent swapping out some monovalent atoms with divalent atoms.

Using the results from a one has:

$$k_F = \left(\frac{3\pi^2 N}{L^3}\right)^{1/3}$$
$$= \left(\frac{3\pi^2 N(x+1)}{L^3}\right)^{1/3}$$

Applying the same steps as in a gives the further refined expression:

$$=\frac{3(\pi^2(1+x))^{2/3}}{a}$$

Want to fill up  $k_{BZ,1}$  so that  $k_{BZ,1} = k_F$ 

$$k_F = \frac{\pi}{a} = k_{BZ,1}$$

solving for x gives:

$$1 + x = \frac{\pi}{a}$$
$$x = \frac{\pi}{a} - 1 \simeq 0.048$$

In percent one has to change 4.8% of the atoms with divalent atoms. I also did this numerically in a for loop". This gave the same result with only a minor deviation in the last digit. The numerical answer yelded 4.74% while

the nummerical value was closer to 4.8%.

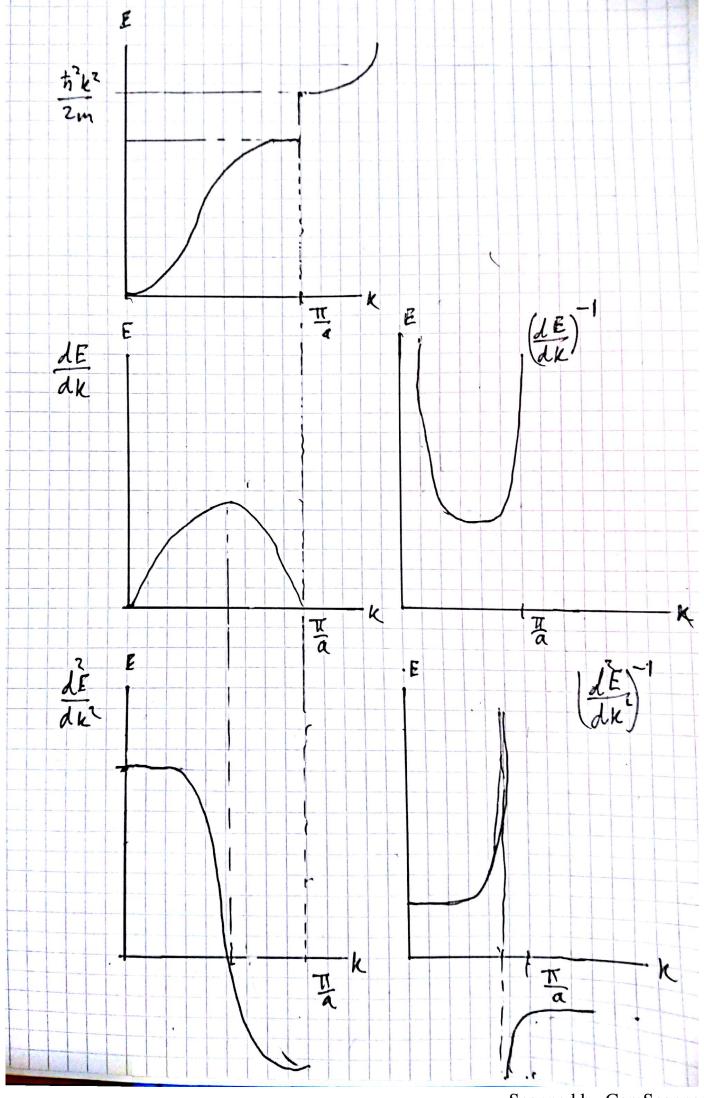
Such alloying would increase the electrical conductivity. More electrons would result in more available electrons for transport. The book presents a formula for electrical conductivity at 6.43,  $\sigma = \frac{ne^2\tau}{m}$ . Here the electrical conductivity is proportional to an increase in the amount of electrons.

#### с-е

I did not do these tasks due to the difficulity of doing c, as explained to you in the group session. I could have done the task with the wrong results as i have seen many others do but i do not see the point in doing this. I have in subtasks a and b showed that i am capable of doing similar calculations as done in c-e.

### 7

Note that in the following plots i have chosen only to illustrate the trend on the possitive side. I have done this do make room for all the plots in one page. The reason why i have chosen this is to make it easier to compare the different plots.



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By using a Taylor expansion around the limits  $k = \pm \frac{\pi}{a}$  one gets the following:

$$\epsilon(k) = \epsilon(k_0) + \frac{\mathrm{d}\epsilon}{\mathrm{d}k}(k - k_0) + \frac{1}{2} \frac{\mathrm{d}^2\epsilon}{\mathrm{d}k^2}(k - k_0)^2 \dots$$

All further factors become very small and can be excluded. The first derivative is approximately zero at the limits. The first term is just a constant factor and can be sat to zero aswell, this will not influence the final result.

$$\epsilon(k) = \frac{1}{2} \frac{\mathrm{d}^2 \epsilon}{\mathrm{d}k^2} (k - k_0)^2$$

Generally the energy is given as  $\epsilon = p^2/2m = \hbar^2 k^2/2m$ . This gives two expressions for the energy, solving for the mass gives:

$$\epsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{1}{2} \frac{\mathrm{d}^2 \epsilon}{\mathrm{d}k^2} (k - k_0)^2$$
$$\frac{\hbar^2 k^2}{m} = \frac{\mathrm{d}^2 \epsilon}{\mathrm{d}k^2} k^2$$
$$m = \hbar^2 \left(\frac{\mathrm{d}^2 \epsilon}{\mathrm{d}k^2}\right)^{-1}$$

The group velocity of a wavefunction is given as  $v_g = \frac{\partial \omega}{\partial k}$ . Using the relation  $\omega = \hbar \epsilon$  gives the group velocity on terms of the energy.  $v_g = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial k}$ . Acceleration is the time derivative of the velocity.

$$a = \frac{1}{\hbar} \underbrace{\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \epsilon}{\partial k}}_{\text{core-rule}}$$
$$a = \frac{1}{\hbar} \frac{\partial^2 \epsilon}{\partial k^2} \frac{\partial \epsilon}{\partial t}$$

Further one can use a result found in the quantum physics lectures.  $\frac{dk}{dt} = \frac{F}{\hbar}$ . From classical physics one also has that F = ma. This gives the final result:

$$F = m^* a = \hbar^2 \left(\frac{\mathrm{d}^2 \epsilon}{\mathrm{d}k^2}\right)^{-1} a$$

a

The effective mass takes into account the wavefunction in which the electron is defined. This wavefunction differs in every case, seen in the illustration of the dispersion relation plottet above. This results in a observed effective mass different from that of the electron at rest.

 $\mathbf{b}$ 

The effective mass is dependent on  $\left(\frac{d^2\epsilon}{dk^2}\right)^{-1}$ . When the second derivative is negative this means that the effective mass is negative. This simply means that the electrons in this region travels in the opposite direction of the electrons with positive effective mass.

This is a concept that physicists and others have a problem with. To circumvent this problem one introduces the concept of holes. Holes has positive mass and positive charge, which is easier to work with. Intuitively this also makes it easier to imagine a traveling wave-packet.

 $\mathbf{c}$ 

 $E(k) = Ak^2$ . Taking the double derivative of this gives:

$$m^* = \hbar^2 \left(\frac{d^2 \epsilon}{dk^2}\right)^{-1} = \left(\frac{d^2}{dk^2} A k^2\right)^{-1}$$
$$m^* = 2\hbar^2 A$$
$$= 1.11212168 * 10^{-32}$$