

# Correction of tutorial QSSP

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10 octobre 2024

Careful : mistakes may subsist !

## 1 The free electron gas

### 1.1 The free electron gas in 2D

#### 1.1.1 Fermi energy and density of states

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

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

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

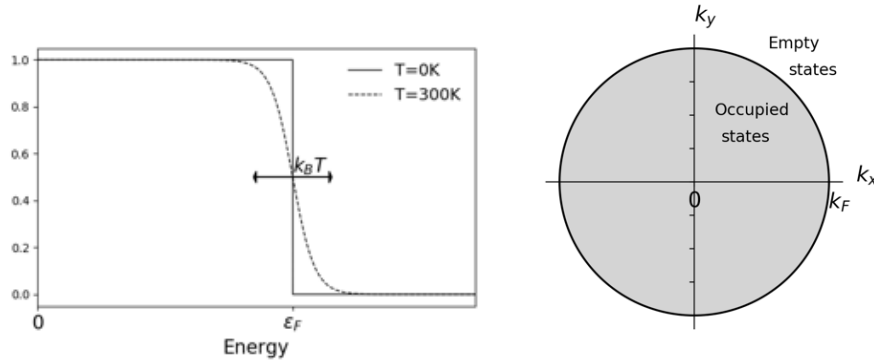


FIGURE 1 –

- 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  $\vec{k} = n_x \frac{2\pi}{L_x} \vec{u}_x + n_y \frac{2\pi}{L_y} \vec{u}_y$  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.

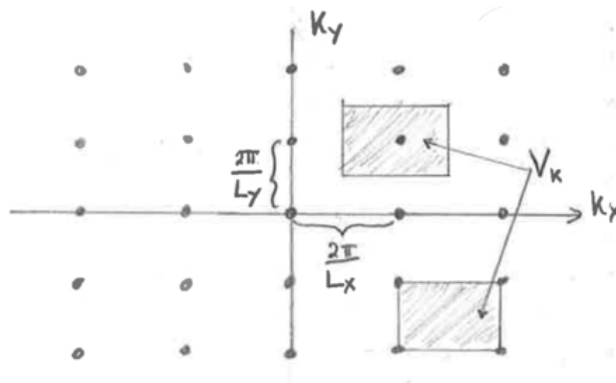


FIGURE 2 –

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

- Determine the surface occupied by 1 state in the k-space :  $S_k = \frac{2\pi}{L_x} \frac{2\pi}{L_y} = \frac{(2\pi)^2}{S}$  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  $g_{2D}(k) = \frac{S}{2\pi^2}$
4. To calculate the density of state in energy space, the previous 2 steps determination of  $g_{2D}(k)$  is required. We then write :

$$g_{2D}(\epsilon)d\epsilon = g_{2D}(k)d^2k \quad (2)$$

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

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

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) :

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

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

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

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

- $k_F = \sqrt{2\pi \frac{N_e}{S}} = 2.9 \cdot 10^9 \text{ m}^{-1}$

- $\epsilon_F = \frac{\hbar^2 k_F^2}{2m_e} = 0.3 \text{ eV}$

- $T_F = \frac{\epsilon_F}{k_B} = 3780 \text{ K}$

The energy to add one electron is much higher than the thermal energy ( $T_F \gg 300\text{K}$ ) so this cannot be considered as a classical Boltzman gas.

7. For  $T \neq 0$  :

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

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

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

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  $\mu$  varies very slowly with the temperature and can be approximated to Fermi energy  $\epsilon_F$ . 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 :

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

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

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

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  $T^2$  would get a straight line with a slope corresponding to  $\beta$  and the y-intercept corresponding to  $\gamma$ .

$\gamma = \frac{N_e \pi^2}{3} k_B \frac{1}{T_F}$ . With a Fermi temperature around  $T_F = 3800$  K (see 1.1.1.6), we get  $\gamma_{theo} = 7 \text{ mJ} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ .  $\gamma_{exp} = 23 \text{ mJ} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ . 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

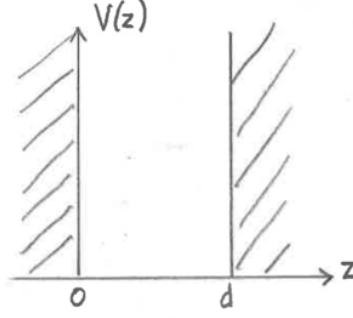


FIGURE 3 –

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

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

Then

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

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

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

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 :  $S_k = \frac{2\pi}{L_x} \frac{2\pi}{L_y} = \frac{(2\pi)^2}{S}$  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  $g_{2D}(k) = \frac{S}{2\pi^2}$
- $n_{2D} = \frac{1}{S} \int_0^{k_F} g_{2D}(k) d^2 k = \frac{k_F^2}{2\pi}$

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

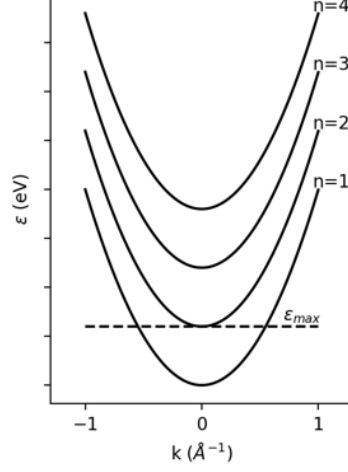


FIGURE 4 –

4. Hamiltonian writes :

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

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

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

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

The 1D dispersion along  $k$  and the 3D dispersion along a 2D plane are plotted in Fig. [5](#).

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

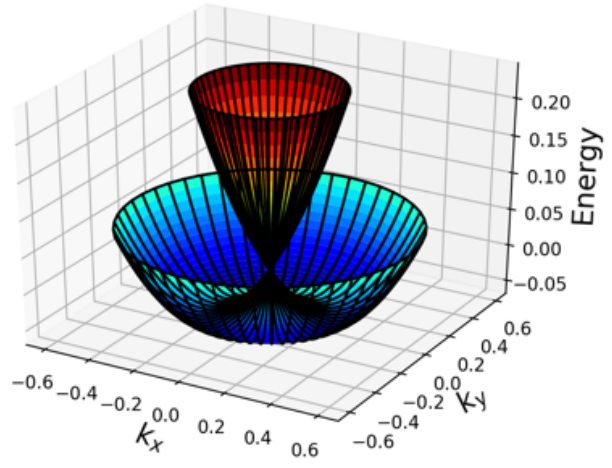
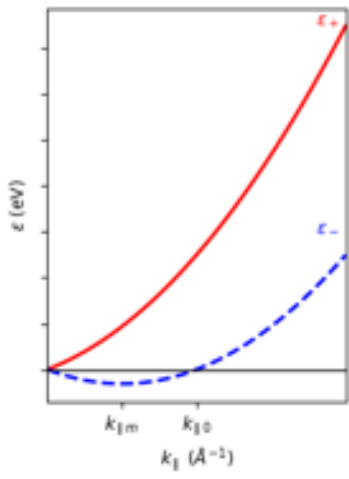


FIGURE 5 –

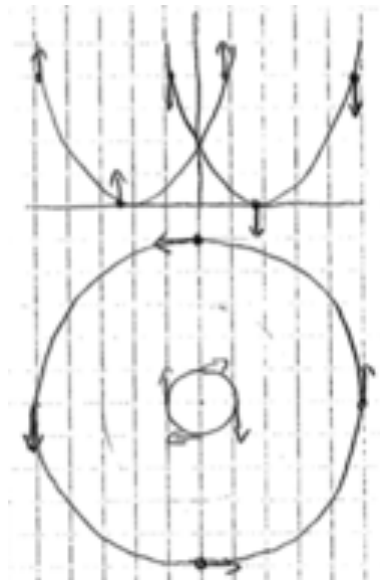


FIGURE 6 –

### 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,  $t \rightarrow -t$ , then  $k \rightarrow -k$ . For spin, if we consider it as a loop current, then  $\uparrow \rightarrow \downarrow$ . For inversion,  $x \rightarrow -x$ , then  $k \rightarrow -k$ , but does not change the spin  $\uparrow \rightarrow \uparrow$

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

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

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

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

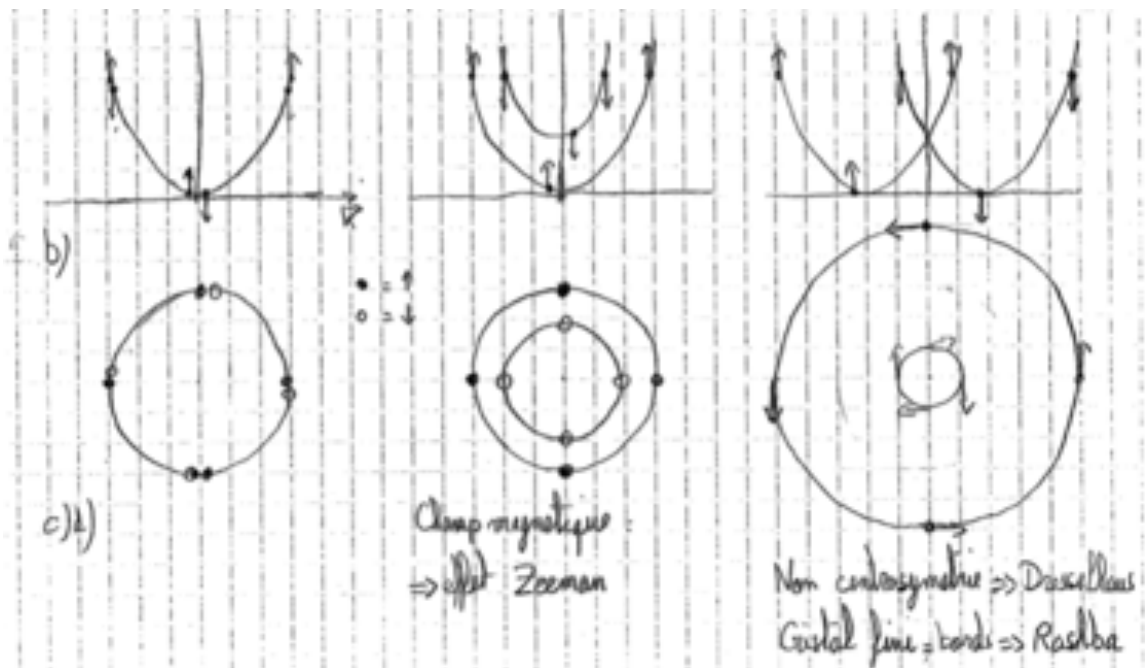


FIGURE 7 –

### 1.3 Pauli Paramagnetism in the 3D electron gas

1. The Schrödinger equation for free electrons in presence of magnetic field can be written :  $\mathcal{H} = \frac{\hbar^2 \hat{p}^2}{2m_e} - \vec{\mu} \cdot \vec{B}$ . 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 :

$$\begin{aligned}\epsilon_{\uparrow} &= \frac{\hbar^2 k^2}{2m_e} + \mu_B B \\ \epsilon_{\downarrow} &= \frac{\hbar^2 k^2}{2m_e} - \mu_B B\end{aligned}\quad (16)$$

- 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  $\Omega$  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

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

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

2. .

$$\begin{aligned}n_{\uparrow} &= \int_{-\infty}^{\infty} g_{\uparrow}(\epsilon) f_{FD}(\epsilon) d\epsilon \\ &\stackrel{T=0}{=} \int_{\mu_B B}^{\epsilon_F} g_{\uparrow}(\epsilon) d\epsilon \\ &= \frac{1}{2} \int_{-\infty}^{\epsilon_F - \mu_B B} g_{\uparrow\downarrow}(\epsilon) d\epsilon\end{aligned}\quad (18)$$

$$\begin{aligned}n_{\downarrow} &= \int_{-\infty}^{\infty} g_{\downarrow}(\epsilon) f_{FD}(\epsilon) d\epsilon \\ &\stackrel{T=0}{=} \int_{-\mu_B B}^{\epsilon_F} g_{\downarrow}(\epsilon) d\epsilon \\ &= \frac{1}{2} \int_0^{\epsilon_F + \mu_B B} g_{\uparrow\downarrow}(\epsilon) d\epsilon\end{aligned}$$

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

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

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

Since for 3d free electrons :

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



4. For Na :  $n_e=2.68 \cdot 10^{28} \text{m}^{-3}$ ,  $\epsilon_F=3.24 \text{eV}$  and  $\rho=0.971 \text{g.cm}^{-3}$   
 $\hbar=1.05 \cdot 10^{-34}$ ,  $m_e=9.1 \cdot 10^{-31}$ ,  $\mu_0 = 4\pi \cdot 10^{-7} \text{m.T.A}^{-1}$  and  $1\text{J}=6.2 \cdot 10^{18} \text{eV}$   
 $\chi=8.4 \cdot 10^{-6}$   
 $\frac{\chi}{4\pi\rho}=6.67 \cdot 10^{-6} \text{cm}^3.\text{g}^{-1}$  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

- $\Psi_{\vec{k}}(x, y, z) = e^{-i\vec{k} \cdot \vec{r}}$ . 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  $n_z \in \mathbb{Z}$
- See Fig. [8](#)

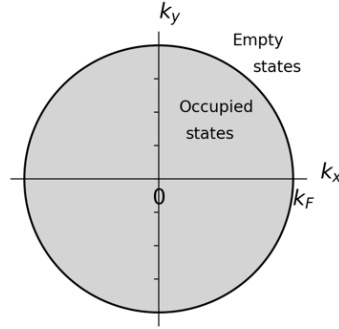


FIGURE 8 –

- 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  $\Omega$  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 :  $g_{3D}(\epsilon) = \frac{1}{\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{\epsilon}$
- $n_{3D} = \int_0^{k_F} g_{3D}(k) d^3k = \int_0^{k_F} \frac{\Omega}{4\pi^3} 4\pi k^2 dk = \frac{\Omega k_F^3}{2\pi^2}$   
 $n_{3D} = \int_0^{\epsilon_F} g_{3D}(\epsilon) d\epsilon = \int_0^{\epsilon_F} \frac{1}{\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{\epsilon} d\epsilon = \frac{2}{3\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \epsilon_F^{\frac{3}{2}}$
- $\epsilon_F = \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m} \approx 7 \text{eV}$

### 1.4.2 Electron surface energy of a nearly 2D plate

- DOS :  $g_{2D}(\epsilon) = \frac{mS}{\pi\hbar^2} = g_0$   
Total energy at T=0 :  $E_e = \int_0^{inf\text{ty}} \epsilon g_{2D}(\epsilon) f_{FD}(\epsilon, \mu, T) d\epsilon = \frac{1}{2} g_0 \epsilon_F^2$   
Number of electrons at T=0 :  $N_e = \int_0^{inf\text{ty}} g_{2D}(\epsilon) f_{FD}(\epsilon, \mu, T) d\epsilon = g_0 \epsilon_F$   
Average energy per electron at T=0 :  $\langle E_e \rangle = \frac{E_e}{N_e} = \frac{1}{2} \epsilon_F$
- $\sin(k_z 0) = \sin(k_z l) = 0 \Rightarrow k_z = n \frac{\pi}{l}$ . 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 :  $V_k = \frac{2\pi}{L_x} \frac{2\pi}{L_y} \frac{\pi}{l} = \frac{4\pi^3}{Sl}$

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

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.  $\Delta\epsilon = \epsilon_F - < E_e > = \frac{1}{2}\epsilon_F$

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

6.  $\frac{\Delta E}{S} = \frac{N^{2D} \Delta\epsilon}{S} = \frac{1}{2\pi} k_F^2 \frac{1}{2} \epsilon_F = f(k_F) \epsilon_k$  with  $f(k) = \frac{1}{4\pi} k_F^2$

### 1.4.3 Surface effects on the electron gas

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

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

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

## 2 Transport phenomena

### 2.1 Electrical conductivity of a metal

1.

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

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

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

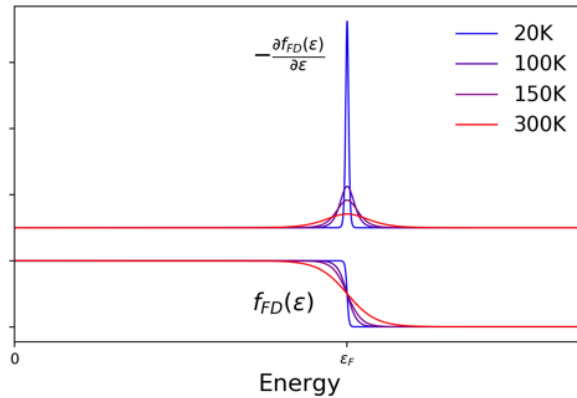


FIGURE 9 –

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

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

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

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 ( $\Theta_D^{Pb, Z=82}=105\text{K}$ ,  $\Theta_D^{Be, Z=4}=1440\text{K}$ ). Here for Na :  $\Theta_D^{Na, Z=11}=158\text{K}$ . 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.  $V_k = \frac{(2\pi)^2}{S}$ ,  $g(k) = \frac{S}{\pi^2}$ ,  $g(\epsilon)d\epsilon = g(k)d^2k$ . From the dispersion relations  $\epsilon(k)$  we find  $\frac{d\epsilon}{dk} = \hbar v_F$  and  $k = \frac{|\epsilon - \epsilon_F|}{\hbar v_F}$ . 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.

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

## 2.2 Thermal conductivity

1. At 1D, accordind to Maxwell-Boltzmann particle velocity distribution, we can write the mean square velocity :  $\frac{1}{2}m \langle v^2 \rangle = \frac{1}{2}k_B T$  so that  $v = \sqrt{\frac{k_B T}{m}}$
2. The energy is purely kinetic so that  $\epsilon = \frac{1}{2}k_B T$  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 :  $\delta x = v\tau$ .

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

3. During a time  $\tau$ , 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.

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

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  $\langle v^2 \rangle = v_x^2 + v_y^2 + v_z^2$  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  $\kappa_{1D}$ . Indeed only one third of the root mean velocity is going in the x direction of the thermal gradient :

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

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

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

$\mathcal{L}_{exp} = \frac{\kappa}{\sigma} = 3 \cdot 10^{-8} \text{W}^2 \text{A}^{-2} \text{K}^{-2}$  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!

## 3 Crystalline Solids

### 3.1 Rectangular lattice

See Fig [10](#) in the case A=B, The conventional rectangular contains 2 primitive unit cells.

### 3.2 Cubic lattice

- *Li* : Motif has 2 Li atoms : (0,0,0) and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . The cube is not a primitive cell. The mode is body centered I. There is 1 motif per unit cell.
- *CsCl* : Motif has 2 atoms : Cs (0,0,0) and Cl  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . The cube is a primitive cell. There is 1 motif per unit cell.
- *BaTiO<sub>3</sub>* : Motif has 5 atoms : Ba (0,0,0), Ti  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ , O  $(\frac{1}{2}, \frac{1}{2}, 0)$ ,  $(\frac{1}{2}, 0, \frac{1}{2})$  and  $(0, \frac{1}{2}, \frac{1}{2})$ . The cube is a primitive cell. There is 1 motif per unit cell.

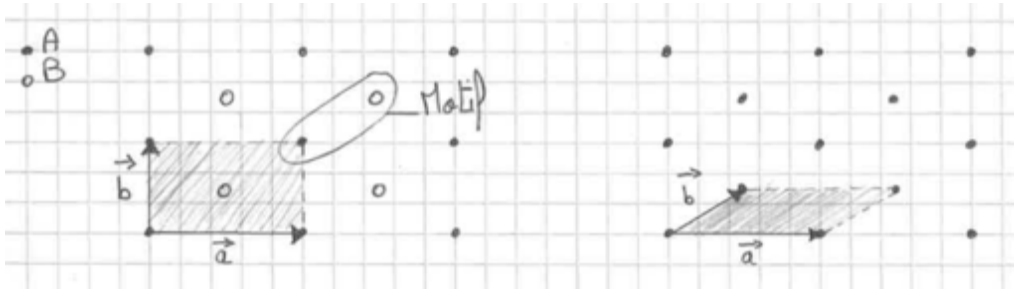


FIGURE 10 –

### 3.3 Hexagonal lattice

1. Different primitive unit cells are represented in Fig. 11 (not shaded).
2. The rectangular lattice is represented in Fig. Fig33 (Left figure, shaded surface). There is 2 unit cell in this conventional cell (multiplicity = 2).  $|\vec{a}_R| = a$  and  $|\vec{b}_R| = 2a \sin(60) = \sqrt{3}a$ .

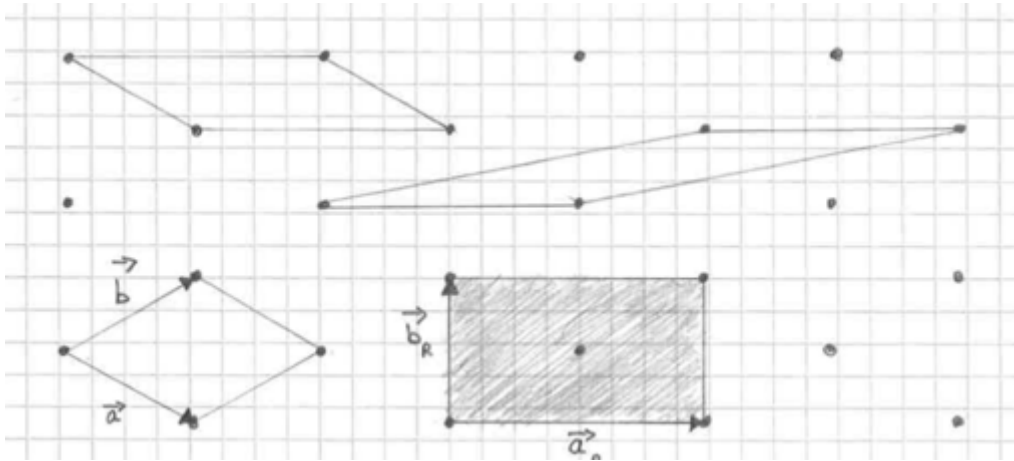


FIGURE 11 –

### 3.4 Honeycomb lattice

1. The Bravais lattice is hexagonal, and the motif is  $C(0,0)$  and  $C(\frac{1}{3}, \frac{1}{3})$
2. See Fig. 12
3.  $|\vec{a}| = |\vec{b}| = 2l \sin(60) = \sqrt{3}l$
4. 3 families of rows are represented in ?? (right figure). The distance between rows for the example in blue is  $d = 2l \sin(60) = \sqrt{3}l$

### 3.5 Reciprocal lattice

#### 3.5.1 2D Rectangular lattice

- 1.

$$\begin{aligned}
 V &= \vec{a} \cdot (\vec{b} \times \vec{c}) = abc \\
 \vec{a}^* &= 2\pi \frac{\vec{b} \times \vec{c}}{V} = \frac{2\pi}{a} \vec{u}_a \\
 \vec{b}^* &= 2\pi \frac{\vec{c} \times \vec{a}}{V} = \frac{2\pi}{b} \vec{u}_b \\
 \vec{c}^* &= 2\pi \frac{\vec{a} \times \vec{b}}{V} = \frac{2\pi}{c} \vec{u}_c
 \end{aligned} \tag{31}$$

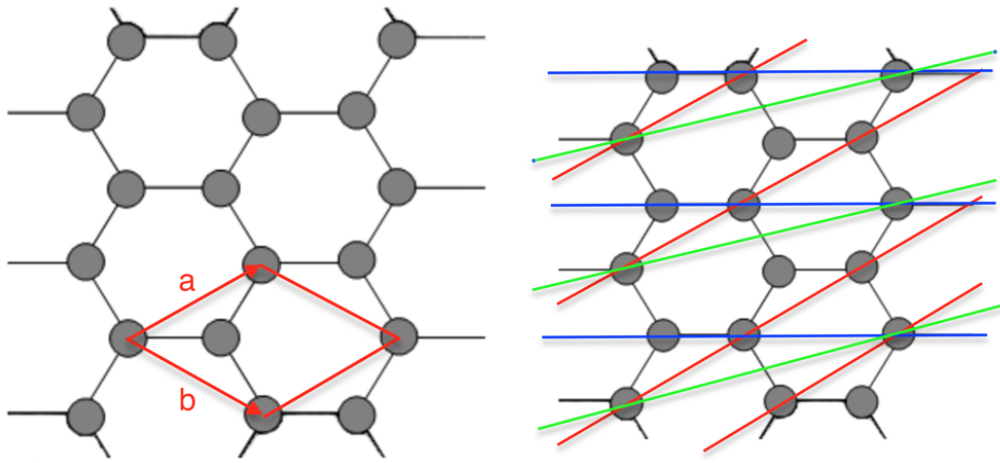


FIGURE 12 -

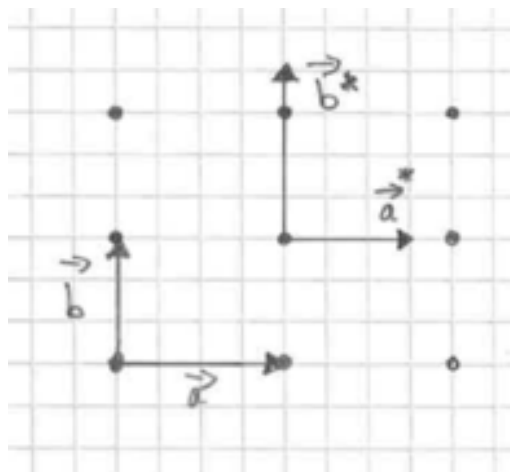


FIGURE 13 -

2. Geometrical construction is plotted Fig. 14.

$\vec{a}_0 = \frac{1}{2}\vec{a} - \frac{1}{2}\vec{b}$  and  $\vec{b}_0 = \frac{1}{2}\vec{a} + \frac{1}{2}\vec{b}$ . Then  $\vec{a}_0^* = \frac{2\pi}{a}\vec{u}_a - \frac{2\pi}{a}\vec{u}_b = \vec{a}^* - \vec{b}^*$  and  $\vec{b}_0^* = \frac{2\pi}{a}\vec{u}_a + \frac{2\pi}{a}\vec{u}_b = \vec{a}^* + \vec{b}^*$

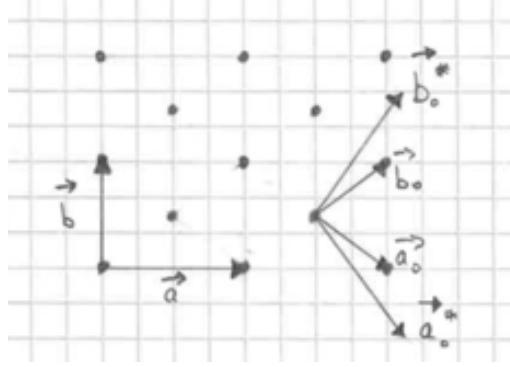


FIGURE 14 –

### 3.5.2 Diffraction on the honeycomb lattice

1. The Bravais lattice is hexagonal, and the motif is  $C(0,0)$  and  $C(\frac{1}{3}, \frac{1}{3})$ . According to Fig. 12,  $\vec{a} = (a \cos(30), a \sin(30), 0) = (\frac{\sqrt{3}}{2}a, \frac{1}{2}a, 0)$  and  $\vec{b} = (a \cos(30), -a \sin(30), 0) = (\frac{\sqrt{3}}{2}a, -\frac{1}{2}a, 0)$  and  $\vec{c} = (0, 0, c)$ .

$$\begin{aligned}
 V &= \vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{\sqrt{3}}{2} a^2 c \\
 \vec{a}^* &= 2\pi \frac{\vec{b} \times \vec{c}}{V} = \frac{2\pi}{\sqrt{3}a} \begin{bmatrix} 1 \\ \sqrt{3} \\ 0 \end{bmatrix} \\
 \vec{b}^* &= 2\pi \frac{\vec{c} \times \vec{a}}{V} = \frac{2\pi}{\sqrt{3}a} \begin{bmatrix} 1 \\ -\sqrt{3} \\ 0 \end{bmatrix} \\
 \vec{c}^* &= 2\pi \frac{\vec{a} \times \vec{b}}{V} = \frac{2\pi}{c} \vec{u}_c
 \end{aligned} \tag{32}$$

The reciprocal lattice is then hexagonal.

2.

$$\begin{aligned}
 S(h, k, l) &= \sum_{i=1}^2 f_i(q) e^{-i2\pi(hx_i + ky_i + lz_i)} \\
 &= f_C(q) e^{-i2\pi(h \cdot 0 + k \cdot 0 + l \cdot 0)} + f_C(q) e^{-i2\pi(h \cdot \frac{1}{3} + k \cdot \frac{1}{3} + l \cdot 0)} \\
 &= f_C(q) \left[ 1 + e^{-i \frac{2\pi}{3}(h+k)} \right]
 \end{aligned} \tag{33}$$

- if  $h+k=3n$  :  $S(h, k, l) = 2f_C(q)$ ,  $|S(h, k, l)|^2 = 4f_C(q)^2$
- if  $h+k=3n+1$  :  $S(h, k, l) = f_C(q) \left[ \frac{1}{2} + i \frac{\sqrt{3}}{2} \right]$ ,  $|S(h, k, l)|^2 = f_C(q)^2$
- if  $h+k=3n+2$  :  $S(h, k, l) = f_C(q) \left[ \frac{1}{2} - i \frac{\sqrt{3}}{2} \right]$ ,  $|S(h, k, l)|^2 = f_C(q)^2$

### 3.6 Reciprocal lattice and diffraction

1. The reciprocal lattice of a tetragonal is tetragonal.

$$\begin{aligned}
 V &= \vec{a} \cdot (\vec{b} \times \vec{c}) = a^2 c \\
 \vec{a}^* &= 2\pi \frac{\vec{b} \times \vec{c}}{V} = \frac{2\pi}{a} \vec{u}_a \\
 \vec{b}^* &= 2\pi \frac{\vec{c} \times \vec{a}}{V} = \frac{2\pi}{b} \vec{u}_b \\
 \vec{c}^* &= 2\pi \frac{\vec{a} \times \vec{b}}{V} = \frac{2\pi}{c} \vec{u}_c
 \end{aligned} \tag{34}$$

2. The Bragg law :  $2d\sin(\theta) = \lambda$ , with  $d = \frac{a}{\sqrt{h^2+k^2+\frac{a^2}{c^2}l^2}}$ . Then :

$$2\theta = 2\arcsin\left(\frac{\lambda\sqrt{h^2+k^2+\frac{a^2}{c^2}l^2}}{2a}\right)$$

3. With :

$$m_n = 1.67 \cdot 10^{-27} \text{ kg}$$

$$\hbar = 1.05 \cdot 10^{-34} \text{ J.s}$$

$$1 \text{ J} = 6.2 \cdot 10^{18} \text{ eV}$$

$$k_B = 1.38 \cdot 10^{-23} \text{ J.K}^{-1}$$

$$\epsilon = k_B T = 38 \text{ meV}$$

$$\epsilon = \frac{\hbar^2}{2m_n} \left(\frac{2\pi}{\lambda}\right)^2 \Rightarrow \lambda = 2\pi \frac{\hbar}{\sqrt{2m_n\epsilon}} = 1.2 \text{ \AA}$$

The experiment was done on a thermal diffractometer :  $\epsilon = 15\text{-}100 \text{ meV}$  ( $\lambda = 2.5\text{-}0.9 \text{ \AA}$ ). Cold diffractometer are used to look at small angles (large  $q$  values) for magnetic peaks for example :  $\epsilon = 0.1\text{-}15 \text{ meV}$  ( $\lambda = 27\text{-}2.5 \text{ \AA}$ ),

$$4. \quad 2\theta_{111} = 2\arcsin\left(\frac{\lambda\sqrt{1+1+\frac{a^2}{c^2}}}{2a}\right) = 2\arcsin\left(\frac{1.2\sqrt{2+\frac{4.8734^2}{3.3103^2}}}{2 \times 4.8734}\right) = 29.1^\circ$$

$$2\theta_{210} = 2\arcsin\left(\frac{\lambda\sqrt{2^2+1+0}}{2a}\right) = 31.96^\circ \quad 2\theta_{200} = 2\arcsin\left(\frac{\lambda\sqrt{2^2+0+0}}{2a}\right) = 31.96^\circ$$

### 3.7 Bravais lattice and structure factor of MnF<sub>2</sub>

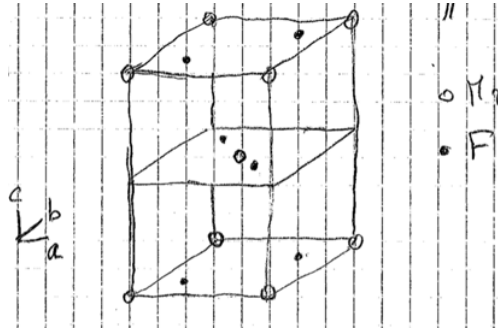


FIGURE 15 -

- 1.
2. There are 2  $MnF_2$  formula per unit cell.
- 3.

$$\begin{aligned} S(h, k, l) &= \sum_{i=1}^2 f_i(q) e^{-i2\pi(hx_i + ky_i + lz_i)} \\ &= f_{Mn} \left[ 1 + e^{-i\pi(h+k+l)} \right] \\ &\quad + f_F \left[ e^{-i2\pi u(h+k)} + e^{i2\pi u(h+k)} + e^{-i2\pi u(h-k)} e^{-i\pi(h+k+l)} + e^{i2\pi u(h-k)} e^{-i\pi(h+k+l)} \right] \\ &= f_{Mn} \left[ 1 + e^{-i\pi(h+k+l)} \right] + 2f_F \left[ \cos(2\pi u(h+k)) + e^{-i\pi(h+k+l)} \cos(2\pi u(h-k)) \right] \end{aligned} \quad (35)$$

with  $g(h, k, l) = e^{-i\pi(h+k+l)}$ .

4. if  $h+k+l$  odd,  $g(h, k, l) = -1$ , then  $S(h, k, l) = 2f_F [\cos(2\pi u(h+k)) - \cos(2\pi u(h-k))]$ . If  $h$  or  $k$  is null then  $S(h, k, l) = 0$ .
5.  $I_{(1,0,0)}$  being null, the first peak should be  $I_{(1,1,0)}$  as observed.



### 3.7.1 X-ray diffraction and measure of the lattice parameter

1.

$$\begin{aligned}
 \frac{S(2,0,2)}{S(3,1,1)} &= \frac{2f_{Mn} + 4f_F \cos(4\pi u)}{2f_F [\cos(8\pi u) - \cos(4\pi u)]} \\
 &= \frac{f_{Mn} + 2f_F \cos(4\pi u)}{f_F [\cos(8\pi u) - \cos(4\pi u)]} \\
 &= \frac{f_{Mn} + 2f_F \cos(4\pi u)}{f_F [\cos(8\pi u) - \cos(4\pi u)]} \\
 &= \frac{\frac{f_{Mn}}{f_F} + 2\cos(x)}{x=4\pi u [\cos(2x) - \cos(x)]}
 \end{aligned} \tag{36}$$

2. Be careful, what we measure is  $I = |S(h, k, l)|^2$ , and for powder, you need to take into account the multiplicity! So  $\frac{I(2,0,2)}{I(3,1,1)} = \frac{m_{202}|S(2,0,2)|^2}{m_{311}|S(3,1,1)|^2}$ . Then from this ratio you can determine the  $\frac{S(2,0,2)}{S(3,1,1)} = 1.22$ .

From the graph,  $f(x) = 1.2$  for  $x = 3.9$  so  $u = 0.31$ .

3.  $\frac{\Delta u}{u} = 0.01 \Rightarrow \frac{\Delta x}{x} = \frac{\Delta u}{u} \Rightarrow \Delta x = 0.01x = 0.04$

So for a variation of % in  $x$ ,  $1 < f(x) < 1.5$  and  $1 < \frac{I(2,0,2)}{I(3,1,1)} < 2.25$ . This ration is very sensitive to the position of F atoms.

### 3.7.2 Neutron scattering and magnetic structure

1.

$$\begin{aligned}
 S(h, k, l)_m &= \sum_{i=1}^2 f_i(q) e^{-i2\pi(hx_i + ky_i + lz_i)} \\
 &= f_{Mn\uparrow} + f_{Mn\downarrow} e^{-i\pi(h+k+l)} \\
 &+ f_F \left[ e^{-i2\pi u(h+k)} + e^{i2\pi u(h+k)} + e^{-i2\pi u(h-k)} e^{-i\pi(h+k+l)} + e^{i2\pi u(h-k)} e^{-i\pi(h+k+l)} \right] \\
 &= f_{Mn\uparrow} \left[ 1 - e^{-i\pi(h+k+l)} \right] + 2f_F \left[ \cos(2\pi u(h+k)) + e^{-i\pi(h+k+l)} \cos(2\pi u(h-k)) \right]
 \end{aligned} \tag{37}$$

Since  $f_{Mn\uparrow} = -f_{Mn\downarrow}$ .

2. With  $f_{Mn\uparrow} \neq -f_{Mn\downarrow}$ , there is no longer extinction for  $h+k+l$  odd and  $h$  or  $k$  null.

3. At low temperature, magnetic order breaks the extinction rule :  $(1,0,0)$  and  $(2,0,1)$  are now allowed and we can see them.

4. If moments are along  $c$ , then we cannot see any magnetic peak for  $\vec{q}$  along  $c$ , like  $(0,0,1)$ . This what is observed.

## 4 The band theory of solids

### 4.1 Tight binding in the one-dimensional atomic chain

To be completed...

### 4.2 Peierls instability

1. We only consider overlap of wavefunction between first neighbours. Closer atoms are thus expected to have a larger overlap :  $1 + \eta$  and most distant one a reduced overlap  $(1 - \eta)$ . The chain period is then  $2a$  and the Brillouin zone is limited to  $[-\frac{\pi}{2a} : \frac{\pi}{2a}]$ .

2. From translational symmetry :

$$\begin{aligned}
\phi_{2m}(x+2a) &= \phi_0(x+2a-2ma) = \phi_0(x+2(m-1)a) = \phi_{2m-2}(x) \\
\phi_{2m+1}(x+2a) &= \phi_0(x+2a-(2m+1)a) = \phi_0(x+(2m-1)a) = \phi_{2m-1}(x) \\
\Psi(x+2a) &= \sum \alpha_m \phi_{2m}(x+2a) + \beta_m \phi_{2m+1}(x+2a) \\
&= \sum_m \alpha_m \phi_{2m-2}(x) + \beta_m \phi_{2m-1}(x) \\
&= \sum_{m'=m-1} \alpha_{m'+1} \phi_{2m'}(x) + \beta_{m'+1} \phi_{2m'+1}(x)
\end{aligned} \tag{38}$$

From Bloch theorem :

$$\Psi(x) = u(x)e^{ikx} \text{ with } u(x+2a) = u(x)$$

$$\text{Then } \Psi(x+2a) = \Psi(x)e^{i2ka}$$

Combining the consequences of translationnal symmetry and Bloch theorem, we thus have by identification :

$$\alpha_{m+1} = e^{i2ka} \alpha_m \text{ and } \alpha_{m+1} = e^{i2ka} \beta_m$$

$$\text{Thus } \alpha_m = e^{i2mka} \alpha_0 \text{ and } \alpha_m = e^{i2mka} \beta_0$$

3.

$$\begin{aligned}
\langle \phi_{2n} | \mathcal{H} | \Psi_k \rangle &= \epsilon_k \langle \phi_0 | \Psi_k \rangle = \epsilon_k e^{i2nka} \alpha_0 \\
&= \sum_m \alpha_m \langle \phi_{2n} | \mathcal{H} | \phi_{2m} \rangle + \beta_m \langle \phi_{2n} | \mathcal{H} | \phi_{2m+1} \rangle \\
&= \alpha_n \epsilon_0 + \beta_0 e^{i2nka} (-t(1-\eta)) + \beta_0 e^{i2(n-1)ka} (-t(1+\eta)) \\
\Rightarrow \epsilon_k \alpha_0 + \beta_0 [t(1-\eta) + t(1+\eta)e^{-i2ka}] &= 0
\end{aligned} \tag{39}$$

$$\begin{aligned}
\langle \phi_{2n+1} | \mathcal{H} | \Psi_k \rangle &= \epsilon_k \langle \phi_0 | \Psi_k \rangle = \epsilon_k e^{i2nka} \beta_0 \\
&= \sum_m \alpha_m \langle \phi_{2n+1} | \mathcal{H} | \phi_{2m} \rangle + \beta_m \langle \phi_{2n+1} | \mathcal{H} | \phi_{2m+1} \rangle \\
&= \alpha_0 e^{i2nka} (-t(1-\eta)) + \alpha_0 e^{i2(n+1)ka} (-t(1+\eta)) + \beta_n \epsilon_0 \\
\Rightarrow \epsilon_k \beta_0 + \alpha_0 [t(1-\eta) + t(1+\eta)e^{i2ka}] &= 0
\end{aligned} \tag{40}$$

We can thus write :

$$\begin{aligned}
&\begin{bmatrix} \epsilon_k & [t(1-\eta) + t(1+\eta)e^{-i2ka}] \\ [t(1-\eta) + t(1+\eta)e^{i2ka}] & \epsilon_k \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\
\Rightarrow \epsilon_k^2 - t^2 [(1-\eta) + (1+\eta)e^{-i2ka}] [(1-\eta) + (1+\eta)e^{i2ka}] &= 0 \\
\Rightarrow \epsilon_k^2 - t^2 [(1-\eta)e^{ika} + (1+\eta)e^{-ika}] [(1-\eta)e^{-ika} + (1+\eta)e^{ika}] &= 0 \\
\Rightarrow \epsilon_k^2 - t^2 [2\cos(ka) + 2i\eta\sin(ka)] [2\cos(ka) - 2i\eta\sin(ka)] &= 0 \\
\Rightarrow \epsilon_k^\pm \underset{k \rightarrow 0}{=} \pm 2t \sqrt{\cos^2(ka) + \eta^2 \sin^2(ka)} &
\end{aligned} \tag{41}$$

To plot it, we can see that  $\epsilon^+(k=0) = 2t$ ,  $\epsilon^-(k=0) = -2t$ ,  $\epsilon^+(k = \frac{2\pi}{a}) = 2t\eta$ ,  $\epsilon^-(k = \frac{2\pi}{a}) = -2t\eta$ .

Also  $\epsilon^\pm = \pm 2t \left[ 1 - \frac{1}{2} k^2 a^2 \right]$ . The plot is represented in Fig. 16.

4. If only one electron occupy each atomic orbital, the the band is half filled : the last occupied state is at  $\epsilon = -2t\eta$ . The system is thus an insulator.

5. Let's calculate the DOS :

- Volume occupied by 1 state in the k-space :  $V_k = \frac{2\pi}{L_x}$

- Number of electron states in this volume :  $g_{1D}(k)V_k = 2^{\uparrow\downarrow} : g_{1D}(k) = \frac{L_x}{\pi}$

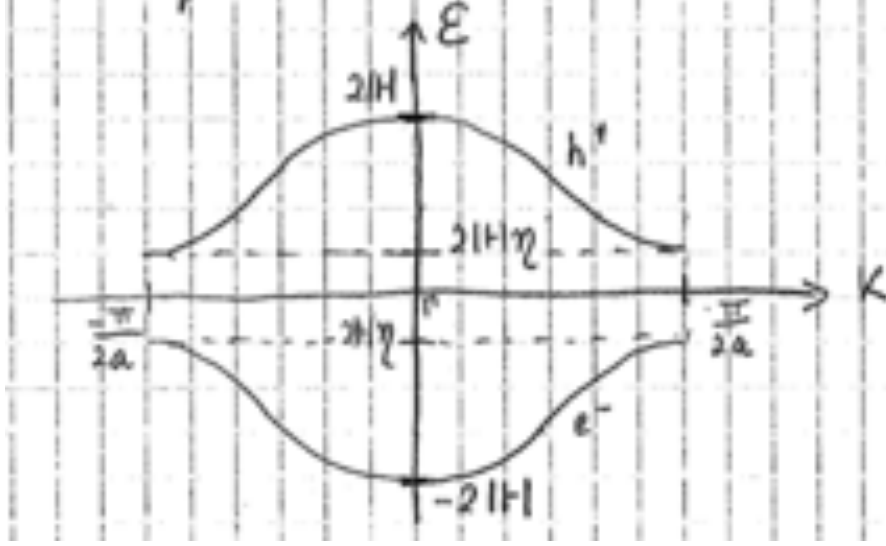


FIGURE 16 –

$$\begin{aligned}
E_1 &= \int_{-k_F}^{k_F} \epsilon_k g_{1D}(k) dk \\
&= \frac{L_x}{\pi} \int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} -2t \sqrt{\cos^2(ka) + \eta^2 \sin^2(ka)} dk \\
&= -\frac{4tL_x}{\pi} \int_0^{\frac{\pi}{2a}} \sqrt{\cos^2(ka) + \eta^2 \sin^2(ka)} dk \\
&= -\frac{4tL_x}{\pi} \int_0^{\frac{\pi}{2a}} \sqrt{1 + (\eta^2 - 1) \sin^2(ka)} dk \\
&= -\frac{4tL_x}{\pi} \int_0^{\frac{\pi}{2}} \sqrt{1 + (\eta^2 - 1) \sin^2(x)} dx \\
&= -\frac{a\pi}{4tL_x} \left[ 1 + \frac{\eta^2}{2} \left( \ln\left(\frac{4}{\eta}\right) - \frac{1}{2} \right) \right]
\end{aligned} \tag{42}$$

6.  $E_1 - E_0 = E_1 - E_1(\eta = 0) = -\frac{2tL_x\eta^2}{a\pi} \left[ \ln\left(\frac{4}{\eta}\right) - \frac{1}{2} \right]$ . This is favorable when  $E_1 - E_0 < 0$ , thus when  $\eta < 4e^{\frac{1}{2}}$
7. Conductivity perpendicular to the chains is 5 order of magnitude weaker than along the chains : we can consider this system as 1D.  $d_{z^2}$  orbitals have a weak overlap. Above 150K, the thermal agitation is greater than the energy gain, and below 150K, the gap opens and KCP becomes insulating.

### 4.3 Square lattice in 2D

1. From Bloch theorem we know

$$\begin{aligned}
\Psi(x+a, y) &= u(x, y) e^{ik_x a} \Psi(x, y) \\
&= \sum_{m,n} c_{m,n} \phi_{m,n}(x+a, y) \\
&= \sum_{m,n} c_{m,n} \phi_{m-1,n}(x, y) \\
&= \sum_{m'=-m-1}^{m'+1} c_{m'+1,n} \phi_{m',n}(x, y)
\end{aligned} \tag{43}$$

Thus  $c_{m+1,n} = c_{m,n} e^{ik_x a} \Rightarrow c_{m,n} = c_{0,n} e^{imk_x a}$ . By extension :  $c_{m,n} = c_{0,0} e^{i(mk_x a + nk_y a)}$

2. Voir Fig. 17

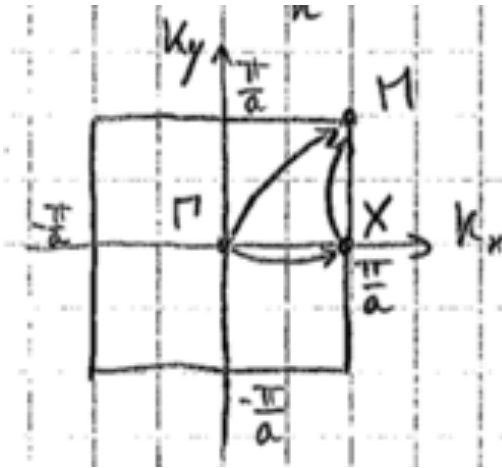


FIGURE 17 -

3.

$$\begin{aligned}
 \langle \phi_{\alpha,\beta} | \mathcal{H} | \Psi_k \rangle &= \epsilon_k \langle \phi_{\alpha,\beta} | \Psi_k \rangle = \epsilon_k e^{i(\alpha k_x + \beta k_y)} c_{0,0} \\
 &= \sum_{m,n} c_{0,0} e^{i(m k_x + n k_y)} \langle \phi_{\alpha,\beta} | \mathcal{H} | \phi_{m,n} \rangle \\
 &= c_{0,0} e^{i\alpha(\alpha k_x + \beta k_y)} \epsilon_0 + c_{0,0} e^{i\alpha((\alpha-1)k_x + \beta k_y)} (-t) + c_{0,0} e^{i\alpha((\alpha+1)k_x + \beta k_y)} (-t) \\
 &\quad + c_{0,0} e^{i\alpha(\alpha k_x + (\beta-1)k_y)} (-t) + c_{0,0} e^{i\alpha(\alpha k_x + (\beta+1)k_y)} (-t) \\
 &= c_{0,0} e^{i(\alpha k_x + \beta k_y)} [e^{i\alpha k_x} + e^{-i\alpha k_x} + e^{i\alpha k_y} + e^{-i\alpha k_y}] \\
 \Rightarrow \epsilon_k &= -2t [\cos(k_x a) + \cos(k_y a)]
 \end{aligned} \tag{44}$$

The bandwidth is  $8t$  (see Fig 18).

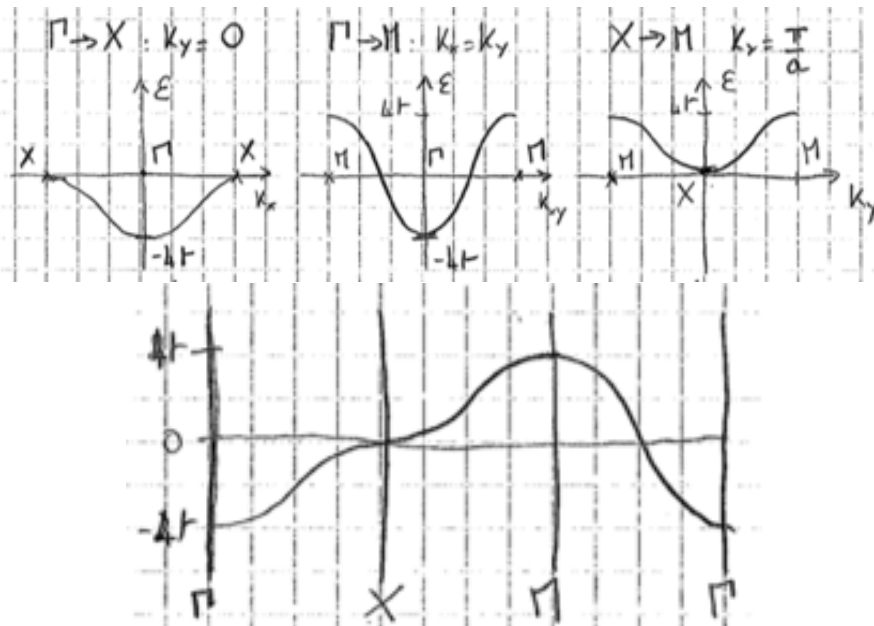


FIGURE 18 -

4. See Fig 19

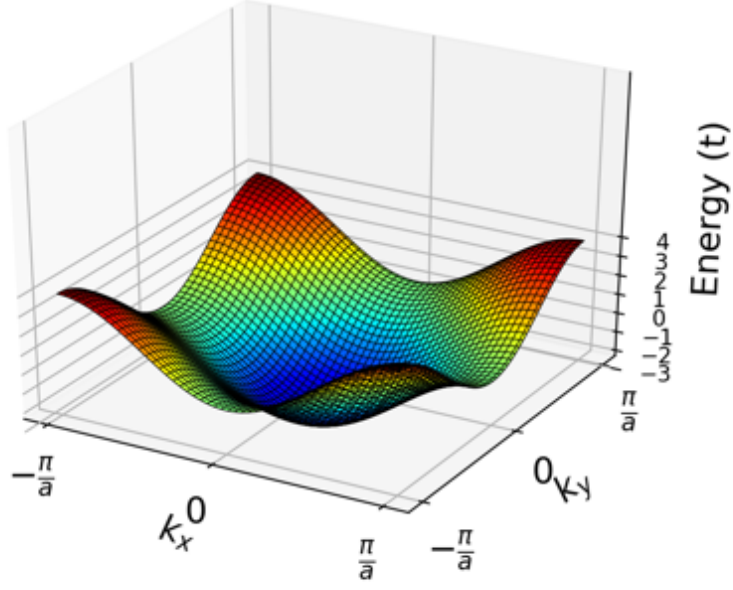


FIGURE 19 –

5. • The band minimum is at  $k_x = k_y = 0$ .

$$\begin{aligned}
 m^*(0,0) &= \hbar^2 \left[ \frac{\partial^2 \epsilon}{\partial k^2} \right]_{k_x \rightarrow 0, k_y = 0}^{-1} \\
 &= \hbar^2 \left[ \frac{\partial^2 (-2t(\cos(k_x a) + 1))}{\partial k^2} \right]_{k_x \rightarrow 0, k_y = 0}^{-1} \\
 &= \hbar^2 [2ta^2 \cos(k_x a)]_{k_x \rightarrow 0, k_y = 0}^{-1} \\
 &= \frac{\hbar^2}{2ta^2}
 \end{aligned} \tag{45}$$

Since the mass is positive, this is considered as an electron.

For the density of state, we know that  $g_{2D}(k) = \frac{S}{2\pi^2}$ .

$$\begin{aligned}
 \epsilon(k) &\underset{k \rightarrow 0}{=} -2t \left[ 2 - \frac{1}{2}k_x^2 a^2 - \frac{1}{2}k_y^2 a^2 \right] \\
 &\underset{k \rightarrow 0}{=} -4t + ta^2 [k_x^2 + k_y^2] \\
 \frac{d\epsilon}{dk} &\underset{k \rightarrow 0}{=} -2ta^2 k \\
 g_{2D}(\epsilon) &\underset{k \rightarrow 0}{=} g_{2D}(k) 2\pi k \frac{dk}{d\epsilon} \\
 &= \frac{S}{2\pi ta^2} \\
 &\underset{k \rightarrow 0}{=} \frac{S}{\pi \hbar^2} m^*(0,0)
 \end{aligned} \tag{46}$$

- The band maximum at  $k_x = k_y = \frac{\pi}{a}$ .

$$\begin{aligned}
m^*\left(\frac{\pi}{a}, \frac{\pi}{a}\right) &= \hbar^2 \left[ \frac{\partial^2 \epsilon}{\partial k^2} \right]_{k_x \rightarrow \frac{\pi}{a}, k_y = \frac{\pi}{a}}^{-1} \\
&= \hbar^2 \left[ \frac{\partial^2 (-2t(\cos(k_x a) + 1))}{\partial k^2} \right]_{k_x \rightarrow \frac{\pi}{a}, k_y = \frac{\pi}{a}}^{-1} \\
&= \hbar^2 [2ta^2 \cos(k_x a)]_{k_x \rightarrow \frac{\pi}{a}, k_y = \frac{\pi}{a}}^{-1} \\
&= \frac{\hbar^2}{2ta^2}
\end{aligned} \tag{47}$$

Since the mass is negative, this is considered as a hole.

For the density of state, we know that  $g_{2D}(k) = \frac{S}{2\pi^2}$ .

$$\begin{aligned}
\epsilon(k) &\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} -2t \left[ \cos\left(\left(\frac{\pi}{a} + (k_x - \frac{\pi}{a})\right)a\right) + \cos\left(\left(\frac{\pi}{a} + (k_y - \frac{\pi}{a})\right)a\right) \right] \\
&\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} -2t \left[ -\cos\left((k_x - \frac{\pi}{a})a\right) - \cos\left((k_y - \frac{\pi}{a})a\right) \right] \\
&\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} 2t \left[ 2 - \frac{1}{2}(k_x - \frac{\pi}{a})^2 a^2 - \frac{1}{2}(k_y - \frac{\pi}{a})^2 a^2 \right] \\
&\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} 4t - ta^2 \left[ (k_x - \frac{\pi}{a})^2 + (k_y - \frac{\pi}{a})^2 \right] \\
\frac{d\epsilon}{dk} &\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} -2ta^2(k_x - \frac{\pi}{a}) \\
g_{2D}(\epsilon) &\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} g_{2D}(k) 2\pi k \frac{dk}{d\epsilon} \\
&\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} \frac{S}{2\pi ta^2} \\
&\underset{k, k_y \rightarrow \frac{\pi}{a}}{=} \frac{S}{\pi \hbar^2} m^*\left(\frac{\pi}{a}, \frac{\pi}{a}\right)
\end{aligned} \tag{48}$$

6. The function  $g(\epsilon) = \frac{2}{\pi} g_0 \ln(\text{rac}16t\epsilon)$  is plotted in Fig 19. We can observe a singularity for  $\epsilon = 0$  : it is the Van Hove singularity, present because of the saddle point in the dispersion.

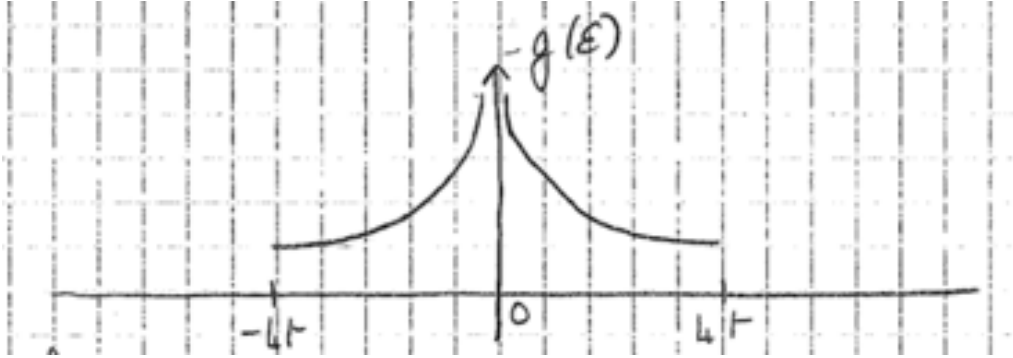


FIGURE 20 –

7. If the atoms are monovalent, 1 electron occupy the surface  $S = a^2$ . So  $1 = \int_0^{k_f} g_{2D}(k) dS_k = \frac{S}{2\pi^2} S_F = \frac{a^2}{2\pi^2} S_F$ . Then Fermi surface  $S_F = \frac{\pi^2}{2a^2} = \left(\frac{\pi}{\sqrt{2}a}\right)^2$ . So the surface is a square of side  $\frac{\pi}{\sqrt{2}a}$  : this correspond to the Fermi surface for  $\epsilon = 0$ , exactly on the Van Hove singularity.
8. In this case, the cuprate fall in the example treated before : it should be metallic. However in reality, this is an insulator, due to the Coulombic repulsion, preventing double occupation of on site, creating a gap.

## 5 Semiconductors

### 5.1 Resistivity of intrinsic semiconductors

- $n_i^2(T) = n_c(T)n_h(T) = N_c N_h e^{-\beta(\epsilon_c - \epsilon_v)} = N_c N_h e^{-\beta\epsilon_g}$
  - $n_i(T) = \sqrt{N_c N_h} e^{-\beta\frac{\epsilon_g}{2}}$  and  $n_i(T) = N_c e^{-\beta(\epsilon_c - \mu)}$  so  $\mu = \frac{\epsilon_g}{2} + \frac{k_B T}{2} \ln\left(\frac{N_h}{N_c}\right)$
1.  $n_i^{Ge} = \sqrt{n_c n_h} = \sqrt{N_c N_h} e^{-\beta\frac{\epsilon_g}{2}} = N_0 \sqrt{\left(\frac{m_c m_h}{m_e^2}\right)^{\frac{3}{2}} e^{-\beta\epsilon_g}} = 2.4e25 \sqrt{(0.55 * 0.29)^{\frac{3}{2}} e^{-0.67/0.025}} = 9e18 e^{-.m^{-3}} = 9 \cdot 10^{12} e^{-.cm^{-3}}$ . For Cu (1 electron per  $\text{\AA}^3$  for the order of magnitude) :  $n^{Cu} = 8.5 \cdot 10^{28} e^{-.m^{-3}} = 8.5 \cdot 10^{22} e^{-.cm^{-3}}$
  2.  $\sigma^{Ge} = n^{Ge} \mu^{Ge} e = n_c^{Ge} \mu_e^{Ge} e + n_h^{Ge} \mu_h^{Ge} e = n_i^{Ge} e (\mu_e^{Ge} + \mu_h^{Ge}) = 0.8 C.V^{-1}.s^{-1}.m^{-1} = 0.8 \Omega^{-1}.m^{-1}$ . For Cu :  $\sigma^{Cu} = n^{Cu} \mu^{Cu} e = 6 \cdot 10^7 C.V^{-1}.s^{-1}.m^{-1} = 6 \cdot 10^7 \Omega^{-1}.m^{-1}$   
Germanium is then a bad conductor.
  3.  $\sigma^{Ge} \propto n_i^{Ge} \mu^{Ge} \propto \beta^{-\frac{3}{2}} e^{-\beta\frac{\epsilon_g}{2}} T^{-\frac{3}{2}} \propto e^{-\beta\frac{\epsilon_g}{2}}$  and  $\rho^{Ge} \propto e^{\beta\frac{\epsilon_g}{2}}$ . For small value of  $\beta$  (large T), resistivity is linear in  $\beta$ . It explains the curve 1. To extract the gap, we need to plot  $\log(\rho)$  as function of  $T^{-1}$  and the slope will be  $\frac{\epsilon_g}{2k_B}$ .

### 5.2 Resistivity of extrinsic semiconductors

1. See Fig. [21](#)

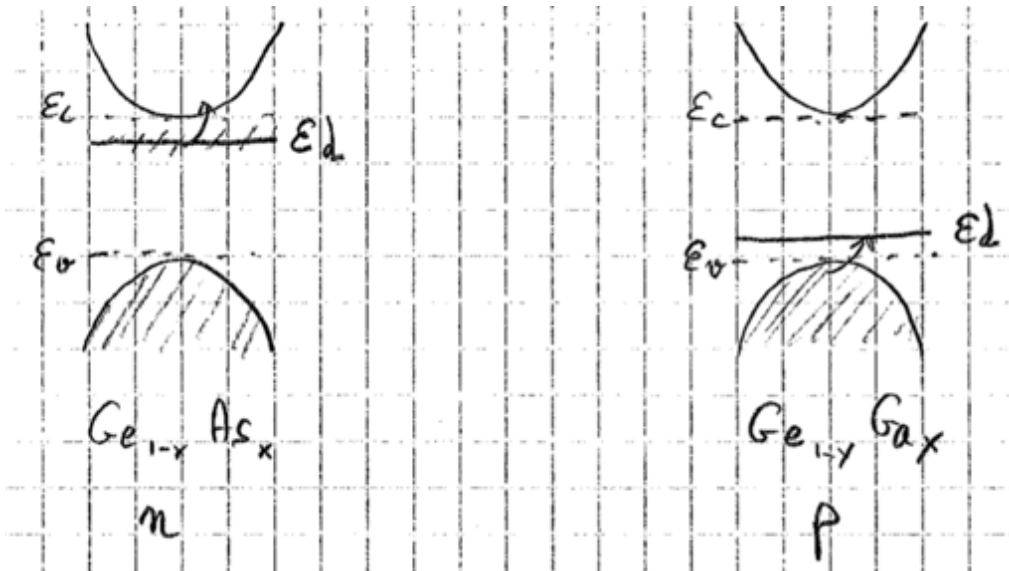


FIGURE 21 –

2. Ga atoms give holes (take electrons) and Sb or As gives electrons. See Fig. [22](#)
3. For n type :  $n_c(T) = n_i(T) + n_d(T) = n_h(T) + n_d(T) \underset{n_d \gg n_h}{=} n_d$   
For p type :  $n_h(T) = n_i(T) + n_a(T) = n_c(T) + n_a(T) \underset{n_a \gg n_c}{=} n_a$
4.  $k_B T \gg \epsilon_c - \epsilon_d \Rightarrow n_d(T) = N_d$  : totally ionized.  
 $k_B T \ll \epsilon_g \Rightarrow n_d \gg n_h$   
So we find :  $\sigma \propto N_d e \mu \propto N_d T^{\frac{3}{2}}$  and thus,  $\ln(\rho) \propto \ln(\beta)$
5. See Fig. [23](#)
6. For doped Ge, we can see that the slope changes at a certain temperature, corresponding to a change from intrinsic to extrinsic behavior, when  $k_B T$  reaches  $\epsilon_g/2$ .

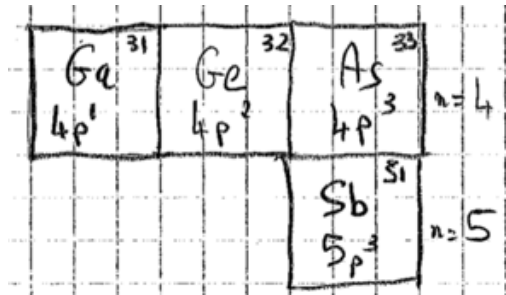


FIGURE 22 -

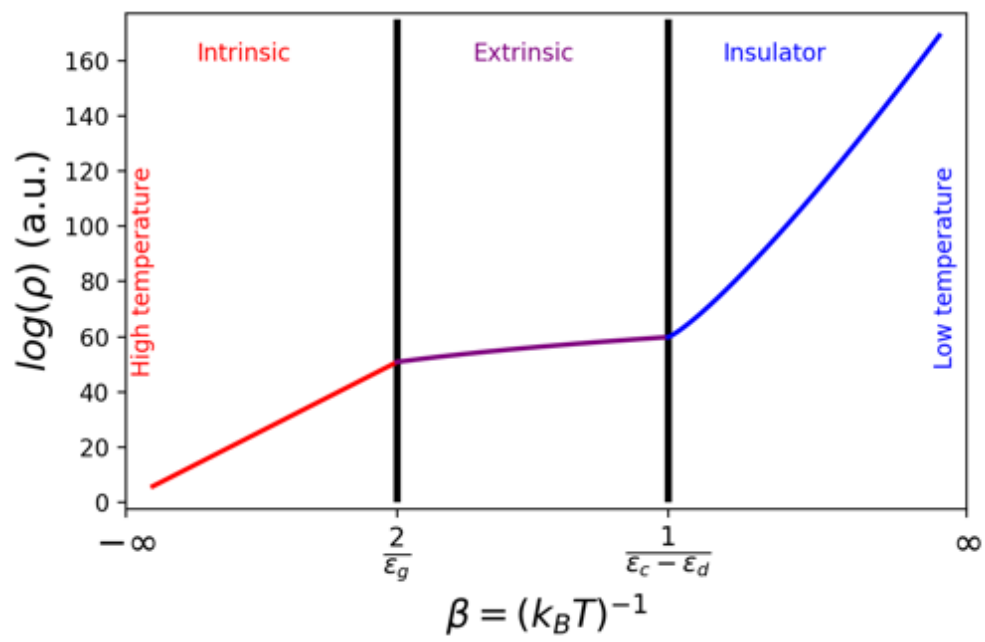


FIGURE 23 -



### 5.3 p-n junctions

1. Electron from the conduction band of the  $p$  side close to the junction will naturally go to the  $n$  region since the conduction band there is lower in energy (first principle : minimization of energy). Symmetrically, holes in the valence band of the  $n$  side will go to the  $p$  side. Thus in the region between, no charge carrier remains : they either go to the  $n$  region (electrons) or the  $p$  region (holes). This region is then depleted and called depletion region.
2. An equivalent model to driving negative charges (electrons) on the right  $n$  region, and positive charges (holes) on the left  $p$  region is to put an electric field so the charges undergo the force  $\vec{F} = q\vec{E}$ . The electric field goes then from  $n$  to the  $p$  region. We can consider that the electric field originates from a potential difference  $V_d$  such as  $\vec{E} = -\nabla V_d$ , with  $V_d = V^n - V^p > 0$ .

3. Thermal scattering :

- electrons ( $e^-$ ) go from  $\epsilon_c^n$  to  $\epsilon_c^p$
- holes ( $h^+$ ) go from  $\epsilon_v^p$  to  $\epsilon_v^n$

Conduction :

- electrons ( $e^-$ ) go from  $\epsilon_c^p$  to  $\epsilon_c^n$
- holes ( $h^+$ ) go from  $\epsilon_v^n$  to  $\epsilon_v^p$

At equilibrium,  $I_{Total}^0 = 0 \Rightarrow I_{P \rightarrow N}^0 + I_{N \rightarrow P}^0 = 0 \Rightarrow I_{P \rightarrow N}^0 = -I_{N \rightarrow P}^0 = I_0 e^{-\frac{eV_d}{k_B T}}$

4. By applying an external tension  $U$ , we modify the potential difference  $V_d$ . The new potential difference is then :  $V' = V_d - U$ . We can thus write :

$$I_{P \rightarrow N} = I_0 e^{-\frac{eV'}{k_B T}} = I_0 e^{-\frac{eV_d}{k_B T}} e^{\frac{eU}{k_B T}} = I_{P \rightarrow N}^0 e^{\frac{eU}{k_B T}}$$

$I_{Total} = I_{P \rightarrow N} + I_{N \rightarrow P} = I_{P \rightarrow N}^0 e^{\frac{eU}{k_B T}} + I_{N \rightarrow P}^0 = I_{P \rightarrow N}^0 \left( e^{\frac{eU}{k_B T}} - 1 \right)$ . The plot Fig. 24 show the current (in unit of  $I_0$ ) as function of  $U$  (in mV) at room temperature. We see that the current is measurable only for positive tension  $U$  : this is the behavior of a diode.

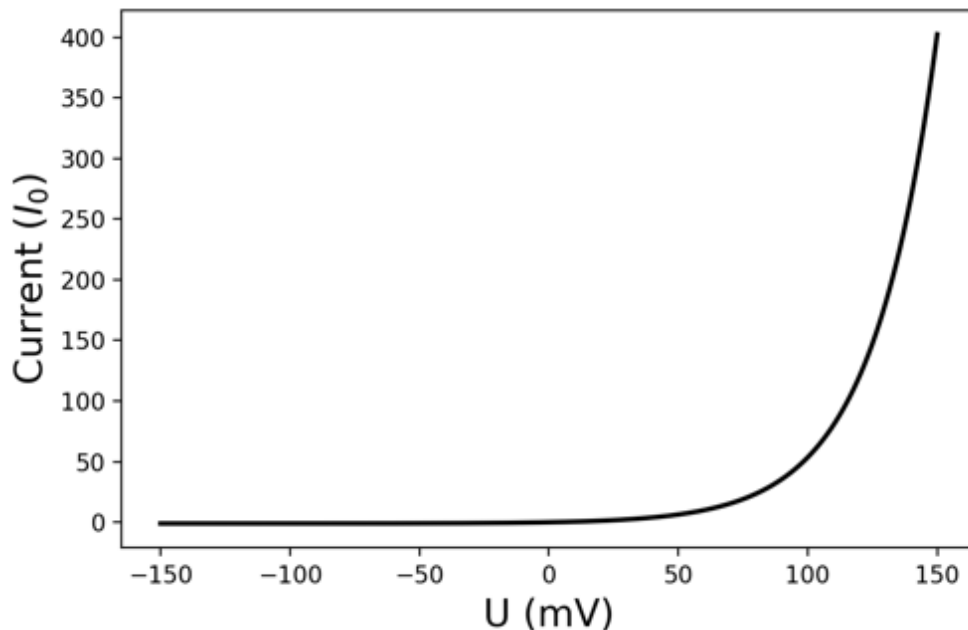


FIGURE 24 –

## 6 Superconductivity

### 6.1 Thermodynamics

To be completed...

**6.1.1 Magnetic field driven transition at  $T=0$**

To be completed...

**6.1.2 H-T phase diagram**

To be completed...

**6.1.3 Specific heat**

To be completed...

**6.2 Magnetic field penetration into a type-I superconducting plate**

To be completed...