Quantum Solid State Physics

QSSP

Book of Exercises

By

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Useful constants :

Planck's constant $\hbar = 1.0546 \times 10^{-34}$ J s
Boltzmann's constant $k_B = 1.3806 \times 10^{-23}$ J/K or $k_B = 8.6173 \times 10^{-5}$ eV /K
free electron mass $m = 9.1094 \times 10^{-31}$ Kg
electron charge $e = 1.601 \times 10^{-19}$ C
permeability in free space $\mu_0 = 4\pi \times 10^{-7}$ m T/A
Bohr magneton $\mu_B = 9.274009 \times 10^{-24}$A m^2
Avogadro's number $N_A = 6.0221409 \times 10^{23}$

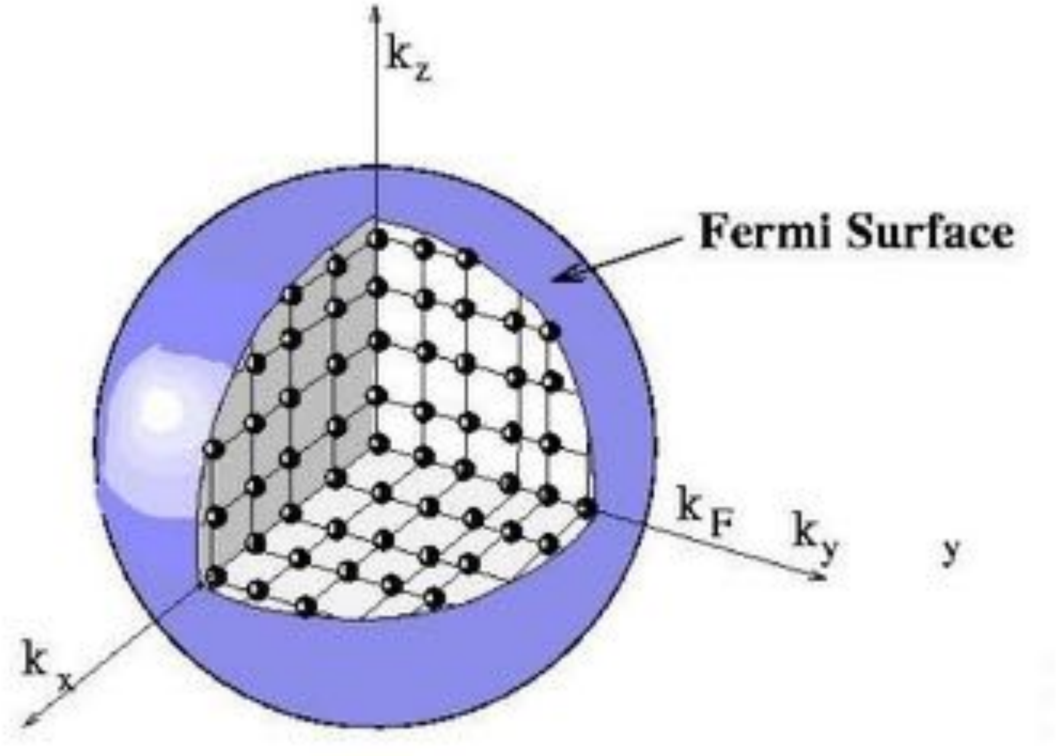
Learn them by heart !

Contents

1

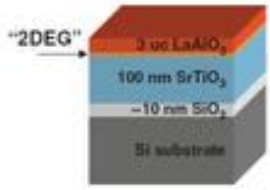
The basic model of metals:

The free electron gas

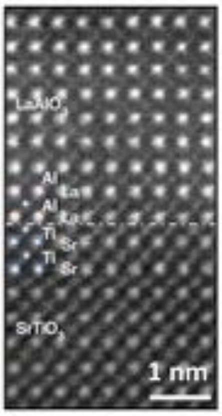


Fermi Surface of the free electron gas in 3D. From http://www.quora.com/What-is-the-relationship-between-boundary-of-the-first-Brillouin-zone-and-the-Fermi-surface-of-a-metal

1.1 The free electron gas in 2D



Let's consider an electron gas in two dimensions (2DEG). This system is for example realized at the interface between two semiconductors or two insulating oxides, like the SrTiO$_3$/LaAlO$_3$ heterostructure displayed in the right-hand-side figure (from http://oxide.engr.wisc.edu/research-alloxide2deg.htm). Other remarkable examples of 2DEG are layered materials (e.g. high temperature copper-oxide superconductors), which are formed by stacking weakly coupled 2D layers.



Here we consider *free* electrons, i.e. we neglect the periodic potential due to the crystal lattice and the electron-electron Coulomb repulsion. The electron energy-momentum relation is then given simply by $\varepsilon = \hbar^2 k^2/2m$.

1.1.1 Fermi energy and density of states

1. Electrons are fermions obeying the Fermi-Dirac statistics. Write down the Fermi-Dirac distribution function $f_{FD}(\epsilon, T, \mu)$ and sketch it schematically for $T = 0$ and $T > 0$. For $T = 0$ draw in the momentum space (k_x, k_y) the region occupied by the electrons, the *Fermi sphere* (i.e. a Fermi disk in 2D). Identify the *Fermi surface* (i.e. a Fermi line in 2D) and the Fermi energy ϵ_F.

2. The electrons live on a 2D square of dimension $L_x \times L_y$. Assuming periodic boundary conditions, also known as Born Von Karman conditions (BVK), write down the quantization conditions on the wave-vector $\vec{k}$.

3. In the limit $L_x >> a_x$ $L_y >> a_y$, where a_x and a_y are typical interatomic distances (this is usually called the *bulk limit*), the wave-vector $\vec{k}$ can be considered as a continuous variable. Infer in this case the the density of states $g(\vec{k})$ in the $\vec{k}$ space.

4. Show that in 2D in the energy space, $g(\varepsilon)$ is a constant g_0 depending only on $\hbar$ and on the free-electron mass m.

5. Express the total number of electrons N_e as an integral formula, involving $g(\varepsilon)$ and the Fermi distribution function $f_{FD}(\epsilon, T, \mu)$. Determine then the relation between the Fermi energy ϵ_F [which is the chemical potential at zero temperature $\epsilon_F = \mu(T = 0)$] and g_0 at $T = 0$. Find also the relation between the corresponding Fermi vector k_F, N_e, $\hbar$ and m.

6. As mentioned above, the high-temperature copper-oxide superconductors can be described as layered materials. Each 2D layer is a square lattice of copper atoms (with an oxygen atom placed between the coppers on each side of the squares, see figure 4.4). The side of each square is $a = 0.384$ nm and there are 0.2 electron per square. Calculate the surface density of electrons in each layer. By considering then just one layer, estimate ϵ_F, k_F and the Fermi temperature T_F ($\epsilon_F = k_B T_F$). Can we consider the electron gas at room temperature as a gas of classical particles?

7. Use again the integral formula relating N_e, $g(\varepsilon)$ and $f_{FD}(\epsilon, T, \mu)$, but this time for $T \neq 0$. For this 2D system, show that the chemical potential $\mu(T)$ is very weakly dependent on

temperature in the limit $\epsilon_F \gg k_B T$. This is true even in three dimensions (even if the correction is larger in 3D than in 2D, it remains small enough). Explain why for any practical purpose we can consider that $\mu(T) \simeq \epsilon_F \; \forall T$.

1.1.2 The specific heat

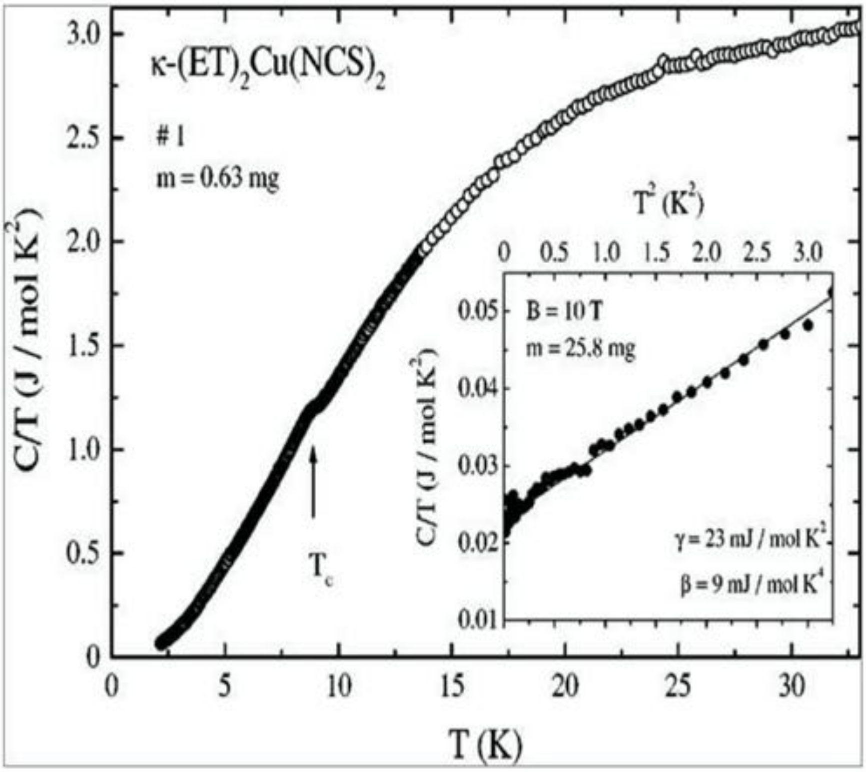


Figure 1.1: $T-$dependence of the specific heat over temperature C/T for the layered superconductor $\kappa(ET)_2Cu(NCS)_2$ ($T_c = 10K$). In the inset, C/T is displayed as a function of T^2 upon the application of 10 Tesla magnetic field which destroys superconductivity. Reference: J. Müller *et al.*, Physical Review B, vol. 65, p.140509 (2002)

The specific heat at constant volume is defined by

$$C_v = \left.\frac{\partial \varepsilon_e}{\partial T}\right|_V ,$$

where ε_e is the total energy and V the total volume of the crystal.

1. Write down an integral formula relating $\varepsilon_e(\mu, T)$, $g(\varepsilon)$ and $f_{FD}(\epsilon, T, \mu)$.

2. The temperature dependence of $\varepsilon_e(\mu, T)$ derives from the Fermi-Dirac distribution function $f_{FD}(\epsilon, T, \mu)$. This latter is a discontinuous function at $T = 0$, therefore its integration at low temperatures requires some attention. We shall use a development introduced by Sommerfeld (1927):

$$\int_0^{+\infty} d\epsilon h(\epsilon) f_{FD}(\epsilon, T, \mu) = H(\mu) + \frac{\pi^2}{6}(k_B T)^2 h'(\mu),$$

where H is the primitive of the h function such that $H(0) = 0$ and h' is the derivative of h. By using this expression show that at low temperatures

$$C_{el} = \frac{\pi^2}{3} k_B^2 g(\epsilon_F) T = \frac{\pi^2}{3} k_B N_e \frac{T}{T_F} = \gamma T,$$

Remember that the $T-$dependence of the $\mu(T)$ is in practice negligible.

3. There is also a contribution to the specific heat due to the lattice vibrations (phonons). At low temperatures, within the Debye model, this contribution is proportional to T^3 whenever $T \ll T_{\text{Debye}}$: $C_{ph} = \beta T^3$. Deduce the form of C/T as a function of T^2 adding the electronic and phononic contributions and explain how we could determine the coefficients γ and β. Let's assume that the lattice parameter a and electron-density given in question 1.1.1.6 are applicable for the material whose specific heat is displayed in figure 1.1. One mole of this material contains 6×10^{23} electrons. Show that the value of γ extracted from the figure has the right order of magnitude as compared to the predictions of the free electron gas. Which information may the actual γ give us on the physical properties of the electrons in the material, which are not predicted by the free electron gas model?

1.2 The Rashba effect:

The spontaneous spin-splitting of the energy in a 2D electron gas

The Rashba effect (first proposed in 1959[1]), is the basis of the spin-effect transistor and of spintronics, i.e. the spin-based electronics. This effect, historically known in compounds with large spin-orbit coupling, has come back on the scene in recent years thanks to advances in the making and control of surface and interfaces, where a 2D electron gas can be confined. The electronic potential asymmetry in the direction perpendicular to the surface/interface can in fact induce a relevant spin-Rashba coupling.

1.2.1 Confinement effect on the spin-orbit coupling of a 2D electron gas

As spin plays a key role, it is first of all convenient to write down explicitly the spin part of the free electron wavefunction by using a spinor (a two-component vector) notation:

$$\psi_{\mathbf{k}}(\mathbf{r}) = (\tilde{A} e^{i\mathbf{k}\cdot\mathbf{r}} + \tilde{B} e^{-i\mathbf{k}\cdot\mathbf{r}}) \begin{pmatrix} \beta_\uparrow \\ \beta_\downarrow \end{pmatrix},$$

where $\beta_\uparrow$ and $\beta_\downarrow$ are respectively the spin up and down components. The scalar in front of the spinor is the usual free electron wavefunction, which here represents only the orbital part.
We shall focus on a 2D electron gas, which is for example realized at the surface of a solid. Differently from the case of the bulk solid described as an infinite crystal, in order to describe a surface, one should impose surface boundary conditions to the electron Schrödinger equation. This produces new electronic surface states. For sake of convenience, here we shall not calculate

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[1] E. I. Rashba and V. I. Sheka, Fiz. Tverd. Tela - Collected Papers (Leningrad), v.II, 162-176 (1959) (in Russian), English translation: Supplemental Material to the paper by G. Bihlmayer, O. Rader, and R. Winkler, Focus on the Rashba effect, New J. Phys. 17, 050202 (2015), http://iopscience.iop.org/1367-2630/17/5/050202/media/njp050202_suppdata.pdf.

explicitly these surface states. Rather, we shall assume that the surface states are well described by a free electron gas, (with electrons having mass m) confined within a layer of width d from the surface by an infinite potential along the z direction (perpendicular to the surface):

$$\begin{aligned} V(z) &= 0 \text{ for } 0 < z < d \\ V(z) &= \infty \text{ everywhere else} \end{aligned}$$

1. Show that the eigenstates of an electron subjected to $V(z)$ can be written as:

   $$\psi_{\mathbf{k}_\parallel, n}(\mathbf{r}) = A \sin(\frac{n\pi z}{d}) e^{i\mathbf{k}_\parallel \cdot \mathbf{r}_\parallel} \begin{pmatrix} \beta_\uparrow \\ \beta_\downarrow \end{pmatrix}, \qquad (1.1)$$

   where $\mathbf{r}_\parallel = (x, y)$, $\mathbf{k}_\parallel = (k_x, k_y)$, $n = 1, 2, 3, \cdots$, and A is a normalization constant (which we won't calculate.)

2. Calculate the associated eigenvalues, which we shall call $E_n(\mathbf{k}_\parallel)$. We call *sub-bands* the electronic bands labeled by the index n.

3. Let's call n_{2D} the electronic surface density. Calculate the limiting density $n_{2D}^\star$ for which only the sub-band of lowest energy is filled. In the following we shall always consider $n_{2D} < n_{2D}^\star$. In this case, the electron system confined by the potential can be effectively assimilated to a real 2D electron gas (2DEG).

4. *Naive derivation of the Rashba Hamiltonian*
   We shall now further simplify the modeling of the 2DEG, by considering a simpler confining potential. This will allow us to simplify the calculation without loosing the salient physical aspects of the problem. The formation of 2DEG at the solid surface can in fact be described by the presence of an effective electric field along z, which mimics the confining potential. Under this point of view, the Rashba effect derives by the inversion symmetry breaking along the z direction produced by an effective electric field. Let's then consider then a constant electric field z, $\mathbf{E} = E_0\hat{\mathbf{z}}$, producing the linear potential:

   $$V_E(z) = -E_0 z \qquad (1.2)$$

   In the reference frame of an electron moving with velocity $\mathbf{v}$ in the 2D plane, the constant electric field is perceived as an effective magnetic field $\mathbf{B} = -(\mathbf{v} \wedge \mathbf{E})/c^2$, where c is the speed of light. This magnetic field then couples with the spin magnetic moment of the electron itself $\boldsymbol{\mu_s} = -g\mu_B\boldsymbol{\sigma}/2$, where g is the Landé factor of the electron ($g = 2$), μ_B is the Bohr magneton and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector whose components are the *Pauli matrices*[2], acting on the spinor part of the electron wavefunction. Show that this spin-$\mathbf{B}$ (*spin-Rashba*) coupling gives a new term in the electron Hamiltonian:

   $$H_R = \alpha(\boldsymbol{\sigma} \wedge \mathbf{k}) \cdot \hat{\mathbf{z}}, \qquad (1.3)$$

   where $\alpha = g\hbar\mu_B E_0/(2mc^2)$ is called *Rashba coupling constant.* As the electric field points in the z direction, the Rashba Hamiltonian can be re-written as:

   $$H_R = \alpha(k_y\sigma_x - k_x\sigma_y). \qquad (1.4)$$

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[2] $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

5. In the following we shall assume $\alpha > 0$. Then the full Hamiltonian of an electron in the 2DEG with wave-vector $\mathbf{k}_{\parallel}$ can be written as:

$$H_R = \frac{\hbar^2 {\mathbf{k}_{\parallel}}^2}{2m} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \alpha(k_y \sigma_x - k_x \sigma_y). \tag{1.5}$$

   The Rashba term lifts the spin degeneracy in the sub-bands of the 2DEG, producing two bands $\epsilon_{\pm}(\mathbf{k})$. Diagonalize the Hamiltonian 1.5, calculate the dispersions $\epsilon_{\pm}(\mathbf{k})$ and sketch them along a given direction in the $\mathbf{k}_{\parallel}$ plane.

6. Determine as a function of α, m and $\hbar$ the wavevector $\mathbf{k}_{\parallel_m}$, where a ring of minima of $\epsilon_{-}(\mathbf{k})$ is obtained in the $\mathbf{k}_{\parallel}$ plane. Determine then as a function of $\mathbf{k}_{\parallel_m}$ the critical electron density n_{2D}^c ("the quantum density") for which the lowest energy branches of $\epsilon_{\pm}(\mathbf{k})$ are completely filled. For $n_{2D} < n_{2D}^c$ electrons occupy only the lower branches, while for $n_{2D} > n_{2D}^c$ electrons occupy both lower and upper band branches. Sketch the Fermi surfaces (lines in 2D in the $\mathbf{k}$ plane) for the two cases $n_{2D} < n_{2D}^c$ and $n_{2D} > n_{2D}^c$, shading the electron occupied regions.

7. From the form of the Rashba coupling in the Hamiltonian 1.5, it is clear that the spin quantum number is not conserved. The $\epsilon_{\pm}(\mathbf{k})$ have therefore both the spin up and the spin down character. By imagining to start from the spin degenerate bands $\alpha = 0$, activate the Rashba coupling $\alpha \neq 0$. Can you guess the spin character on different $\epsilon_{\pm}(\mathbf{k})$ branches? Can you mark the spin orientation on the Fermi surface? For this latter case it is better to think to the Rashba interaction in terms of the coupling between $\mathbf{B}$ and $\mu_{\mathbf{s}}$.

8. *Numerical application*:
   The figure 1.2 in the bottom shows the Rashba splitting measured in the band dispersion of Au(111) by Angle Resolved Photo-Emission Spectroscopy. Let's take from this $k_{\parallel_m} \sim 0.012$. Estimate the quantum density and a value of the Rashba coupling α (in eV·m). Show that you cannot account for the quantitative value 110 meV of the splitting between the lower and upper bands obtained at the k_F^+ of the upper band. A rough estimation is sufficient. You may consider the electron mass of Au(111) equal to the free electron mass $m\,c^2 = 0.511 \times 10^6$ eV and $\hbar\,c = 0.197 \times 10^{-6}$ eV·m. Have you any idea why our modeling does not work quantitatively in this case[3]?

1.2.2 Hand-waving approach to the Rahba coupling: Symmetry effects on the electronic energies in a solid

Let's consider electrons with wavevector $\mathbf{k}$ and spin up ($\uparrow$) or down ($\downarrow$) living in a three dimensional solid. We shall consider the effects of two fundamental symmetries on the electron energies $E(|\mathbf{k}, \uparrow\rangle)$ and $E(|\mathbf{k}, \downarrow\rangle)$. In the following questions you are asked to give qualitative answers without a demonstration.

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[3] Hint: You may read the following research articles about this open problem and see if you have an understanding of the quantitative mismatch of the band slitting found above:
G. Bihlmayer et al., Surface Science 600, 3888 (2006).
M. Nagano et al., J. Phys.: Condens. Matter 21, 064239 (2009).

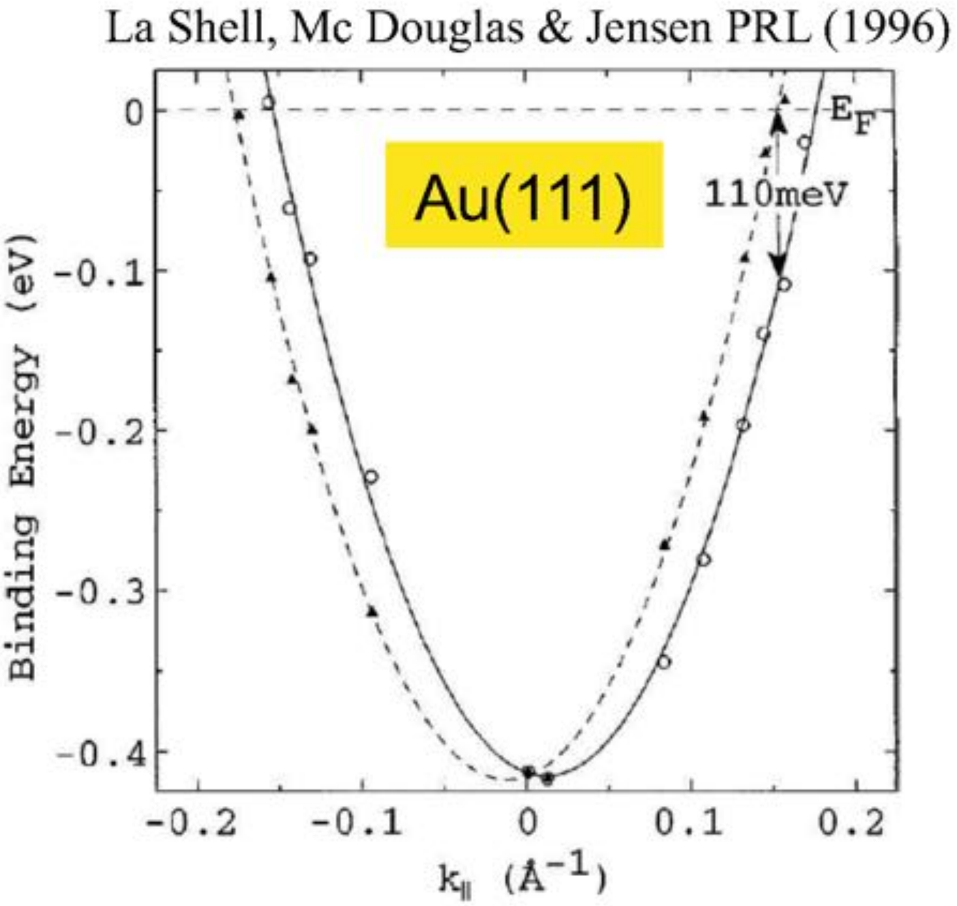

Figure 1.2: Band splitting in Au(111) due to Rahsba spin-orbit coupling

1. When the time-reversal symmetry (TRS) is respected, the system Hamiltonian is invariant under all transformation of physical quantities which depend on the time-reversal, like for example the momentum or the velocity of the electrons.
   (a) How does the electron state $|\mathbf{k}, \uparrow\rangle$ change under a time-reversal transformation? (*Hint:* by analogy, consider the spin as the magnetic moment created by a small current loop).
   (b) Let's consider the electrons in the solid as a free electron gas. If TRS is respected, how does the energy of the state $|\mathbf{k}, \uparrow\rangle$ changes under a time-reversal transformation? Write this down explicitly.
2. In the majority of materials, the crystal lattice obeys to the *inversion symmetry* (IS). In this case the system Hamiltonian is invariant under the coordinate transformation $\mathbf{r} \to -\mathbf{r}$.
   (a) Write down how the state $|\mathbf{k}, \uparrow\rangle$ changes under the $\mathbf{r}$ inversion.
   (b) In the case of a free electron gas, if IS is respected, how does the energy of the state $|\mathbf{k}, \uparrow\rangle$ changes under a time-reversal transformation? Write this down explicitly.

3. Show now that in a system where TRS and IS are respected the electronic states must be spin degenerate.

4. In order to lift the spin degeneracy then, at least one between the TRS and IS should be broken. For convenience sake, let's consider again the energy-momentum (dispersion) relation of the free electron gas (for which all $\mathbf{k}$ directions are equivalent).

   (a) Choose for example the k_z direction and sketch the dispersion relations $E(|\mathbf{k},\uparrow\rangle)$ and $E(|\mathbf{k},\downarrow\rangle)$ in the cases (i) the TRS and IS are respected, (ii) only the TRS is broken and (iii) only the IS is broken. Mark the spin character on the bands that you draw.

   (b) For the three cases i,ii,iii) considered above, draw the Fermi-energy cuts in the $k_z - k_y$ plane. In the case when only the IS is broken, could you say what is the spin orientation on these Fermi lines ?

   (c) Give a practical example on how we could break the TRS.

   (d) The IS is in fact broken in materials known to be non-centro-symmetric. In this case a spin splitting of the bands is observed, and this phenomenon is known as the *Dresselhaus effect*. Show that for any real material, even for a material which is centro-symmetric, the IS is actually broken. In which part of the material could this take place? This is the second well-known case of IS breaking, known as *Rashba effect*.

1.3 Pauli Paramagnetism in the 3D electron gas

We consider a free electron gas of density n in three dimensions (3D). We want to study the magnetic properties at zero temperature ($T = 0$ K) originating from the spins of the electrons. We shall denote $n_\uparrow$ and $n_\downarrow$ the density of electrons respectively with spin $\uparrow$ and $\downarrow$ along the quantization axis Oz. We shall call $g(\mathbf{k}) = g_\uparrow(\mathbf{k}, \mathbf{B} = 0) + g_\downarrow(\mathbf{k}, \mathbf{B} = 0)$ and $g(\epsilon) = g_\uparrow(\epsilon, \mathbf{B} = 0) + g_\downarrow(\epsilon, \mathbf{B} = 0)$ the density of states (per unit volume), in the momentum and energy spaces respectively, of the unpolarized gas (for $\mathbf{B} = 0$ T, we have $n_\uparrow = n_\downarrow = \frac{n}{2}$). We assume BVK conditions.

1. Under an external magnetic field $\mathbf{B}$ directed along the Oz direction, an electron of spin $S = \pm 1/2$ gains an extra energy $-m_z B$, where $m_z = -g\mu_B S_z$ is the projection along Oz of the electron magnetic moment associated with the spin, $g = 2$ is the Landé factor and μ_B is the Bohr magneton. Write down the new electron energies $\epsilon_{k,\uparrow}$ and $\epsilon_{k,\downarrow}$ of the electrons with spin $\uparrow$ and $\downarrow$ respectively upon application of $\mathbf{B}$. Calculate the corresponding density of states (per unit volume) $g_\uparrow$ et $g_\downarrow$, first in the momentum space and then in the energy space. We consider here only the effect of $\mathbf{B}$ on the electron spin and neglect its effect on the momentum (orbital effects).

2. Write down the integral expression of $n_\uparrow$ and $n_\downarrow$ as a function of $g_\uparrow(\epsilon, \mathbf{B})$ and $g_\downarrow(\epsilon, \mathbf{B})$ respectively. Remember that $T = 0$ K. Think well how to fix the integration boundaries for the two spin species (because of the applied field we expect one of the two spin species to be favoured with respect to the other). Do not try to solve explicitely the integrals. Rather, infer an integral expression of $\Delta n = n_\downarrow - n_\uparrow$ as a function of $g(\epsilon)$, the total density of states (per unit volume) of the unpolarized gas (realized when $B = 0$ T).

3. Compare the magnetic energy acquired by an electron under a magnetic field $-m_z B$ with the typical magnitude of the Fermi energy. Infer an approximate expression of Δn by using a first order Taylor expansion in the magnetic energy (again do not try to solve explicitely the integral). From this latter, calculate then the magnetization M_z and finally the magnetic susceptibility $\chi = \mu_0 M_z / B$ as a function of μ_B and the density of states at the Fermi level $g(\epsilon_F) = 3n/2\epsilon_F$. This magnetic susceptibility is known as *Pauli susceptibility.* A more involved calculation can show that the Pauli susceptibility weakly depends on temperature. The expression obtained here is however correct in the $T = 0$ limit.

4. In the case of sodium, the electron density is $n = 2.68 \times 10^{28}$ m^{-3} and the Fermi energy $\epsilon_F = 3.24$ eV. Calculate for this case the $T = 0$ value of the magnetic susceptibility and compare it with the value that can be extracted from Fig. 1.3, where we display the ratio $\frac{1}{4\pi}\frac{\chi}{\rho}$ for various metals. Here ρ is the material density ($\rho = 0.971$ g.cm^{-3} for sodium).

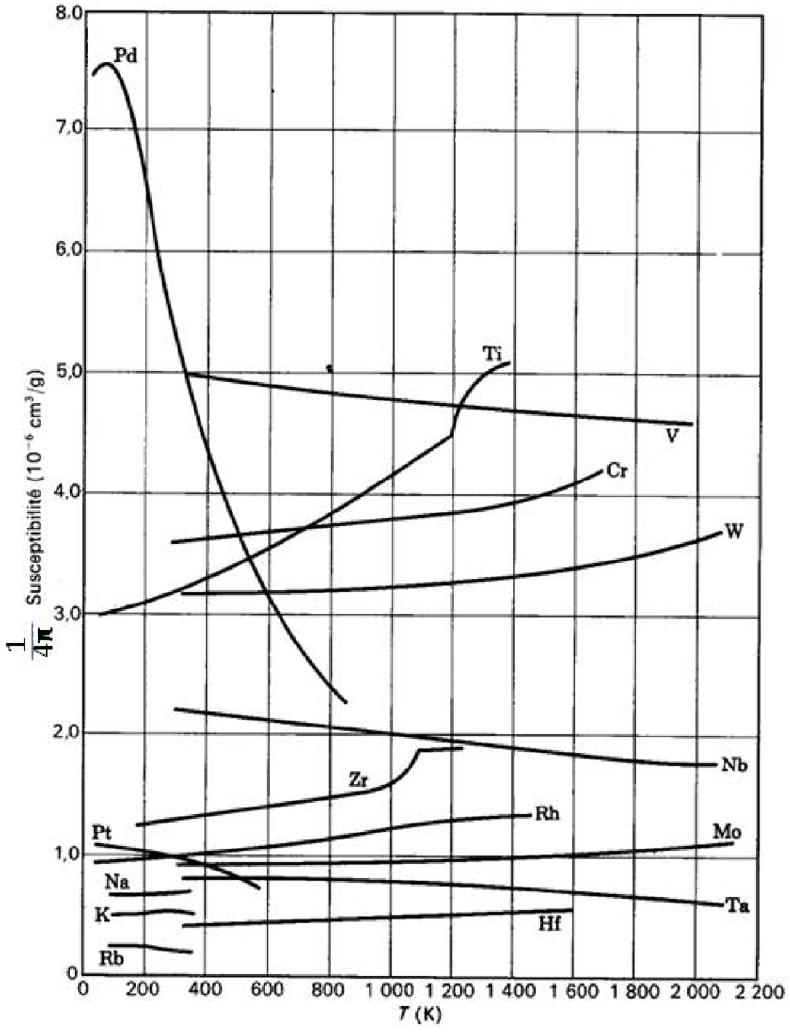

Figure 1.3: Magnetic susceptibility of various metals as a function of temperature

1.4 The free electron gas from 3D to 2D

1.4.1 Electron gas in 3D

We consider a free electron gas in 3D of density n_{3D}, occupying a volume $\Omega = L^2 \times l$. We impose periodic boundary conditions (B.V.K.) in the three spatial directions x, y, z.

1. Write down the expression for the wavefunction $\psi_{\vec{k}}(x, y, z)$ and give the quantization rules applied on the momentum vector $\vec{k}$, specifying the values allowed (positive, negative or zero) for each component of $\vec{k}$.
2. Draw a scheme in the momentum space of the occupied states at $T = 0$. Mark on the scheme the Fermi vector $\vec{k}_F$.
3. Write down the density of states $g_{3D}(\vec{k})$ in momentum space and show that in the energy space $g_{3D}(\epsilon) = A\sqrt{\epsilon}$. Calculate the exact expression of A.
4. By writing the integral expression relating n_{3D} and $g_{3D}(\epsilon)$ at $T = 0$, find the relation between n_{3D} and the Fermi energy ϵ_F.
5. Calculate ϵ_F (in eV) and $\vec{k}_F$ for the case of copper, $n_{3D} = 8 \times 10^{28}\ m^{-3}$.

1.4.2 Electron surface energy of a nearly 2D plate

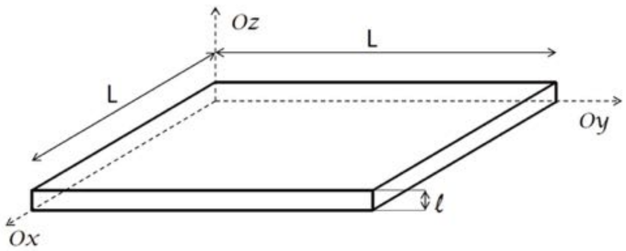

Figure 1.4: Plate scheme

1. Let's first consider a free electron gas of density n_{2D} uniformly distributed on a 2D surface. Consider the density of states $g_{2D}(\epsilon)$ in the energy space and evaluate the average energy per electron as a function of ϵ_F at $T = 0$.

2. We shall now consider the effects of the surfaces on the electron gas living in a thin plate of thickness l, lying the $x - y$ plane perpendicularly to the Oz axis (see Fig. 1.4). To this purpose we apply periodic boundary conditions only on the x and y directions and close boundaries along the z direction. In this case the electron wave-function must go to zero at the surfaces: $\psi(x, y, 0) = \psi(x, y, l) = 0$. A suitable form of the electron wave-function is:
$$\psi(x, y, z) = Be^{ik_x x}\, e^{ik_y y}\, \sin(k_z z)$$
What are the quantization conditions on k_x, k_y and k_z? Explain why the occupied states in the momentum space at $T = 0$ form now a hemisphere. Which hemisphere should one

consider, the one with a north pole or the one with the south pole? Why the base at $k_z = 0$ is now unoccupied? The electrons that originally lived on the $k_z = 0$ base, where have they gone?

3. Show that the new density of states in the momentum space $g'_{3D}(\vec{k})$ is twice as much the the density of states $g_{3D}(\vec{k})$ of the 3D system with periodic boundary conditions in all the three spatial directions. Explain why the Fermi momentum k_F is in practice unchanged.

4. For electrons living on the $k_z = 0$ base of the hemisphere the average energy per particle is the one of a 2D electron gas with periodic boundary conditions (see the question 1 above). Evaluate the average gain in energy per electron $\Delta\epsilon$ when the $k_z = 0$ base is emptied by the creation of the plate surfaces. This gain of energy is required to go from the 3D electron system to a nearly 2D electron plate system, i.e. it is the energy required to create the surfaces.

5. We can assimilate the density of states of the $k_z = 0$ empty disk to that of a 2D electron gas occupying a L^2 surface. By using then the momentum-space density of states $g_{2D}(\vec{k})$ of the 2D electron gas, evaluate the number of electrons that at $T = 0$ migrate from the base of the hemisphere, when the plate surfaces are formed. These electrons acquire an average extra energy $\Delta\epsilon$.

6. Infer the total gain of energy ΔE, then the surface energy $\Delta E/L^2$, which we shall write as $\epsilon_F \times f(k_F)$, where f is a function of k_F to be determined. Verify the units of your formula. Evaluate this energy for copper in J/m^2 units.

1.4.3 Surface effects on the electron gas

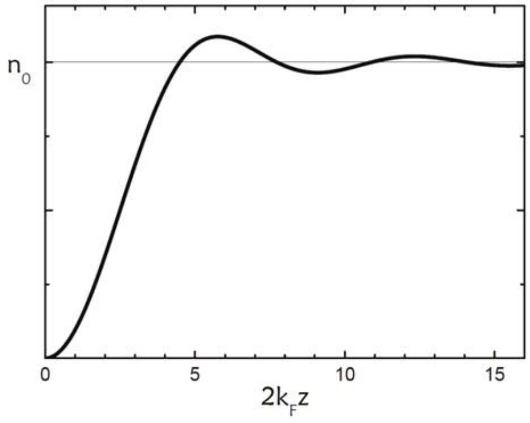

Figure 1.5: $n(z)$ close to the plate surface

Generally, the local density of electrons in a metal can be written as

$$n(x, y, z) = \int_{|\vec{k}|<k_F} |\psi(x, y, z)|^2 \, g(\vec{k}) \, dk_x dk_y k_z$$

1. Show that for periodic boundary conditions in 3D the density n_0 is homogeneous. Give its value as function of k_F.

2. By treating rigorously a nearly 2D plate geometry (see Fig.1.4), we find

$$n(z) = n_0 \left(1 - 3\frac{\sin(2k_F z) - 2k_F z\cos(2k_F z)}{(2k_F z)^3}\right)$$

Find the distance at which $n(z) = n_0$ for the first time starting from $z = 0$ (extract this from Fig.1.5), and compare it to the inter-atomic distance. What conclusion can you draw about the surface effects on the electron gas in a material, like a thin plate?

2

Transport phenomena

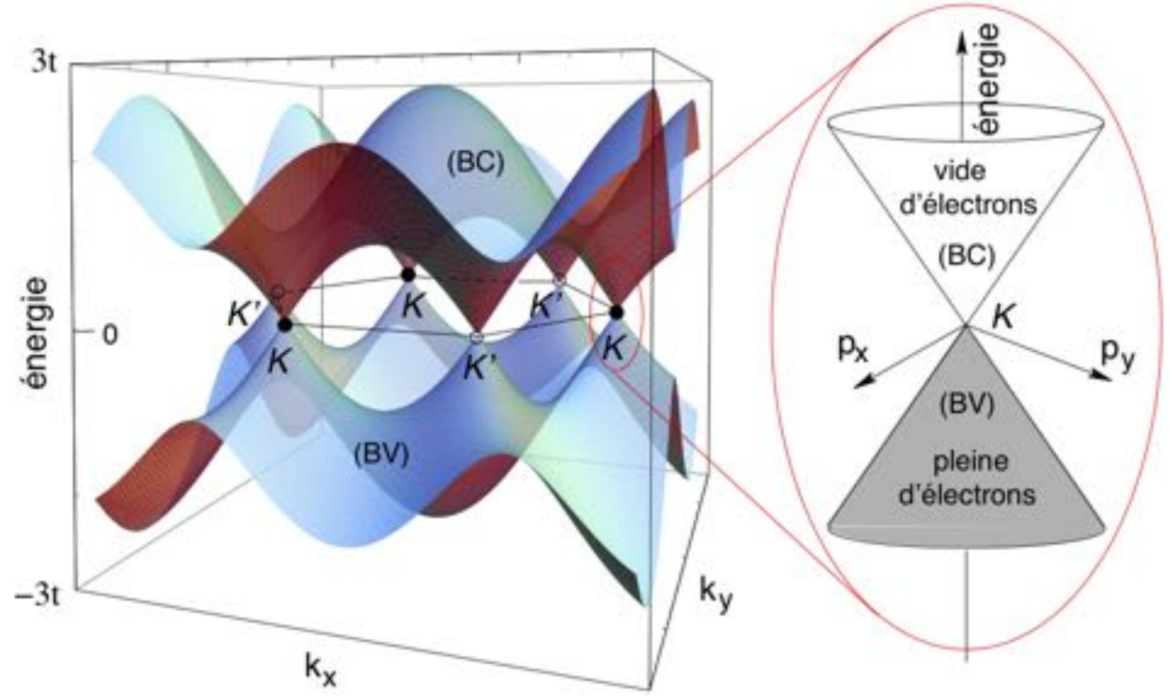

Figure 2.1: Electronic band structure of graphene, from the review article of J. N. Fuchs: https://arxiv.org/abs/1306.0380

2.1 Electrical conductivity of a metal

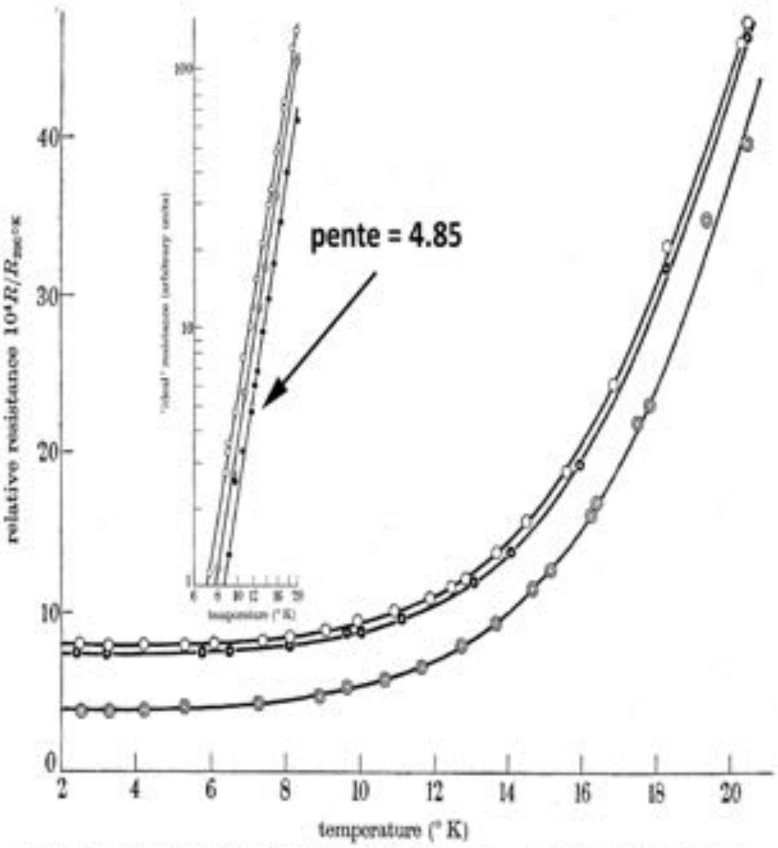

FIGURE 4. Resistance of sodium below 20° K. Specimens: ◐, Na2; ⊚, Na3; ○, Na4.

Figure 2.2: Resistivity of a sodium sample as a function of temperature. From D.K.C. MacDonald et K. Mendelssohn, Proc. Roy. Soc. A, vol. 202, p.523 (1950)

We shall study the temperature dependence of the electrical conductivity in a standard metal. To this purpose, we consider the Boltzmann theory of gases, which is able to well describe the electronic transport in the semiclassical regime. Within this framework the electrical conductivity can be written as:

$$\sigma = e^2\tau \int d\varepsilon\, g(\varepsilon)\, \frac{v^2}{d} \left(-\frac{df^0(\varepsilon)}{d\varepsilon}\right) \tag{2.1}$$

where d is the spatial dimension.

1. Starting from equation (2.1), show that in the low temperature limit $\sigma = e^2\tau\, g(\varepsilon_F)\, \frac{v_F^2}{d}$.
2. In the $d = 2$ case, rewrite $g(\varepsilon)$ as a function of the electron density n_e and the Fermi energy ε_F. Derive the Drude conductivity formula (though we perform a calculation in 2D, this result remains valid in any dimension).
3. The parameter which most depends on temperature is the collision time τ. At very low temperatures τ is nearly temperature independent because the scattering process is

dominated by impurities. At higher temperature the dominant scattering is due to lattice vibrations. Then, according to the number of excited vibrational modes, $\tau \propto T^{-5}$ for $T \ll \theta_D$ and $\tau \propto T^{-1}$ for $T \gg \theta_D$, where θ_D is a characteristic temperature of phonons (for Na θ_D=158 K). According to you, can the Drude formula and the temperature dependence of τ account for the behavior of the resistance of sodium displayed in Fig. 2.2? Explain your reasoning.

2.1.1 Electrical conductivity of graphene

Graphene is a 2D sheet of carbon atoms forming a honeycomb lattice (see Fig. 3.3), displaying a variety of extraordinary properties. For example it is about 207 times stronger than steel, it is nearly transparent (this is usually a property of insulators, can you say why?), but conducts heat and electricity efficiently (differently from insulators). The electronic structure of graphene displays "Dirac cones" (see Fig. 2.1) with the Fermi level located at the vertex of the cones. This structure is halfway between the one of a metal and the one of an insulator (where the Fermi level is located in the middle of a gap), conveying graphene unusual transport properties.
Let's then consider the following parametrization of the electronic band structure of graphene close to the the Fermi level:

$$\begin{aligned} \varepsilon_+(\vec{k}) &= \varepsilon_F + \hbar v_F\, k, \text{si } \varepsilon > \varepsilon_F \\ \varepsilon_-(\vec{k}) &= \varepsilon_F - \hbar v_F\, k, \text{si } \varepsilon < \varepsilon_F \end{aligned} \tag{2.2}$$

where $v_F \approx 10^6\ m.s^{-1}$ is the Fermi velocity and $k = ||\vec{k}||$ is the norm of the wavevector $\vec{k} = (k_x, k_y)$.

- Calculate the density of states $g(\varepsilon)$ and show that it is proportional to $|\varepsilon - \varepsilon_F|$ (we shall call $S = L^2$ the total surface of the system).
- Calculate the temperature dependence of the conductivity within the framework of Boltzmann theory and compare it to the one of a standard metal. We can neglect the temperature dependence of the chemical potential. You may first prove that at finite temperature

  $$-\frac{df^0(\varepsilon)}{d\varepsilon} = \frac{\beta}{4ch^2\left(\frac{\beta(\varepsilon-\varepsilon_F)}{2}\right)}.$$

  and use the following relation:

  $$\int_0^\infty dx\, \frac{x}{ch^2 x} = \ln 2.$$

2.2 Thermal conductivity

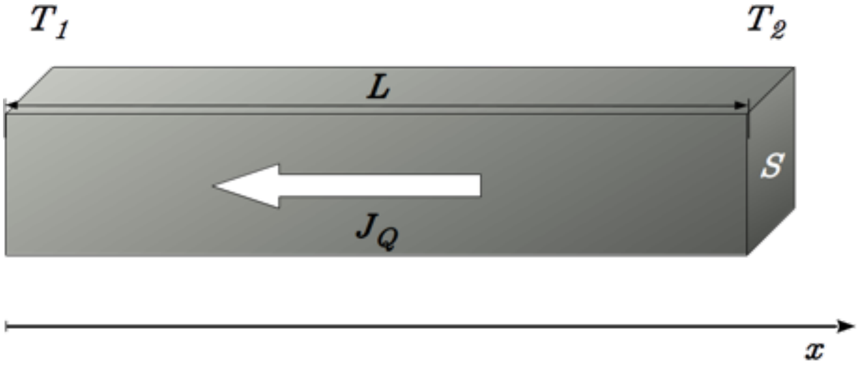

Figure 2.3: Metallic bar subjected to a temperature gradient: $T_2 > T_1$.

Upon the application of a gradient of temperature to a metal, electrons which are free to move set up a heat flow. We shall calculate here the thermal conductivity originating from this electronic contribution to the thermal current using a simplified approach, the Drude model. A more realistic calculation would imply to use Boltzmann transport theory, however this would be much more involving.
Within the Drude model, thermal exchange is ensured by the collisions that electrons experience with the lattice of ions. We shall introduce a time parameter τ, indicating the averaged time between two subsequent collisions. For convenience's sake, we consider a thin metallic bar long L and of section S, such that $S << L^2$ (see Fig. 2.3). Here we suppose that the bar is isolated, so that there is no electrical current circulating. Upon application of a temperature gradient $\vec{\nabla} T$ along the $x-$axis direction ($T_2 > T_1$), a thermal current $\vec{j}_Q$ sets in the in the opposite direction. In the limit of weak temperature gradient (linear response limit) this phenomenon is well described by the Fourier law $\vec{j}_Q = -\kappa \vec{\nabla} T$, where κ is the thermal conductivity.

1. Write down the root mean square velocity v of an electron in 1D as a function of temperature. The Drude approach assumes that electrons are classical particles.

2. Evaluate the change of energy of an electron with velocity v within the time interval $[t, t+\tau]$ between two collisions, as a function of v, τ, the specific heat c and the temperature gradient $\nabla_x T$.

3. Given the total electron density n, evaluate the number of electrons $n_+ (n_-)$ moving from the left(right) hand side to the right(left) hand one, crossing the section S during a time interval τ.

4. Evaluate the heat $Q = S \tau \vec{j}_Q . \vec{x}$ crossing the section S in a time τ. Deduce then the heat-current density $\vec{j}_Q$ and the thermal conductivity κ_{1D} in this 1D case.

5. Let's now consider a 3D system and suppose that the velocity distribution is homogeneous in space. Show that the thermal conductivity in 3D can be written as $\kappa = \frac{1}{3} v^2 \tau c_v = \frac{1}{3} v l_e c_v$ where c_v is the molar specific heat and l_e is the mean free path.

6. Calculate the Wiedemann-Franz ratio between the thermal conductivity κ and the electrical Drude conductivity $\sigma = \frac{ne^2\tau}{m}$

   $$\frac{\kappa}{\sigma} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 T = \mathcal{L}T \tag{2.3}$$

   $\mathcal{L}$ is called the *Lorentz number*.

7. Evaluate $\mathcal{L}$ for copper: at $T = 0$ °C, $\sigma = 6.45\ \times 10^7 \Omega^{-1}\mathrm{m}^{-1}$ and $\kappa = 385$ W m^{-1} K^{-1}. Is this value comparable to the one obtained within the Drude calculation above?

8. Actually it is know that the Drude model is too crude to explain many important properties of the electron gas, which are in reality quantum particles. The Drude approach for instance underestimates the electron velocity of a factor 100. However it also overestimates of a factor 100 the specific heat, so that the order of magnitude of the Wiedemann-Franz ratio calculated within the Drude approach is roughly correct. We will do a more precise estimation now. Using a Boltzmann approach one obtains the same result as the Drude calculation but the electron velocity v is replaced with the Fermi velocity v_F. At the same time (see section 1) the specific heat of an electron gas is $c_v = \frac{\pi^2}{2} n_e k_B \frac{T}{T_F}$ where n_e is the electron density an T_F the Fermi temperature. Show that the Wiedemann-Franz law is now written as:

   $$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T = \mathcal{L}T \tag{2.4}$$

   and compare this improved theoretical calculation with the experimental value of copper calculated in question 7 above.