



WS16/17 Condensed Matter Physics I

Exercise 3. Lattice transport + Electrons I.

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Notice: In solving the proposed exercises clearly motivate the passages to reach the result. The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results. When you are asked to “evaluate” something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e. $\omega_c = 1.76 H$ (Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.

2.1 Lattice thermal conductivity

In intrinsic silicon, the thermal conductivity is mainly due to the lattice contribution, and the acoustic phonons in particular. In figure 1, the measured thermal conductivity of a Silicon sample is shown, along with the specific heat.

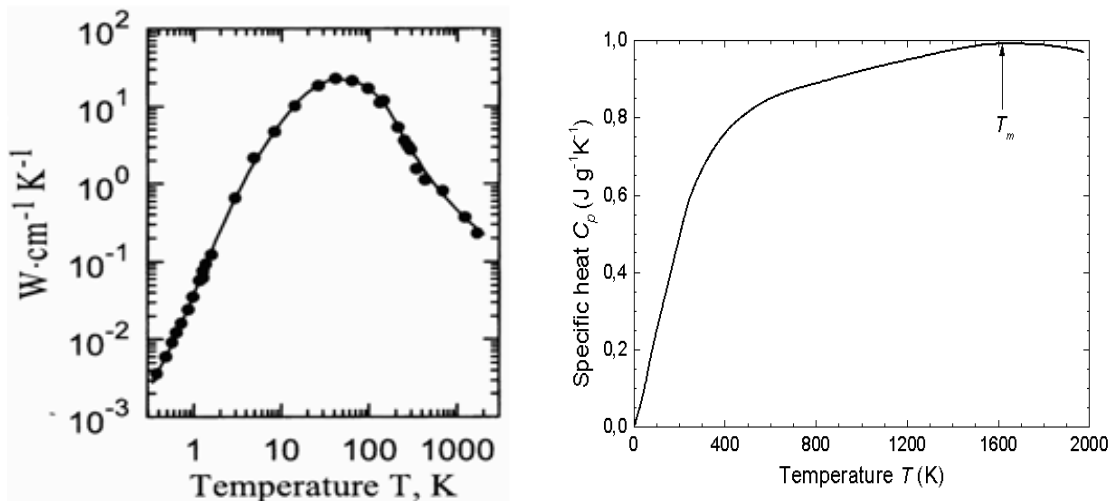


Figure 1: Thermal conductivity and specific heat of of Silicon.

The data show four different behaviors: i) a low temperature region below 5 K where k increases rapidly with temperature; ii) a plateau region centered around between 10 K and

40 K; iii) a crossover region between 100 K and 400 K where the conductivity starts decreasing; and iv) a high temperature region above 400 K.

1. From the data it is clear that the low temperature conductivity in region i) follows a power law behavior. Estimate the value of the exponent of this power law and comment the result in the light of the model for the thermal conductivity

$$k = \frac{1}{3} C v l$$

shown during the lectures. (Here C is the specific heat, v is the sound velocity and l is the mean free path).

[The bi-logarithmic plot clearly shows that the thermal conductivity follows a T^3 behavior at low temperature. This means that its behavior is dominated by the specific heat, and the mean free path is constant in this temperature range.]

2. By using the low temperature thermal conductivity data, give an estimate of the low temperature mean free path of phonons in silicon. (assume the low-T mean free path is temperature-independent and obtain the specific heat and phonon velocity data for Silicon from literature or other online references). Comment the result.

[From literature we get that the (angle averaged) velocity of longitudinal sound waves in silicon is $8.97 \times 10^3 \text{ m s}^{-1}$. From the plot we get that $k(T = 10 \text{ K}) = 2 \times 10^{-2} \text{ W cm K}^{-1}$ and from literature we get $C_p(T = 10 \text{ K}) = 3 \times 10^{-4} \text{ J g}^{-1} \text{ K}^{-1}$ and the density is $\rho = 2.33 \text{ g cm}^{-3}$ therefore:

$$l(T = 10 \text{ K}) = 3 \frac{k(T=10 \text{ K})}{\rho C_p(T=10 \text{ K}) v} = 1 \mu\text{m}.]$$

3. The conductivity shows a plateau around 40 K, i.e. in a region where the specific heat is still growing rapidly with temperature. Give a qualitative reason of such a different behavior.

[This means the mean free path starts to be suppressed by inelastic scattering mechanisms.]

4. The decrease in the thermal conductivity in the region iv) shows also a power law behavior. Give an rough estimate of the exponent of the power law. What is the main scattering mechanism responsible for this decrease? Comment in the light of the known properties of silicon (i.e. Debye temperature)

[The power law is between 1 and 2. This means umklapp scattering is the main high temperature limit to mean free path. This is consistent since T is above silicon Debye temperature of 640 K.]

2.2 Free electrons in Sodium

(10 pts)

Sodium (Na) in normal conditions of temperature and pressure is a metal with BCC structure, with a density of 0.97 g cm^{-3} , mass number of about 23 and Fermi energy E_F of about 3 eV.

1. Calculate the Fermi temperature T_F , Fermi velocity and average kinetic energy of the electrons at 0 K.

[Since the Fermi Energy is $E_F = 3 \text{ eV}$ this corresponds to a Fermi temperature of $T_F = E_F/k_B = 3.6 \times 10^4 \text{ K}$; by extracting the rs parameter and the number density (Ashcroft eq. 2,.26) we calculate the Fermi velocity to be (Ashcroft eq. 2,24) $v_F = 1.1 \times 10^8 \text{ cm s}^{-1}$. The average kinetic energy (per electron - Ashcroft eq. 2.31) is simply $E = 3/5E_F = 1.8 \text{ eV}$.]

2. Calculate the average kinetic energy at room temperature. What is the difference with its value at 0 K?

[The average kinetic energy is the energy density divided by the number density. Therefore, from the energy density as a function of temperature (for $T \ll T_F$) (Ashcroft eq. 2.79) we get:

$$E(T) = 3E_F/5 + g(E_F)(k_B T)^2 \pi^2 / 6n$$

By inserting the value of the DOS at Fermi (Eq. 2.65) we finally get:

$$E(T) = 3E_F/5 + (k_B T)^2 \pi^2 / 4 E_F.$$

Since $E_F = 3 \text{ eV}$ and $k_B T = 0.025 \text{ eV}$ at 300 K we get

$$E(T = 300K) = 1.8 + 2 \times 10^{-4} \text{ eV}$$

the relative correction for the average energy is negligible because the Fermi temperature is high.

3. If you would consider the electron gas as a classical gas. What would be the average kinetic energy at 0 K? And at room temperature?

[The average kinetic energy of a classical electron gas is $3k_B T/2$. Therefore at 0 K for a classical gas is of course zero and at 300 K it would be 37.5 meV.]

4. From the given Fermi energy, calculate the density n of free electrons present in the metal.

[As mentioned in point 1, the r_s parameter from the Fermi energy (Ashcroft eq. 2.26) is about 4; therefore the number density obtained is $n_{el}=2.6 \times 10^{22} \text{ cm}^{-3}$.]

5. Calculate the number density of Na atoms and then the average number of free electrons per atom. Is it what you expect? Comment.

[From the mass density given and the mass number we get an atomic number density of approximately $n_{at}= 7.8 \times 10^{22} \text{ cm}^{-3}$, this would mean that there is one third of electron per atom! This is an unphysical result, therefore the density given for sodium MUST be wrong. Is in fact the density of aluminium.]

2.3 Electronic Density of States

(10 pts)

1. Derive the expression of the Density of electronic states for a two dimensional electron gas.

[From the density of states definition in two dimensions (2 is the spin degeneracy)

$$g_2(\epsilon) = \frac{2}{4\pi^2} \int d\mathbf{k} \delta(\epsilon - \hbar^2 k^2/2m) = \\ = \frac{4\pi}{4\pi^2} \int dk k \delta(\epsilon - \hbar^2 k^2/2m) = \frac{m}{\pi\hbar^2} \int du \delta(\epsilon - u) = \frac{m}{\pi\hbar^2}.$$

2. Considering the electron density n as a parameter, study the behavior of the chemical potential as a function of temperature. Discuss high and low T limits.

[From the definition of number density (Ashcroft eq. 2.67):

$$n = \int_0^\infty d\epsilon g(\epsilon) f(T, \epsilon) = g_2 \int_0^\infty d\epsilon \frac{1}{e^{\beta(\epsilon-\mu)} + 1}.$$

Since the DOS $g_2 = \frac{m}{\pi\hbar^2}$ is constant we can solve the integral analytically. By performing the change of variable $x = \beta(\epsilon - \mu)$ and successively $u = e^x$, obtaining

$$n = \frac{g_2}{\beta} \int_{-\beta\mu}^\infty \frac{d\epsilon}{e^x + 1} = \frac{g_2}{\beta} \int_{e^{-\beta\mu}}^\infty \frac{du}{u} \frac{1}{u + 1} = \frac{g_2}{\beta} \log(e^{\beta\mu} + 1).$$

We invert the equation to get an expression for the chemical potential:

$$\mu(T) = k_B T \log(e^{n/g_2 k_B T} - 1)$$

The limit for $T \rightarrow 0$ is $\mu(T) \rightarrow n/g_2$, this is the Fermi energy. Note: the behavior of the chemical potential around zero temperature is non-analytic, i.e. cannot be expanded in a power law series.

In the limit for $T \rightarrow \infty$ the chemical potential diverges as $\mu(T) \approx k_B T \log\left(\frac{n}{g_2 k_B T}\right)$.

This would mean that the chemical potential at a certain point goes to zero for $T_0 = n/g_2 k_B \log 2 = T_F / \log 2$, and subsequently is negative. This would mean that there are not any occupied states anymore! This is, of course, impossible, and indicates that, when the temperature approaches the value of the Fermi energy at $T=0$ the (equilibrium) density is not anymore constant.

3. Derive the expression for the density of electronic states for a four-dimensional electronic gas.

[From the definition:

$$g_4(\epsilon) = \frac{2}{(2\pi)^4} \int d^4 \mathbf{k} \delta(\epsilon - \hbar^2 k^2 / 2m) = \frac{2}{(2\pi)^4} \frac{2\pi^2}{\Gamma(2)} \int dk k^3 \delta(\epsilon - \hbar^2 k^2 / 2m) = \frac{m^2}{2\pi^2 \hbar^4} \epsilon.]$$

Here, we used the D-dimensional solid angle for $D=4$, where in general $\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}$.

2.4 Conductance Quantization in 1D ballistic quantum wires. (20 pts)

A Quantum Point Contact (QPC) is a low narrow channel joining two two-dimensional electron gas reservoirs, each maintained at two different chemical potentials μ_1 and μ_2 (see figure 1) by a voltage difference V .

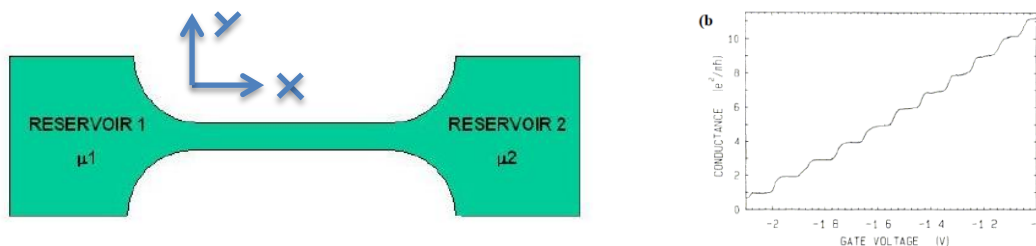


Figure 2: left, schematic of the quantum point contact between the two reservoirs. Left: Measurement of the conductance between a gated QPC grown on a semiconductor heterostructure. Here the gate voltage controls the width of the contact. From van Wees et al. PRL 60, 848 (1988).

Let us calculate the conductance for a very narrow QPC by assuming ballistic transport through the contact (i.e. that the free electron conductance is limited only by the geometry of the contact itself). Let us treat the QPC as a 1D free electron gas otherwise.

1. Due to the chemical potential difference electrons will be moving from one end of the contact to the other. Using the electron velocity, charge and density of states in 1D $\frac{dn}{d\epsilon}$ write an expression for the current density. Verify and justify through physical arguments that $j = ev(\mu_1 - \mu_2) \frac{dn}{d\epsilon}$.

[An electron with charge e and velocity v will contribute with a current ev . The number of states contributing to the conduction is given by the chemical potential imbalance at the end of the two ends of the wire which can be approximated by $(\mu_1 - \mu_2) \frac{dn}{d\epsilon}$. Therefore we get $j = ev(\mu_1 - \mu_2) \frac{dn}{d\epsilon}$.]

2. By substituting the values for the DOS and the potential difference obtain an expression for the conductance $G=j/V$. Verify that your result has indeed the dimension of a conductance. Comment the result. Does the conductivity depends on the material properties? Why this striking result would not necessarily hold in calculating the conductivity for a two dimensional electron gas? Evaluate it and obtain an evaluation of the corresponding resistivity in KOhm.

[$G = e^2 v \frac{dn}{d\epsilon}$. Now In 1D the DOS is $\frac{dn}{d\epsilon} = \frac{1}{\hbar\pi} \sqrt{\frac{m}{2E}} = \frac{1}{\hbar\pi} \frac{1}{v}$, therefore $G = \frac{e^2}{\hbar\pi} = \frac{2e^2}{h}$

i.e. the velocity terms in the current and in the DOS cancel each other, leaving a material independent constant. This correspond to a conductance of $G_0 = 7.75 \times 10^{-5} S$, corresponding to a resistance $\Omega_0 = 12.9 KOhm$.]

The result found in the preceding point applies for a perfectly 1D channel. When the contact is made larger along the y direction more single 1D channel open. Therefore we expect a quantization of the conductivity as a function of the contact width. This fundamental result has been measured in 1988 by van Wees and collaborators [Figure 1 right and PRL 60, 848 (1988)]. Download and read the paper.

3. Model the electrons in the contact as 2D electrons free along the x direction and confined by a hard box potential along the y direction. Obtain the quantization condition for k_y . How many different k_y values are possible for an electron on the Fermi circle for a given width W of the channel?

[The quantization condition for a hard box is of course $k_y = \pm n\pi/W$, $n = (1,2, \dots)$ i.e. the Fermi circle is cut by horizontal lines at constant k_y , which are denser the

wider is the box. The number of channels (i.e. of allowed k_y states) is N_c , i.e. the largest integer smaller than $k_F W / \pi$.]

4. A more rigorous treatment of the conductivity is given in the paper (Equation 2), involving the calculation of the average of the absolute value of k_x over the Fermi circle. Justify and evaluate the integral (Equation 3 of the paper) giving all the fundamental passages, and arrive at the result of Equation 4.

[We have that

$$\langle |k_x| \rangle = \frac{1}{2\pi k_F} \int d^2 k |k_x| \delta(k - k_F) \frac{2\pi}{W} \sum_n \delta\left(k_y - \frac{n\pi}{W}\right)$$

i.e. we have to evaluate the average value of the longitudinal wave vector on the Fermi circle intersected by the $k_y = \text{constant}$ lines. The pre factor is just the length of the Fermi circle, the first dirac delta locates us on the circle itself, while the second deltas save only the points where the Fermi line intersects the allowed $k_y = \text{constant}$ lines. The factor $\frac{2\pi}{W}$ is a jacobian there to make the sum of the distribution dimensionless.pv]