1 The free electron gas

1.1 The free electron gas in 2D

1.1.1 Fermi energy and density of states

1. The Fermi-Dirac distribution is $f_{FD}(\epsilon, \mu, T) = \dfrac{1}{e^{\frac{\epsilon - \mu}{k_B T}} + 1} = \dfrac{1}{e^{\beta(\epsilon - \mu)} + 1}$

   The Shrödinger equation for free electrons reads : $\dfrac{\hbar \hat{P}^2}{2m} \Psi = \epsilon \Psi$ thus eignenvalue is

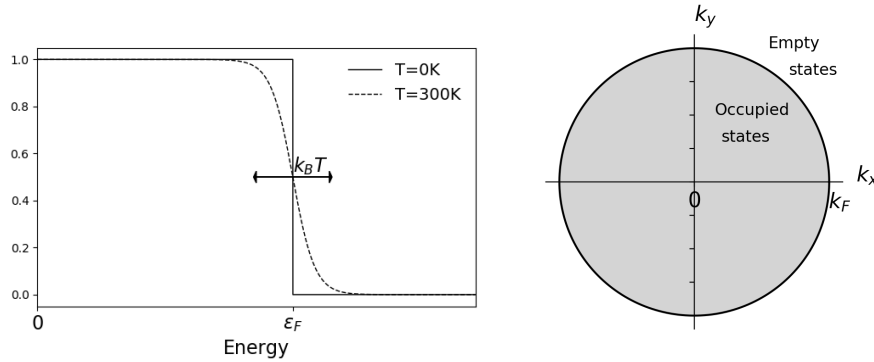$$\epsilon = \frac{\hbar^2 k^2}{2m} \qquad (1)$$

FIGURE 1 –

2. In a 2D square of dimension L_x and L_y along $\vec{u}_x$ et $\vec{u}_y$ respectively, electrons wavevectors take the form $\vec{k} = n_x \dfrac{2\pi}{L_x} \vec{u}_x + n_y \dfrac{2\pi}{L_y} \vec{u}_y$ with n_x and n_y integers. This comes from the fact that both wavefunction and its derivative is null at the borders of the box.
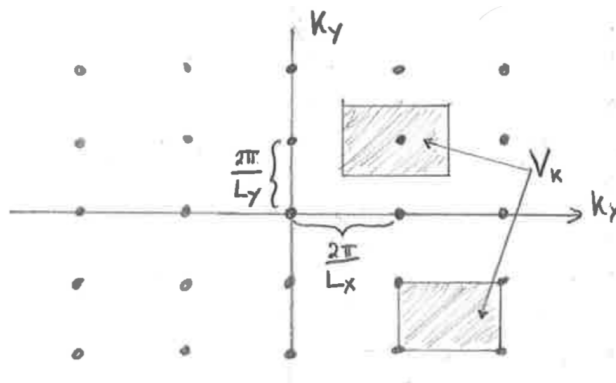

FIGURE 2 –

3. To calculate the density of state in the k space, 2 steps :

- Determine the surface occupied by 1 state in the k-space : $S_k = \dfrac{2\pi}{L_x}\dfrac{2\pi}{L_y} = \dfrac{(2\pi)^2}{S}$ with S the surface of the box in the real space (S=$L_x L_y$).
- Write the number of electron states in this volume : $g_{2D}(k)S_k = 2^{\uparrow\downarrow}$ due to spin degeneracy. Then $g_{2D}(k) = \dfrac{S}{2\pi^2}$

4. To calculate the density of state in energy space, the previous 2 steps determination of $g_{2D}(k)$ is required. We then write :
$$g_{2D}(\epsilon)d\epsilon \quad = g_{2D}(k)d^2k \tag{2}$$

We can write $d^2k = 2\pi k dk$ since the k-space filling is isotropic (sphere) in k space : $\epsilon = \dfrac{\hbar^2 k^2}{2m}$. Using $\dfrac{d\epsilon}{dk} = \dfrac{\hbar^2 k}{m}$ we can deduce :

$$
\begin{aligned}
g_{2D}(\epsilon) \quad &= g_{2D}(k)2\pi k \dfrac{dk}{d\epsilon} \\
&= \dfrac{S}{2\pi^2}2\pi k \dfrac{m}{\hbar^2 k} \\
&= \dfrac{mS}{\pi\hbar^2} \\
&= g_0
\end{aligned}
\tag{3}
$$

5. Total number of electron can be calculated by summing over all energies the product of density of electron state (number of state available at one energy : $g_{2D}(\epsilon)$) with the probability of occupying this state (defined by Fermi-Dirac distribution) :

$$
\begin{aligned}
N_e \quad &= \int_0^\infty g_{2D}(\epsilon)f_{FD}(\epsilon,\mu,T)d\epsilon \\
&\underset{T=0}{=} \int_0^{\epsilon_F} g_{2D}(\epsilon)d\epsilon \\
&\underset{T=0}{=} g_0\epsilon_F
\end{aligned}
\tag{4}
$$

using 1, we can write : $k_F = \sqrt{2\pi\dfrac{N_e}{S}}$

6. $S = a^2$, N_e=0.2, $\hbar$=1.05 10^{-34}, m_e=9.1 10^{-31}, k_B=1.38 10^{-23}J.K^{-1} and 1J=6.2 10^{18}eV

- $n_e = \frac{N_e}{S}$=1.36 10^{18}m^{-2}

- $k_F = \sqrt{2\pi\frac{N_e}{S}}$=2.9 10^9m^{-2}
- $\epsilon_F = \frac{\hbar^2 k_f^2}{2m_e}$=0.3eV
- $T_F = \frac{\epsilon_F}{k_B}$=3780 K
  The energy to add one electron is much higher than the thermal energy (T_F»300K) so this cannot be considered as a classical Boltzman gas.

7. For T$\neq$0 :

$$
\begin{aligned}
N_e &= \int_0^\infty g_{2D}(\epsilon) f_{FD}(\epsilon, \mu, T) d\epsilon \\
&= g_0 \int_0^\infty \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}} + 1} d\epsilon \\
&\underset{x=\beta(\epsilon-\mu)}{=} \frac{g_0}{\beta} \int_{-\beta\mu}^\infty \frac{dx}{e^x + 1} \\
&= \frac{g_0}{\beta} \int_{-\beta\mu}^\infty \frac{e^x dx}{1 + e^{-x}} \\
&= \frac{g_0}{\beta} \left[ln(1 + e^{-x}) \right]_{-\beta\mu}^\infty \\
&= \frac{g_0}{\beta} ln(1 + e^{\beta\mu}) \\
&= \frac{g_0}{\beta} ln(e^{\beta\mu}(e^{-\beta\mu} + 1)) \\
&= \mu g_0 + \frac{g_0}{\beta} ln(1 + e^{-\beta\mu}) \\
&\underset{\epsilon_F \approx \mu >> \beta^{-1}}{=} \mu g_0 + g_0 k_B T e^{-\beta\mu}
\end{aligned}
\tag{5}
$$

The hypothesis that $\epsilon_F \approx \mu$ is reasonnable as it is exactly equal at T=0. Let's see how μ changes as function of temperature :

$$
\begin{aligned}
\mu &= \frac{N_e}{g_0} - k_B T e^{-\frac{\epsilon_F}{k_B T}} \\
&\underset{eq.4}{=} \epsilon_F (1 - \frac{k_B T}{\epsilon_F} e^{-\frac{\epsilon_F}{k_B T}})
\end{aligned}
\tag{6}
$$

Since $\frac{\epsilon_F}{k_B T}$>10, the temperature correction (second term) is less than 0.001%. We then can confirm that the chemical potential μ varies very slowly with the temperature and can be approximated to Fermi energy ϵ_F. This is convenient for all the calculation using the Fermi-Dirac equation.

1.1.2   The specific heat

1. The total energy can be written as the sum over all energies of : i) the number of electrons states at given energy, ii) the energy of these electrons and iii) the probability of occupying this state (defined by Fermi-Dirac distribution) :

$$
\epsilon_e = \int_0^\infty g_{2D}(\epsilon) f_{FD}(\epsilon, \mu, T) \epsilon d\epsilon
\tag{7}
$$

2. Identifying $h(\epsilon) = \epsilon$ then $h'(\epsilon) = \frac{dh(\epsilon)}{d\epsilon} = 1$ and $H(\epsilon) = \int_0^\epsilon h(\epsilon') d\epsilon' = \frac{\epsilon^2}{2}$, we can apply Sommerfeld development to eq. 7 :

$$
\epsilon_e = g_0 \frac{\epsilon_F}{2} + g0 \frac{\pi^2}{6} (k_B T)^2
\tag{8}
$$

Using eq. 8, we can derive the specific heat :

$$
\begin{aligned}
C_v &= \frac{d\epsilon_e}{dT} \\
&= \frac{N_e \pi^2}{3\epsilon_F} k_B^2 T \\
&= \frac{N_e \pi^2}{3} k_B \frac{T}{T_F} \\
&= \gamma T
\end{aligned}
\tag{9}
$$

3. Summing both electronic and phononic contribution to the specific heat we get : $C_v = C_v^{e^-} + C_v^{ph} = \gamma T + \delta T^3$. Plotting $\frac{C_V}{T} = \gamma + \beta T^2$ as function of T^2 sould get a straight line with a slope corresponding to β and the y-intercept corresponding to γ.

$\gamma = \dfrac{N_e \pi^2}{3} k_B \dfrac{1}{T_F}$. With a Fermi temperature around T_F=3800 K (see 1.1.1.6), we get γ_{theo}=7mJ.mol^{-1}.K^{-1}. γ_{exp}=23mJ.mol^{-1}.K^{-1}. This is the good order of magnitude. The factor 3 may be ascribed to the heavier effective mass of electron. The notion of effective mass of electron will be further discussed in the tight binding model.

1.2 The Rashba effect

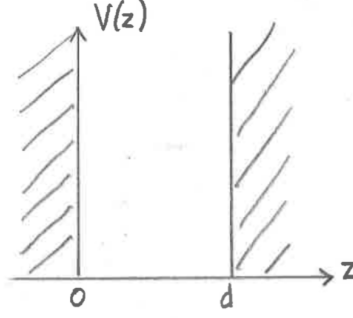### 1.2.1 Confinement effect on the spin-orbit coupling of a 2D electron gas

FIGURE 3 –

1. Hamiltonian is $\mathcal{H} = \dfrac{p^2}{2m}$. The general solution is of the form : $\Psi(\vec{r}, \vec{\sigma}) = [A_1 e^{i\vec{k}.\vec{r}} + A_2 e^{-i\vec{k}.\vec{r}}]$ without considering the spin. With the boundaries conditions and decomposing $\vec{k} = \vec{k}_\parallel + \vec{k}_\perp$:

$$
\begin{aligned}
\Psi(z=0)=0 \quad &\Rightarrow A_1 e^{i\vec{k}_\parallel.\vec{r}_\parallel} + A_2 e^{-i\vec{k}_\parallel.\vec{r}_\parallel} = 0 \\
\Psi(z=d)=0 \quad &\Rightarrow A_1 e^{i\vec{k}_\parallel.\vec{r}_\parallel} e^{k_z d} + A_2 e^{-i\vec{k}_\parallel.\vec{r}_\parallel]} e^{-k_z d} = 0 \\
&\Rightarrow -A_2 e^{-i\vec{k}_\parallel.\vec{r}_\parallel} e^{k_z d} + A_2 e^{-i\vec{k}_\parallel.\vec{r}_\parallel]} e^{-k_z d} = 0 \\
&\Rightarrow -A_2 e^{-i\vec{k}_\parallel.\vec{r}_\parallel} 2i sin(k_z d) = 0 \\
&\Rightarrow k_z d = n\pi, \ n \in \mathbb{Z}
\end{aligned}
\tag{10}
$$

Then

$$
\Psi(z) \quad = A sin(\dfrac{n\pi}{d}) e^{-i\vec{k}_\parallel.\vec{r}_\parallel} \begin{bmatrix} \beta_\uparrow \\ \beta_\downarrow \end{bmatrix}
\tag{11}
$$

2. Solving the Schrödinger equation : $\mathcal{H}\Psi_n = \dfrac{p^2}{2m}\Psi_n$ gives :

$$
\epsilon_n = \dfrac{\hbar^2}{2m}\left[k_\parallel + \left(\dfrac{n\pi}{d}\right)^2 \right]
\tag{12}
$$

3. First we need to calculate the 2D density of state in the k space :
   - Determine the surface occupied by 1 state in the k-space : $S_k = \dfrac{2\pi}{L_x}\dfrac{2\pi}{L_y} = \dfrac{(2\pi)^2}{S}$ with S the surface of the box in the real space (S=$L_x L_y$).
   - Write the number of electron states in this volume : $g_{2D}(k)S_k = 2^{\uparrow\downarrow}$ due to spin degeneracy. Then $g_{2D}(k) = \dfrac{S}{2\pi^2}$
   - $n_{2D} = \dfrac{1}{S}\displaystyle\int_0^{k_F} g_{2D}(k)d^2k = \dfrac{k_F^2}{2\pi}$

   Only the first band (n=1) is filled if $\epsilon_{n=1}(k_\parallel = k_F) < \epsilon_{n=0}(k=0) \Rightarrow k_F < \dfrac{\pi}{d} \Rightarrow n_{2D} < \dfrac{\pi}{2d^2}$
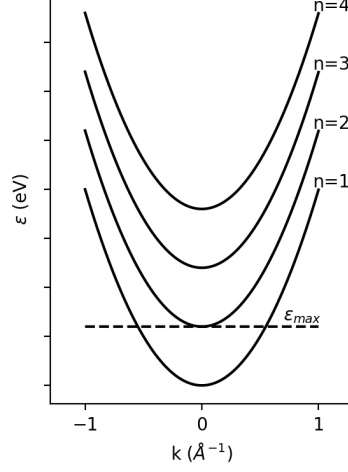
FIGURE 4 –

4. Hamitonian writes :

$$
\begin{aligned}
\mathcal{H} &= -\vec{\mu}.\vec{B} \\
&= -g\mu_B \vec{S}.\frac{\vec{v} \times \vec{E}}{c^2} \\
&= \frac{g\mu_B}{c^2} \vec{S}.(\frac{\hbar \vec{k}}{m^*} \times \vec{u}_z) \\
&= \frac{g\mu_B \hbar}{m^* c^2} \vec{S}.(\vec{k} \times \vec{u}_z) \\
&= \frac{g\mu_B \hbar}{m^* c^2} (\vec{S} \times \vec{k}).\vec{u}_z \\
&= \frac{g\mu_B \hbar}{2m^* c^2} (\vec{\sigma} \times \vec{k}).\vec{u}_z \\
&= \alpha(\vec{\sigma} \times \vec{k}).\vec{u}_z
\end{aligned}
\tag{13}
$$

5. The Hamiltonian car be written in a matrix form :

$$
\mathcal{H} = \frac{\hbar^2 k_\parallel^2}{2m^*} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \alpha\sigma_x k_y - \alpha\sigma_y k_x = \begin{bmatrix} \frac{\hbar^2 k_\parallel^2}{2m^*} & \alpha(k_y + ik_x) \\ \alpha(k_y - ik_x) & \frac{\hbar^2 k_\parallel^2}{2m^*} \end{bmatrix}
\tag{14}
$$

$$
\begin{aligned}
& det(\mathcal{H} - \lambda\mathcal{I}) = 0 \\
\Rightarrow \quad & \left(\frac{\hbar^2 k_\parallel^2}{2m^*} - \epsilon\right)^2 - \alpha^2(k_y + ik_x)(k_y - ik_x) \\
\Rightarrow \quad & \epsilon_\pm = \frac{\hbar^2 k_\parallel^2}{2m^*} \pm \alpha k_\parallel
\end{aligned}
\tag{15}
$$

The 1D dispersion along k and the 3D dispersion along a 2D plane are plotted in Fig. 5.

6. ϵ_- has a minimum when $\frac{\partial \epsilon_-}{\partial k_\parallel} = 0 \Rightarrow \frac{\hbar^2 k_{\parallel m}}{m^*} = \alpha \Rightarrow k_{\parallel m} = \frac{m^* \alpha}{\hbar^2}$

Only the lower energy branch ϵ_- is filled when $\epsilon_-(k_{max}) = 0 \Rightarrow k_{max} = \frac{2\alpha m^*}{\hbar^2}$. We can deduce the density of state for this branch from question 3 : $n_{2D\pm}(k) = \frac{1}{2}n_{2D}(k)$ since only 1 electron per state is allowed when spin degeneracy is lifted. Thus $n_{2D}^c(k_{max}) = \frac{k_{max}^2}{4\pi}$.

7. Mixing up and down spins, with the linear k_x and k_y dependence induce a rotation of the spin direction in the (x,y) plane, as represented in Fig. 6.

8. $k_{\parallel m} = 0.012\text{Å}^{-1}$. Using expression from question 6 : $\alpha = \frac{\hbar^2 k_{\parallel m}}{m^*}$=1.8 10^{-11}eV.m.
$\Delta\epsilon(k_F) = \epsilon_+(k_F) - \epsilon_-(k_F) = \alpha k_F$=27meV with k_F=0.15Å^{-1}.Recheck the numbers...
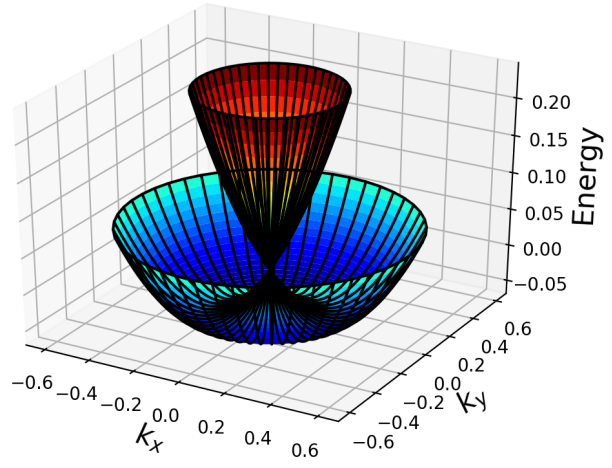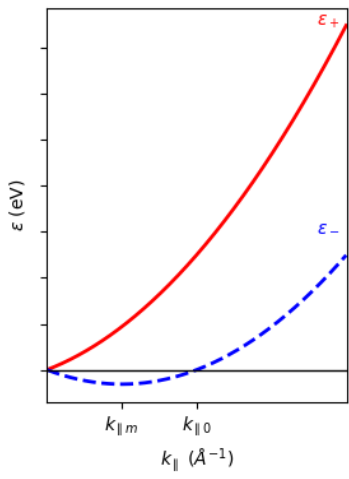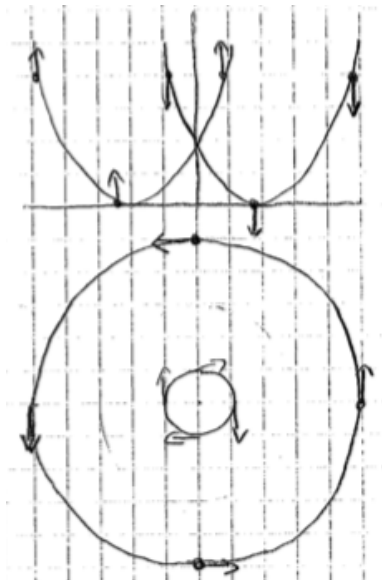
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FIGURE 5 –

FIGURE 6 –

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

Let's recall that $\vec{k}$ is related to the momentum and thus velocity, and thus the time derivative of the position. Thus if we reverse time, $t \to -t$, then $k \to -k$. For spin, if we consider it as a loop current, then $\uparrow \to \downarrow$. For inversion, $x \to -x$, then $k \to -k$, but does not change the spin $\uparrow \to \uparrow$

1. (a) $\mathcal{T}|\vec{k}, \uparrow> = |-\vec{k}, \downarrow>$
   (b) If TRS is respected then $[\mathcal{H}, \mathcal{T}]=0$:

   - $\mathcal{H}\mathcal{T}|\vec{k}, \uparrow> = \mathcal{H}|-\vec{k}, \downarrow> = \epsilon_{-\vec{k},\downarrow}|-\vec{k}, \downarrow>$

   - $\mathcal{T}\mathcal{H}|\vec{k}, \uparrow> = \mathcal{T}\epsilon_{\vec{k},\uparrow}|\vec{k}, \uparrow> = \epsilon_{\vec{k},\uparrow}|-\vec{k}, \downarrow>$

   Thus $\epsilon_{\vec{k},\uparrow} = \epsilon_{-\vec{k},\downarrow}$

2. (a) $\mathcal{I}|\vec{k}, \uparrow> = |-\vec{k}, \uparrow>$
   (b) If IS is respected then $[\mathcal{H}, \mathcal{I}]=0$:

   - $\mathcal{H}\mathcal{I}|\vec{k}, \uparrow> = \mathcal{H}|-\vec{k}, \uparrow> = \epsilon_{-\vec{k},\uparrow}|-\vec{k}, \uparrow>$

   - $\mathcal{I}\mathcal{H}|\vec{k}, \uparrow> = \mathcal{I}\epsilon_{\vec{k},\uparrow}|\vec{k}, \uparrow> = \epsilon_{\vec{k},\uparrow}|-\vec{k}, \uparrow>$

   Thus $\epsilon_{\vec{k},\uparrow} = \epsilon_{-\vec{k},\uparrow}$

3. If both TRS and IS are respected then : $\epsilon_{\vec{k},\uparrow} = \epsilon_{-\vec{k},\downarrow} = \epsilon_{\vec{k},\downarrow}$: there is spin degeneracy.

4. See Fig. 7
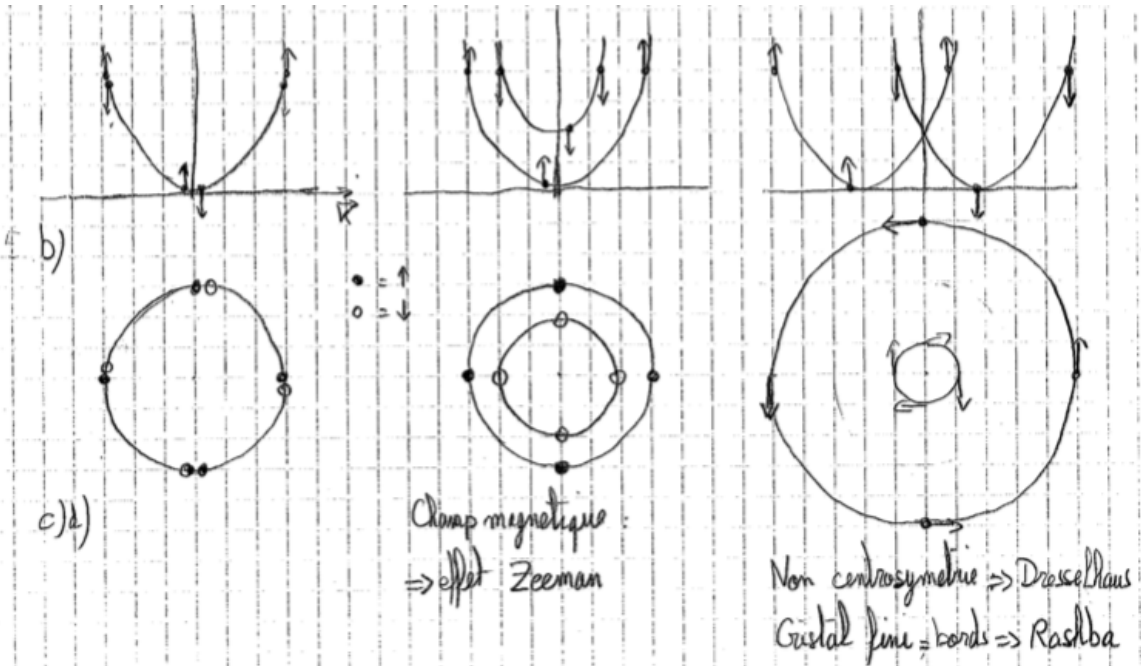
FIGURE 7 –

1.3 Pauli Paramagnetism in the 3D electron gas

1. The Shrödinger equation for free electrons in presence of magnetic field can be written : $\mathcal{H} = \frac{\hbar \hat{P}^2}{2m_e} - \vec{\mu}B$. Eigenfunction of free electron are also eigenfunction of this Hamiltonian, then only eigenvalue changes. Writing the spin magnetic moment $\vec{\mu} = -g\mu_B \vec{S}$ (and the projection $\mu_z = -g\mu_B \vec{S}_z$), and $\vec{B} = B\vec{u}_z$ we

can see that :

$$\epsilon_\uparrow = \frac{\hbar^2 k^2}{2m_e} + \mu_B B$$
$$\epsilon_\downarrow = \frac{\hbar^2 k^2}{2m_e} - \mu_B B \qquad (16)$$

- Determine the volume occupied by 1 state in the k-space : $V_k = \frac{2\pi}{L_x}\frac{2\pi}{L_y}\frac{2\pi}{L_z} = \frac{(2\pi)^3}{\Omega}$ with Ω the surface of the box in the real space ($\Omega = L_x L_y L_z$).
- Write the number of electron states in this volume : $g_\uparrow(k)V_k = 1^\uparrow$. Then $g_\uparrow(k) = \frac{\Omega}{(2\pi)^3}$
- $g_\uparrow(\epsilon)d\epsilon = g_\uparrow(k)d^3k$. With $d^3k = 4\pi k^2 dk$, eq. 16 and $k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{\epsilon_\uparrow - \mu_B B}$

Thus

$$g_\uparrow(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon_\uparrow - \mu_B B}$$
$$= \frac{1}{2}g_{\uparrow\downarrow}(\epsilon - \mu_B B)$$
$$g_\downarrow(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon_\downarrow + \mu_B B} \qquad (17)$$
$$= \frac{1}{2}g_{\uparrow\downarrow}(\epsilon + \mu_B B)$$

with $g_{\uparrow\downarrow}(\epsilon)$ the density for B=0.

2. .

$$n_\uparrow = \int_{-\infty}^{\infty} g_\uparrow(\epsilon)f_{FD}(\epsilon)d\epsilon$$
$$\underset{T=0}{=} \int_{\mu_B B}^{\epsilon_F} g_\uparrow(\epsilon)d\epsilon$$
$$= \frac{1}{2}\int_0^{\epsilon_F - \mu_B B} g_{\uparrow\downarrow}(\epsilon)d\epsilon$$
$$n_\downarrow = \int_{-\infty}^{\infty} g_\downarrow(\epsilon)f_{FD}(\epsilon)d\epsilon \qquad (18)$$
$$\underset{T=0}{=} \int_{-\mu_B B}^{\epsilon_F} g_\downarrow(\epsilon)d\epsilon$$
$$= \frac{1}{2}\int_0^{\epsilon_F + \mu_B B} g_{\uparrow\downarrow}(\epsilon)d\epsilon$$

$$\Delta n = (n_\downarrow - n_\uparrow)$$
$$= \frac{1}{2}\int_{\epsilon_F - \mu_B B}^{\epsilon_F + \mu_B B} g_{\uparrow\downarrow}(\epsilon)d\epsilon \qquad (19)$$

3. μ_B=0.06meV.T^{-1}, and typical magnetic field B=10T. Then $\mu_B B \approx$ 1meV $\ll \epsilon_F \approx$5eV). Then we can considerate the density of state constant near the Fermi level : $g_{\uparrow\downarrow}(\epsilon) \approx g_{\uparrow\downarrow}(\epsilon_F)$:

$$\Delta n = g_{\uparrow\downarrow}(\epsilon_F)\mu_B B$$
$$M = \mu_B \Delta n$$
$$= g_{\uparrow\downarrow}(\epsilon_F)\mu_B^2 B$$
$$\chi = \frac{\partial M}{\partial H} \qquad (20)$$
$$= \mu_0 \frac{\partial M}{\partial B}$$
$$= \mu_0 g_{\uparrow\downarrow}(\epsilon_F)\mu_B^2$$
$$= \mu_0 \mu_B^2 \frac{3}{2}\frac{n}{\epsilon_F}$$

Since for 3d free electrons :

$$n = \int_0^{\epsilon_F} g_{\uparrow\downarrow}(\epsilon)d\epsilon$$
$$= \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{1}{3\pi^2}\epsilon_F^{\frac{3}{2}} \qquad (21)$$
$$= \frac{2}{3}\epsilon_F g_{\uparrow\downarrow}(\epsilon_F)$$

8

4. For Na : n_e=2.68 10^{28}m^{-3}, ϵ_F=3.24eV and ρ=0.971 g.cm^{-3}
   $\hbar$=1.05 10^{-34}, m_e=9.1 10^{-31}, $\mu_0 = 4\pi\ 10^{-7}$m.T.A^{-1} and 1J=6.2 10^{18}eV
   χ=8.4 10^{-6}
   $\frac{\chi}{4\pi\rho}$=6.67 10^{-6}cm^3.g^{-1} in agreement with the Fig 1.3 of the tutorial.

1.4 The free electron gas from 3D to 2D

1.4.1 Electron gas in 3D

1. $\Psi_k(x,y,z) = e^{-i\vec{k}.\vec{r}}$. In a 3D box of dimension L_x, L_y and L_z, electrons wavevectors take the form
   $\vec{k} = n_x \frac{2\pi}{L_x}\vec{u}_x + n_y \frac{2\pi}{L_y}\vec{u}_y + n_z \frac{2\pi}{L_z}\vec{u}_z$ with n_x, n_y and $n_z \in \mathbb{Z}$
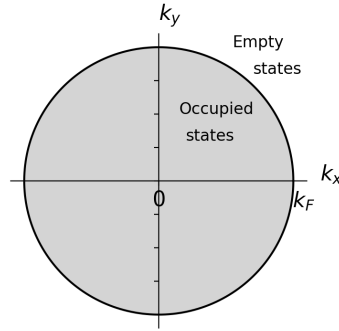
2. See Fig. 8.

FIGURE 8 –

3. The volume occupied by 1 state in the k-space : $V_k = \frac{2\pi}{L_x}\frac{2\pi}{L_y}\frac{2\pi}{L_z} = \frac{(2\pi)^3}{\Omega}$ with Ω the surface of the box in
   the real space ($\Omega=L_x L_y L_z$).
   The number of electron states in this volume : $g_{3D}(k)V_k = 2^{\uparrow\downarrow}$ due to spin degeneracy. Then $g_{3D}(k) = \frac{\Omega}{4\pi^3}$
   $g_{3D}(\epsilon)d\epsilon = g_{3D}(k)d^3k$. With $d^3k = 4\pi k^2 dk$, $k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{\epsilon}$ and $\frac{\partial\epsilon}{\partial k} = \frac{\hbar^2 k}{m}$, we have : $g_{3D}(\epsilon) = \frac{1}{\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon}$

4. $n_{3D} = \int_0^{k_F} g_{3D}(k)d^3k = \int_0^{k_F} \frac{\Omega}{4\pi^3}4\pi k^2 dk = \frac{\Omega k_F^3}{2\pi^2}$
   $n_{3D} = \int_0^{\epsilon_F} g_{3D}(\epsilon)d\epsilon = \int_0^{\epsilon_F} \frac{1}{\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon}d\epsilon = \frac{2}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\epsilon_F^{\frac{3}{2}}$

5. $\epsilon_F = \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}}\frac{\hbar^2}{2m} \approx 7$eV

1.4.2 Electron surface energy of a nearly 2D plate

1. DOS : $g_{2D}(\epsilon) = \dfrac{mS}{\pi\hbar^2} = g_0$

   Total energy at T=0 : $E_e = \displaystyle\int_0^{infty} \epsilon g_{2D}(\epsilon)f_{FD}(\epsilon,\mu,T)d\epsilon = \frac{1}{2}g_0\epsilon_F^2$

   Number of electrons at T=0 : $N_e = \displaystyle\int_0^{infty} g_{2D}(\epsilon)f_{FD}(\epsilon,\mu,T)d\epsilon = g_0\epsilon_F$

   Average energy per electron at T=0 :$< E_e >= \dfrac{E_e}{N_e} = \frac{1}{2}\epsilon_F$

2. $sin(k_z 0) = sin(k_z l) = 0 \Rightarrow k_z = n\dfrac{\pi}{l}$. Here n>0 : since $sin(-k_z z) = -sin(k_z z)$: k_z and $-k_z$ describe
   the same state! So we are restricted to only half a sphere in reciprocal space. Which hemisphere we
   choose is nor relevant. At the base : $k_z = 0 \Rightarrow \Psi(k_z = 0) = 0$ The electron at the base occupy now the
   next available state at the Fermi level.

3. Volume occupied by 1 state : $V_k = \dfrac{2\pi}{L_x}\dfrac{2\pi}{L_y}\dfrac{\pi}{l} = \dfrac{4\pi^3}{Sl}$

Number of electron occupying this state : $g_{3D}(k)'V_k = 2^{\uparrow\downarrow} \Rightarrow g_{3D}(k)' = \dfrac{V}{2\pi^3} = 2g_{3D}(k)$.

Since the DOS is multiplied by two, but we divide the sphere in 2 to have only hemisphere available, the two factors 2 compensate one another : the fermi vector do not change (you can make the calculation of k_F and k_F' to convince yourself by calculating the number of electron in both cases N_e).

4. $\Delta\epsilon = \epsilon_F - \langle E_e \rangle = \dfrac{1}{2}\epsilon_F$

5. Number of electron at $k_z = 0$: $N^{2D} \displaystyle\int_0^{k_F} g_{2D}(k)2\pi k\,dk = \dfrac{S}{2\pi}k_F^2 = \dfrac{S}{\pi}\dfrac{m}{\hbar^2}\epsilon_F$

6. $\Delta E = N^{2D}\Delta\epsilon$

$\dfrac{\Delta E}{S} = \dfrac{1}{2\pi}k_F^2\dfrac{1}{2}\epsilon_F = f(k_F)\epsilon_k$ with $f(k) = \dfrac{1}{4\pi}k_F^2$

1.4.3 Surface effects on the electron gas

1. Born Von Karman conditions implies : $\Psi = \dfrac{1}{\sqrt{V}}e^{i\vec{k}.\vec{r}}$

$n(x,y,z) = \dfrac{1}{V}\displaystyle\int_{k<k_F} g(k)4\pi k^2 dk = \dfrac{1}{V}\int_{k<k_F}\dfrac{V}{4\pi^3}4\pi k^2 dk = \dfrac{k_F^3}{3\pi^2} = n_0$

2. $n(z) = n_0$ when $2k_F z = 4.5 \Rightarrow z = \dfrac{2.25}{k_F} \approx 2\text{Å}$. The surface effects disappear for few layers deep.

2 Transport phenomena

2.1 Electrical conductivity of a metal

1.

$$\sigma = e^2\tau \int_{-\infty}^{-\infty} g(\epsilon)\frac{v(\epsilon)^2}{d}\left(-\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon}\right)d\epsilon \tag{22}$$

$$\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon} = -\beta\frac{e^{\beta(\epsilon-\mu)}}{(e^{\beta(\epsilon-\mu)}+1)^2} \tag{23}$$

The result is plotted in Fig. 9. As we can see, $\dfrac{\partial f_{FD}(\epsilon)}{\partial \epsilon}\bigg|_{T=0} = \delta(\epsilon - \epsilon_F)$. Then we can write :
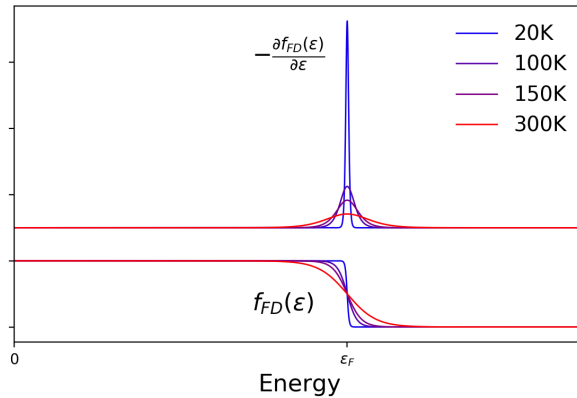

FIGURE 9 –

$$\begin{aligned}\sigma &= e^2\tau \int_{-\infty}^{-\infty} g(\epsilon)\frac{v(\epsilon)^2}{d}\delta(\epsilon - \epsilon_F)d\epsilon \\ &= e^2\tau g(\epsilon_F)\frac{v(\epsilon_F)^2}{d}\end{aligned} \tag{24}$$

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2. $V_k = \dfrac{(2\pi)^2}{S}$, $g(k) = \dfrac{S}{\pi^2}$, $g(\epsilon) = \dfrac{mS}{\pi\hbar^2}$, then $n = \displaystyle\int_0^{\epsilon_F} g(\epsilon)d\epsilon = g(\epsilon_F)\epsilon_F$.

$$
\begin{aligned}
\sigma & = e^2 \tau g(\epsilon_F)\frac{v(\epsilon_F)^2}{d} \\
& = e^2 \tau \frac{n}{\epsilon_F}\frac{m}{m}\frac{v(\epsilon_F)^2}{2} \\
& = \frac{e^2 \tau n}{m}
\end{aligned}
\tag{25}
$$

This comes back to the Drude model result for conductivity.

3. $\tau^{imp} \propto T^{-5}$ and $\tau^{ph} \propto T^{-1}$. The Debye temperature is linked to the typical energy of the phonons. Since phonons are vibration of the lattice, we can expect Debye temperature (phonon energy) to be smaller for heavy materials ($\Theta_D^{Pb,Z=82}$=105K, $\Theta_D^{Be,Z=4}$=1440K). Here for Na : $\Theta_D^{Na,Z=11}$=158K. Resistivity can be written : $\rho \propto \frac{1}{\sigma} \propto \frac{1}{\tau} \propto T^5$ in the case that conductivity is only limited by impurities. Then in a log plot, the slope should be equal to 5 : $log(\rho) = A + 5T$. This is the case here.

2.1.1 Electrical conductivity of graphene

1. $V_k = \dfrac{(2\pi)^2}{S}$, $g(k) = \dfrac{S}{\pi^2}$, $g(\epsilon)d\epsilon = g(k)d^2k$. From the dispersion relations $\epsilon(k)$ we find $\dfrac{d\epsilon}{dk} = \hbar v_F$ and $k = \dfrac{|\epsilon - \epsilon_F|}{\hbar v_F}$. Then

$$
\begin{aligned}
g(\epsilon) & = g(k)2\pi k\frac{dk}{d\epsilon} \\
& = \frac{S}{2\pi^2}2\pi k\frac{1}{\hbar v_F} \\
& = \frac{S}{\pi}\frac{|\epsilon - \epsilon_F|}{\hbar^2 v_F^2}
\end{aligned}
\tag{26}
$$

2.

$$
\begin{aligned}
-\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon} & = \beta\frac{e^{\beta(\epsilon-\mu)}}{(e^{\beta(\epsilon-\mu)} + 1)^2} \\
& = \beta\frac{1}{(e^{\frac{\beta}{2}(\epsilon-\mu)} + e^{-\frac{\beta}{2}(\epsilon-\mu)})^2} \\
& = \frac{\beta}{4ch^2(\frac{\beta}{2}(\epsilon - \mu))}
\end{aligned}
\tag{27}
$$

We will consider that $v(\epsilon) = v_F$ and $\mu = \epsilon_F$ in the range where $-\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon}$ is non zero.

$$
\begin{aligned}
\sigma & = e^2 \tau \int_{-\infty}^{-\infty} g(\epsilon)\frac{v(\epsilon)^2}{d}\left(-\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon}\right)d\epsilon \\
& = \frac{e^2 \tau}{2}\int_{-\infty}^{-\infty}\frac{S}{\pi}\frac{|\epsilon - \epsilon_F|}{\hbar^2 v_F^2}\frac{\beta}{4ch^2(\frac{\beta}{2}(\epsilon - \epsilon_F))}d\epsilon \\
& = \frac{e^2 \tau S \beta}{8\hbar^2 \pi}\int_{-\infty}^{-\infty}\frac{|\epsilon - \epsilon_F|}{ch^2(\frac{\beta}{2}(\epsilon - (\epsilon_F)))}d\epsilon \\
(X = \tfrac{\beta}{2}(\epsilon - \epsilon_F)) \quad & = \frac{e^2 \tau S \beta}{8\hbar^2 \pi}\int_{-\infty}^{-\infty}\frac{2}{\beta}\frac{|X|}{ch^2(X)}\frac{2}{\beta}dX \\
& = \frac{e^2 \tau S}{\pi\hbar^2}ln(2)
\end{aligned}
\tag{28}
$$

2.2 Thermal conductivity

1. At 1D, accordind to Maxwell-Boltzmann particle velocity distribution, we can write the mean square velocity : $\dfrac{1}{2}m < v^2 > = \dfrac{1}{2}k_B T$ so that $v = \sqrt{\dfrac{k_B T}{m}}$

2. The energy is purely kinetic so that $\epsilon = \dfrac{1}{2}k_B T$ so that the specific heat can be easily expressed : $C_v = \frac{d\epsilon}{dT} = \frac{1}{2}k_B$. We can then write the variation of energy between time t and $t + \tau$, the time between

2 collisions. During this time we can express the distance travelled by the electron : $\delta x = v\tau$.

$$
\begin{aligned}
\epsilon &= \frac{1}{2}k_B T \\
\delta\epsilon &= \frac{1}{2}k_B \frac{\partial T}{\partial x}\delta x \\
&\underset{\delta x = v\tau}{=} C_v \nabla_x T v\tau
\end{aligned} \tag{29}
$$

3. During a time τ, the same amount goes from left to right and from right to left : $n_- = n_+ = n\frac{1}{2}Sv\tau$: half the density goes left (hence the n/2 term), $v\tau$ being the distance traveled by the electron to reach S from the left or right side of the section S.

4. The left and right electron do not have the same energy. The exchange of electrons from right and left side is thus accompanied with a heat exchange Q.

$$
\begin{aligned}
Q &= n_+\delta\epsilon_+ - n_-\delta\epsilon_- \\
&= n\frac{1}{2}Sv\tau C_v \nabla_x T v\tau - n\frac{1}{2}Sv\tau C_v(-\nabla_x T)v\tau \\
&= nSv\tau C_v \nabla_x T v\tau \\
&= nSv^2\tau^2 C_v \nabla_x T
\end{aligned} \tag{30}
$$

Thus $\vec{j}_Q = \frac{Q}{S\tau} = nv^2\tau C_v \nabla_x T$ and $\kappa_{1D} = \frac{j_Q}{\nabla_x T} = nv^2\tau C_v$

Be careful here, at 3D $\epsilon = \frac{3}{2}k_B T$ so $C_v^{3D} = \frac{3}{2}k_B$!

5. The mean free path is defined as the distance travelled by the electron without collision. We can thus write : $l_e = v\tau$. Since $<v^2> = v_x^2 + v_y^2 + v_z^2$ then the $v_{1D}^2 = \frac{1}{3}v_{3D}^2$, thus we just have to replace v^2 by $\frac{v^2}{3}$ in the expression of κ_{1D}. Indeed only one third of the root mean velocity is going in the x direction of the thermal gradient :

$\kappa_{3D} = \frac{1}{3}nv^2\tau C_v = \frac{1}{3}nvl_e C_v$

6. $\frac{\kappa}{\sigma} = \frac{\frac{1}{3}nvl_e c}{\frac{ne^2\tau}{m}} = \frac{\frac{1}{3}nvv\tau \frac{3k_B}{2}m}{ne^2\tau} = \frac{mv^2}{2}\frac{k_B}{e^2} = \frac{3K_B T}{2}\frac{k_B}{e^2} = \frac{3}{2}\left(\frac{K_B}{e}\right)^2 T = \mathcal{L}T$

7. $\mathcal{L}_{theo} = \frac{3}{2}\left(\frac{K_B}{e}\right)^2 = 1.1\ 10^{-8}\text{W}^2\text{A}^{-2}\text{K}^{-2}$

$\mathcal{L}_{exp} = \frac{\kappa}{\sigma} = 3\ 10^{-8}\text{W}^2\text{A}^{-2}\text{K}^{-2}$ The experiment value is close to the calculated one !

8. We no longer take $C_v = \frac{3}{2}k_B$ but $C_v = \frac{\pi^2}{2}n_e k_B \frac{T}{T_F}$

$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{K_B}{e}\right)^2 T$

$\mathcal{L}_{theo} = \frac{\pi^2}{3}\left(\frac{K_B}{e}\right)^2$

This changes the previous result by a factor 2.2 !