

# Solid State Physics - Homework

Rachele Cicioni  
mat. 2057053

Academic Year 2021-2022

## Homework 1

a) The primitive vectors of the crystal are:

$$\vec{a}_1 = a \left( -\frac{\sqrt{3}}{2} \hat{i} - \frac{1}{2} \hat{j} \right)$$

$$\vec{a}_2 = a \hat{j}$$

$$\vec{a}_3 = c \hat{k}$$

Since  $|\vec{a}_1| = |\vec{a}_2|$  and the angle between the vectors  $\vec{a}_1$  and  $\vec{a}_2$  is  $120^\circ$ , the lattice of the crystal is an hexagonal Bravais lattice.

b) The volume of the primitive cell can be calculated by the formula:

$$V = |\vec{a}_1 \cdot (\vec{a}_2 \wedge \vec{a}_3)| = |\vec{a}_1 \cdot \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & a & 0 \\ 0 & 0 & c \end{vmatrix}| = \frac{\sqrt{3}}{2} a^2 c$$

c) The primitive vectors of the reciprocal space are:

$$\vec{b}_1 = \frac{2\pi}{V} (\vec{a}_2 \wedge \vec{a}_3) = \frac{2\pi}{V} \cdot (ac \hat{i}) = \frac{4\pi}{\sqrt{3}a} \hat{i}$$

$$\vec{b}_2 = \frac{2\pi}{V} (\vec{a}_3 \wedge \vec{a}_1) = \frac{2\pi}{V} \cdot \left( \frac{1}{2} ac \hat{i} - \frac{\sqrt{3}}{2} ac \hat{j} \right) = \frac{2\pi}{a} \left( \frac{\hat{i}}{\sqrt{3}} - \hat{j} \right) = \frac{4\pi}{\sqrt{3}a} \left( \frac{1}{2} \hat{i} - \frac{\sqrt{3}}{2} \hat{j} \right)$$

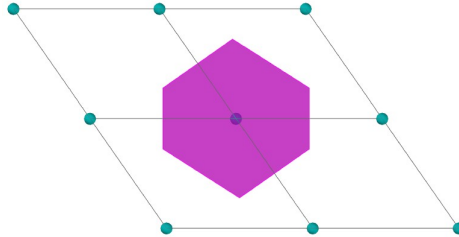
$$\vec{b}_3 = \frac{2\pi}{V} (\vec{a}_1 \wedge \vec{a}_2) = \frac{2\pi}{V} \cdot \left( -\frac{\sqrt{3}}{2} a^2 \hat{k} \right) = -\frac{2\pi}{c} \hat{k}$$

d) The Bravais lattice of the reciprocal lattice of the hexagonal Bravais lattice is also an hexagonal. To prove this in our case, we note that:

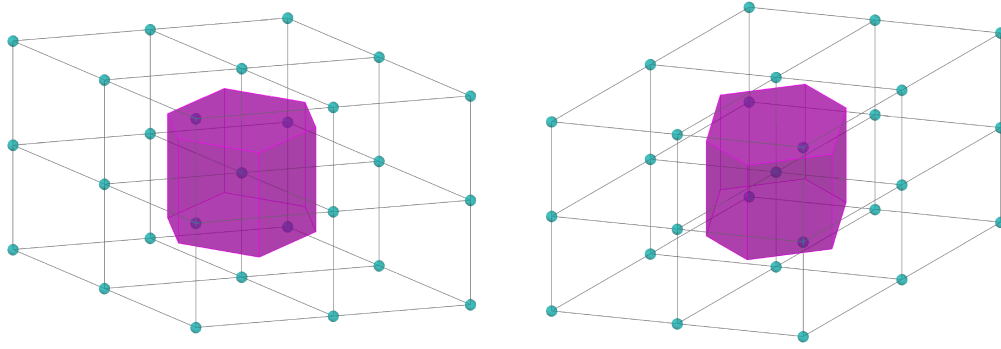
$$|\vec{b}_1| = |\vec{b}_2| = \frac{4\pi}{\sqrt{3}a}$$

and the angle between  $\vec{b}_1$  and  $\vec{b}_2$  is  $60^\circ$ .

e) The first Brillouin zone of the lattice is a prism with the base shown in **Figure 1**. The **Figure 2** shows the first Brillouin zone from different angles.



**Figure 1:** Projection of the first Brillouin zone along the axis xy.



**Figure 2:** First Brillouin zone of the reciprocal lattice.

f) Now let's consider a Si crystal with such structure, with  $a = 2\text{\AA}$  and  $c = 2.5\text{\AA}$ . Since the atomic weight of Si is  $A=28.1$ , the weight of an atom of Silicon is:

$$m = 28.1 \cdot 1.66 \cdot 10^{-24} g = 46.65 \cdot 10^{-24} g$$

The volume occupied by a single atom is the volume found in point (b) to which we substitute the values  $a$  and  $c$ :

$$V = \frac{\sqrt{3}}{2} a^2 c = 8.66 \text{\AA}^3 = 8.66 \cdot 10^{-24} \text{cm}^3$$

With the volume and the mass it's possible to compute the density of Silicon:

$$\rho = \frac{m}{V} = 5.39 g/\text{cm}^3$$

## Homework 2

a) The two atoms of Argon are neutral atoms since Argon is a rare gas. The potential that describes the interaction between a pair of Argon atoms is the Lennard-Jones potential.

$$V_{LJ} = 4E_b \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] = \frac{a}{r^{12}} - \frac{b}{r^6}$$

where:

$$a = 4E_b \sigma^{12}$$

$$b = 4E_b \sigma^6$$

The value of  $\sigma$  is obtained from the equilibrium condition

$$\left. \frac{dV}{dr} \right|_{r=r_0} = 0$$

and considering that the value of the potential  $V(r) \Big|_{r=r_0}$  is the binding energy  $E_b$ .

From these considerations  $\sigma$  is:

$$\sigma = \frac{r_0}{2^{\frac{1}{6}}} = 3.34 \cdot 10^{-10} m = 3.34 \text{\AA}$$

The value of  $a$  and  $b$  are:

$$a = 4E_b\sigma^{12} = 1.18 \cdot 10^9 K \text{\AA}^{12}$$

$$b = 4E_b\sigma^6 = 8.45 \cdot 10^5 K \text{\AA}^6$$

b) Now we consider a linear chain on  $N$  atoms of Ar with a distance  $R$  from each other like in **Figure 3**.



**Figure 3:** Linear chain of  $N$  atoms.

The Lennard-Jones potential  $V(r)$  represents the energy of an atom, given its distance  $r$  from another atom. For a linear chain the total energy is the sum of the energies of each atom.

$$U(r) = \frac{1}{2} \sum_{i=1}^N V_i(r) = \frac{N}{2} V(r)$$

The factor  $\frac{1}{2}$  avoids the double counts. The term  $V(r)$  is energy of a single atom which is the same for each atom in the limit  $N \rightarrow \infty$ . In a linear chain of Argon, the energy  $V(r)$  is given by the Lennard-Jones potential:

$$\begin{aligned} V(r) &= 2 \left[ \frac{a}{R^{12}} - \frac{b}{R^6} + \frac{a}{(2R)^{12}} - \frac{b}{(2R)^6} + \frac{a}{(3R)^{12}} - \frac{b}{(3R)^6} + \dots \right] \\ &= \frac{2a}{R^{12}} \left( 1 + \frac{1}{2^{12}} + \frac{1}{3^{12}} + \dots \right) - \frac{2b}{R^6} \left( 1 + \frac{1}{2^6} + \frac{1}{3^6} + \dots \right) \\ &= \frac{2a}{R^{12}} \left( \sum_{i=1}^N \frac{1}{i^{12}} \right) - \frac{2b}{R^6} \left( \sum_{i=1}^N \frac{1}{i^6} \right) \end{aligned}$$

For  $N \rightarrow \infty$ , the energy  $V(r)$  becomes:

$$V(r) = \frac{2a}{R^{12}} - 1.017 \frac{2b}{R^6}$$

And so the total energy of a linear chain of  $N$  atoms of Argon is:

$$U(R) = N \left[ \frac{a}{R^{12}} - 1.017 \frac{b}{R^6} \right]$$

c) For the equilibrium value of the lattice constant  $R_0$  it is necessary to calculate the derivative of the energy  $U(R)$  and set it equal to 0.

$$\frac{d}{dR} \left( N \left[ \frac{a}{R^{12}} - 1.017 \frac{b}{R^6} \right] \right) = \frac{-12aN}{R^{13}} + \frac{1.017 \cdot 6bN}{R^7} = 0$$

$$R_0 = \sqrt[6]{\frac{2a}{1.017b}}$$

From the value  $R_0$  we can obtain the cohesive energy, i.e. the total energy  $U(r)$  evaluated in  $R_0$  divided by the number of atoms  $N$ :

$$\frac{U(R_0)}{N} = \frac{a}{R_0^{12}} - 1.017 \frac{b}{R_0^6} = -\frac{\gamma^2 b^2}{4a}$$

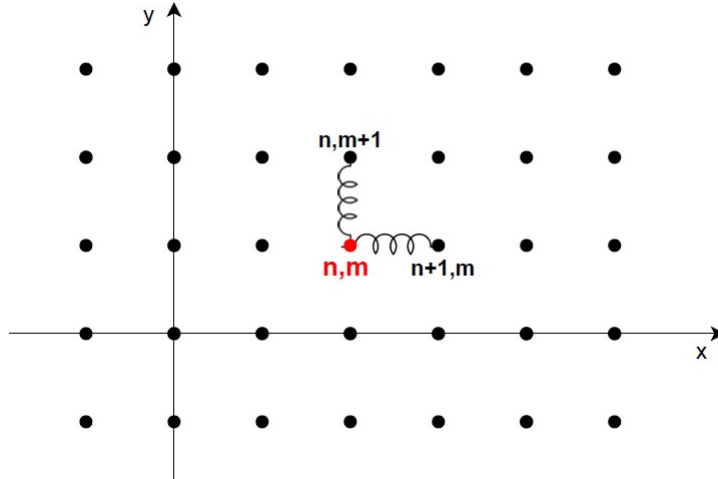
where  $\gamma=1.017$ .

d) The compressibility  $K$  of the crystal is:

$$K = \left[ L \left( \frac{d^2 U}{dL^2} \right) \right]^{-1} = \left[ \frac{R}{N} \frac{d^2 U}{dR^2} \right]^{-1} = \left[ \frac{6(26a - 7\gamma b R^6)}{R^{13}} \right]^{-1}$$

### Homework 3

a) We have a two-dimensional monoatomic crystal in a square Bravais lattice. The **Figure 4** schematically shows the interactions that will be considered, i.e. an harmonic interaction between the nearest-neighbour.



**Figure 4:** Square lattice with harmonic interactions.

The equation of motion to solve is:

$$M \frac{d^2 u_{n,m}(x, y)}{dt^2} = - \frac{\partial U_{n,m}}{\partial u_{n,m}}$$

The potential energy  $U_{n,m}$  for the  $(n, m)$ -atom is:

$$\begin{aligned} U_{nm} &= \frac{\tilde{K}}{2} [(u_{n,m} - u_{n+1,m})^2 + (u_{n-1,m} - u_{n,m})^2 + (u_{n,m} - u_{n,m+1})^2 + (u_{n,m-1} - u_{n,m})^2] \\ &= \tilde{K} (u_{n+1,m} - 2u_{n,m} + u_{n-1,m} + u_{n,m+1} - 2u_{n,m} + u_{n,m-1}) \end{aligned}$$

For the solution  $u_{n,m}$  we can consider a plane wave:

$$u_{n,m} = \varepsilon_{nm} e^{i(k_x n a + k_y m a - \omega t)}$$

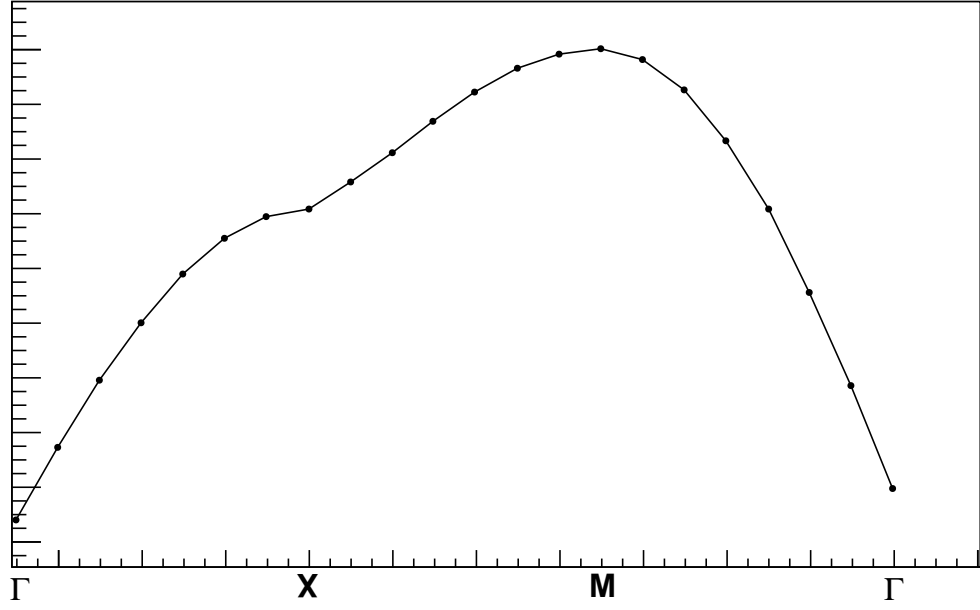
Replacing it in the equation of motion we have:

$$M \omega^2 u_{n,m} = u_{n,m} \tilde{K} (4 - 2 \cos k_x a - 2 \cos k_y a)$$

And therefore the dispersion relation is:

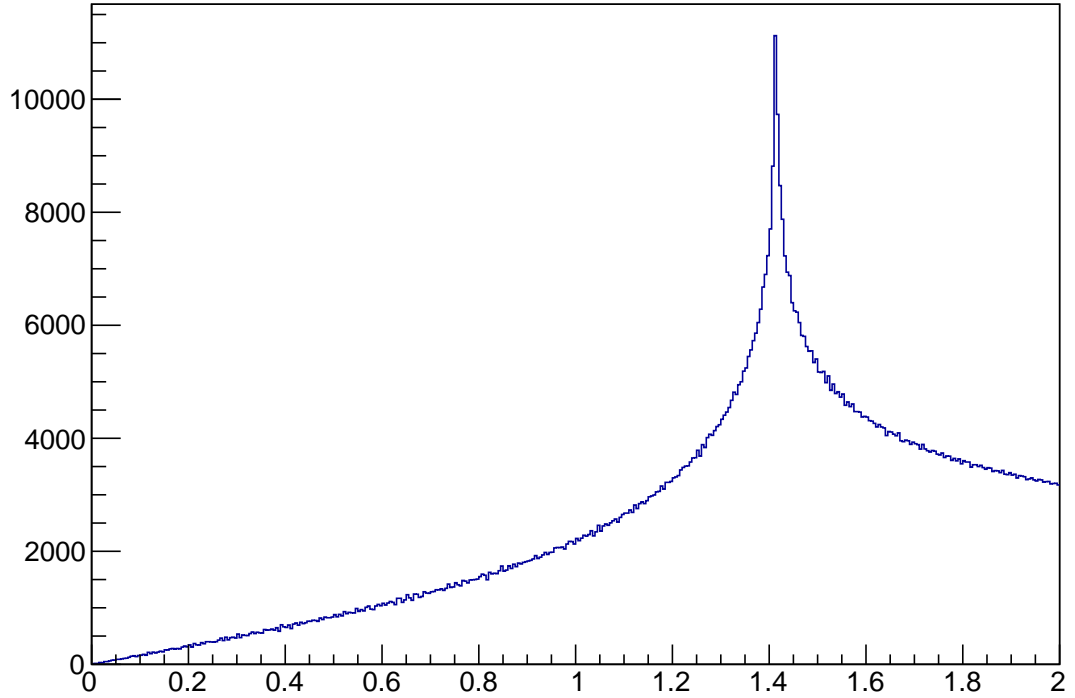
$$\omega(k_x, k_y) = \sqrt{\frac{2\tilde{K}}{M} \left( 2 - \cos k_x a - \cos k_y a \right)}$$

b) We can plot the dispersion relation  $\omega(k_x, k_y)$  along a path  $\Gamma - X - M - \Gamma$ . For this plot of  $\omega(k_x, k_y)$  we calculate the value of  $\omega(k_x, k_y)$  at several points along the path and insert the obtained values into a graph. The resulting plot is shown in **Figure 5**.



**Figure 5:** Plot 1-dim of  $\omega(k_x, k_y)$ .

c) To Obtaining the vibrational density of states  $D(\omega)$ , several values of  $\omega(k_x, k_y)$  are calculated in many  $(k_x, k_y)$  points (in this case 1000000 points) and the values obtained are inserted in a histogram. The density of the vibrational states obtained is shown in the **Figure 6**.



**Figure 6:** Vibrational density of states  $D(\omega)$

## Homework 4

a) The number of normal modes for a given value of the wavevector  $k$  are  $= D \cdot M$ , where  $D$  is the dimension and  $M$  is the number of atoms per cell. In this case  $D = 2$ ,  $M = 1$ . So, the total number of normal modes for a given value of  $k$  are two. These are both acoustic modes, one transverse and one longitudinal.

b) With the Debye approximation we can consider  $\omega = kv_s$ . For the density of states, the volume element  $\frac{L^3}{(2\pi)^3}$  of the three-dimensional case becomes a surface element  $\frac{L^2}{(2\pi)^2}$ .

$$D(\omega) = \frac{L^2}{(2\pi)^2} \frac{1}{v_s} \int_{circ} dl = \frac{L^2}{2\pi} \frac{k}{v_s} = \frac{L^2}{2\pi} \frac{\omega}{v_s^2}$$

c) The Debye frequency  $\omega_D$  is obtaining considering that the total number of normal modes are equal to the sum of the number of modes of the integral of the density of the states:

$$2N = \sum_s \int_0^{\omega_D} D(\omega) d\omega = \frac{L^2}{2\pi} \frac{2}{v^2} \frac{\omega_D^2}{2}$$

$$\omega_D = \sqrt{\frac{4\pi N v^2}{L^2}}$$

In the calculation, it was considered:

$$\sum_s \frac{1}{v_s^2} = \frac{1}{v_T^2} + \frac{1}{v_L^2} = \frac{2}{v^2}$$

where  $v$  is the sound velocity. The value of the Debye temperature  $T_D$  is:

$$T_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar}{k_B} \sqrt{\frac{4\pi N v^2}{L^2}} \simeq 90K$$

d) The heat capacity  $C_v$ , considering the Debye approximation for  $D(\omega)$ , is:

$$\begin{aligned} C_v &= \frac{d}{dT} \left[ \sum_s \int_0^{\omega_D} d\omega D(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \right] \\ &= \frac{d}{dT} \left[ \int_0^{\omega_D} d\omega \frac{L^2 \omega^2}{\pi v^2} \frac{\hbar}{e^{\hbar\omega/k_B T} - 1} \right] \\ &= \frac{d}{dT} \left[ \int_0^{T_D/T} \frac{L^2 k_B^3 T^3}{\pi v^2 \hbar^2} \frac{x^2}{e^x - 1} dx \right] \end{aligned}$$

where  $x \equiv \frac{\hbar\omega}{k_B T}$ . For  $T \ll T_D$  we can do an approximation:

$$\int_0^\infty \frac{x^2}{e^x - 1} dx = 2.404 \equiv \alpha$$

And so:

$$C_v = \frac{3L^2 k_B^3}{\pi v^2 \hbar^2} \alpha T^2$$

## Homework 5

a) In the *Fermi gas model* the Fermi energy  $E_F$  is:

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

where  $n$  is the number of electrons for unit of volume. The potassium has one valence electron, so the value of  $n$  can be calculate with the density  $\rho$  and the atomic number  $A$ , converted into kg. In this way we get the number of electrons per unit of volume.

$$n = \frac{\rho}{A} = 1.4 \cdot 10^{28} m^{-3}$$

Substituting this value in the previous equation we get:

$$E_F = 2.12eV$$

With the value of  $k_F$  it's possible to estimate even the Fermi velocity  $v_F$ :

$$v_F = \frac{\hbar k_F}{m} = 863513 m/s$$

b) It is possible to calculate the electronic contribution to the specific heat knowing the Fermi temperature  $T_F$ .

$$T_F = \frac{E_F}{k_B} = 24599K$$



Now, with the Fermi temperature, it's possible to calculate the heat capacity per unit of volume and unit of moles:

$$\frac{C_{el}}{Tn} = \frac{\pi^2}{2} \frac{k_B^2}{E_F} N_a = 1.67 mJ/(molK^2)$$

This value is a little bit different from  $2.08 mJ/(molK^2)$ , however these are of the same order of magnitude.

c) Equaling the expression of  $C_{el}$  with the expression of  $C_{lat}$  it's possible to obtain the expression of  $T$  for which the two contributions are comparable.

$$\frac{12}{5} \pi^4 N_a k_B \left( \frac{T}{T_D} \right)^3 = \frac{\pi^2}{2} \frac{k_B^2}{E_F} N_a T$$

$$T = \sqrt{\frac{5}{24\pi^2} \frac{T_D^3}{T_F}} = 0.79 K$$

d) From the value of the measured resistivity  $\rho$ , it's possible to evaluate the mean-free-path  $\lambda$  in this way:

$$\lambda \sim v_F \tau$$

where  $v_F$  is the Fermi energy and  $\tau$  is the scattering time. The value of  $\tau$  can be calculated with the experimental value of  $\rho$ .

$$\tau = \frac{m}{ne^2 \rho} = 3.52 \cdot 10^{-14} s$$

where  $m$  is the mass of electron,  $n$  the density of electrons and  $e$  the electronic charge. And so the mean-free-path is equal to:

$$\lambda = v_F \tau = 3.04 \cdot 10^2 \text{\AA}$$

We can compare the mean-free-path with the average electron-electron distance, that is:

$$d \simeq \frac{1}{n^{1/3}} = 4.15 \text{\AA}$$

So the relation between mean-free-path and  $d$  is  $\lambda \sim 100d$ .

## Homework 6

a) The possible energy levels for a two-dimensional square lattice, in the approximation of *free electrons*, are:

$$E(\vec{k}) = \frac{\hbar^2(\vec{k} - \vec{G})^2}{2m}$$

Since the energy bands are periodic in the reciprocal lattice, we can reduce to the first Brillouin zone. For the plot of the energy bands in the direction [11], we have that the components of  $\vec{k}$ ,  $k_x$  and  $k_y$  vary in the intervals  $[-\frac{\pi}{a}, \frac{\pi}{a}]$ . Expressing the energy in units of  $\frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$  and the vectors  $\vec{k}$  and  $\vec{G}$  in units of  $(\frac{2\pi}{a})$ , the first six energy bands are represented in **Figure 7**.

b) The Fermi energy is:

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

It is possible to express  $k_F$  as a function of the number of electrons per unit cell  $n_v$ , considering that  $n_v$  is the area of the Fermi circumference (the Fermi sphere of the three-dimensional case is, in this case, a circumference on the space  $(k_x, k_y)$  divided by the area of a unit cell in the reciprocal space, considering that in each cell of the reciprocal space we have two electrons of opposite spin.

$$n_v = 2 \frac{\pi k_F^2}{(\frac{2\pi}{a})^2}$$

And so:

$$k_F^2 = \frac{n_v}{a^2} 2\pi$$

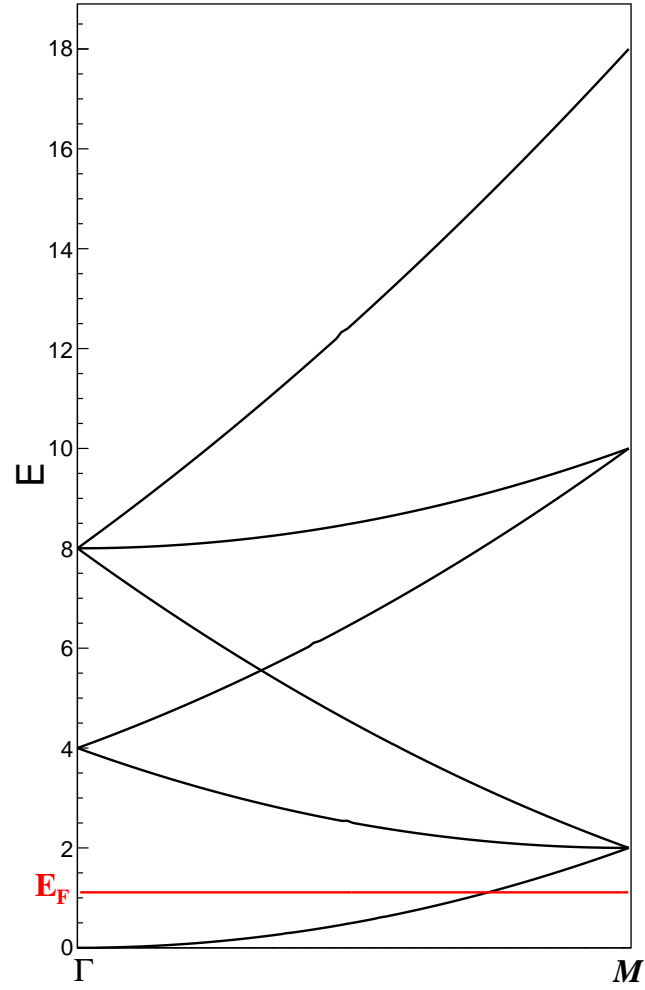
Substituting this expression in the equation of the Fermi energy we have:

$$E_F = \frac{\hbar^2}{2m} \frac{n_v}{a^2} 2\pi \cdot \frac{(2\pi)^2}{a^2} \frac{a^2}{(2\pi)^2}$$

In units of  $\frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$  the energy becomes:

$$E_F = \frac{n_v}{2\pi}$$

In the **Figure 7** the Fermi level is represented with a red line, assuming  $n_v = 7$ .



**Figure 7:** First six energy bands for two-dimensional square lattice. The energy is in units of  $\frac{\hbar^2}{2m} \left(\frac{2\pi}{a}\right)^2$ .

## Homework 7

a) The energy bands of the electrons in a one-dimensional lattice are obtainable by solving the central equation which can be written in matrix notation:

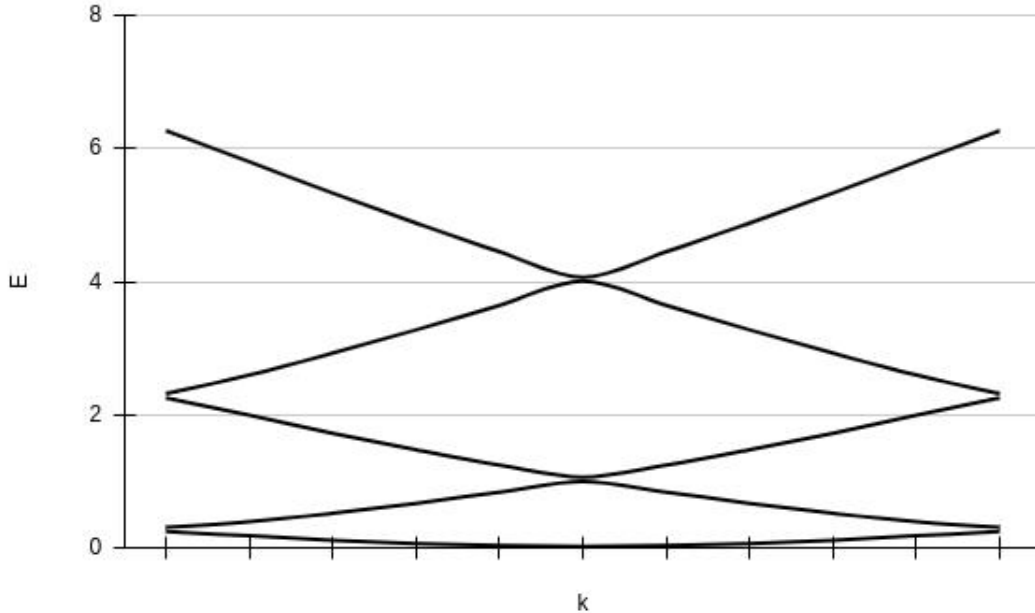
$$\hat{A}(k)\vec{C} = E_n(k)\vec{C}$$

By diagonalizing the matrix  $A$ , it is possible to obtain the different energy levels  $E_n(k)$ . The generic element of matrix  $A$ , considering the energy in the units of  $\frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$  and the vectors in units of  $(\frac{2\pi}{a})$ , is:

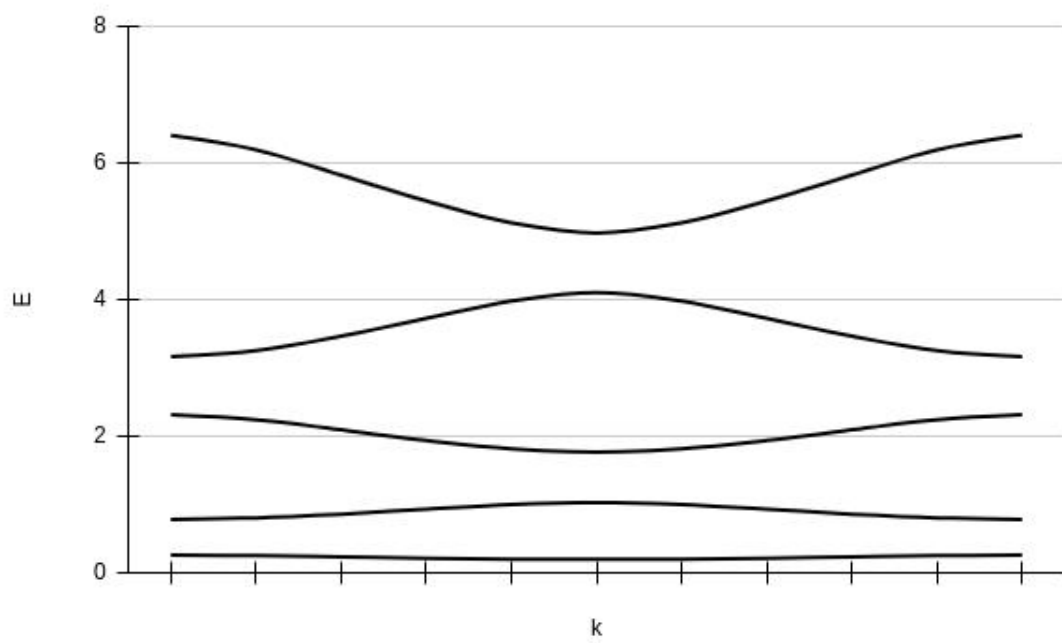
$$A_{lm} = (k_u - l)\delta_{lm} - V_0 \frac{\sigma}{a} \sqrt{\pi} \exp\left\{-\pi^2 \frac{\sigma^2}{a^2} (l - m)^2\right\}$$

where  $k_u$  is the value of  $k \in 1^{st}$  B.Z. in units of  $(\frac{2\pi}{a})$ . To find the eigenvalues of the matrix, one must choose the  $k$  values and the size  $d$  of the matrix. The calculation is more accurate for larger  $d$ . The routine *dsyev* of *lapack* was used. By executing the code, a problem of segmentation fault was found in the computation of eigenvalues for matrices with dimensions greater than 7, due to the physical limit of the computer's memory. For this reason we considered a matrix  $(7 \times 7)$ . Reducing ourselves to the first Brillouin zone, 10 values of  $k$  were considered. The points obtained were reported in a graph that approximated the energy bands. Two values were considered for the potential  $V_0$ . The **Figure 8** shows the bands in the "quasi-free" electron regime, where  $V_0 = 0.5$  (in units of  $\frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$ ), while **Figure 9** shows the bands in the "tight-binding" regime in which  $V_0 = 7.0$ .

As expected, in both cases there is the creation of an energy gap near to the cross point. In the case of "tight-binding" approximation the bands are more squashed.



**Figure 8:** Energy bands in "quasi-free" electron regime for a one-dimensional lattice.



**Figure 9:** Energy bands in "tight-binding" electron regime for a one-dimensional lattice.