Mid-term assessment test of Condensed Matter Physics - January 14th 2020
Prof. S. Caprara

Exercise 1: Tight binding.

Consider the two-dimensional centered rectangular Bravais lattice shown in Fig. 1. Each lattice site hosts an atom with one valence electron, occupying an s-type orbital, whose wave function $\phi_s(\boldsymbol{r})$ is real. The lattice parameters of the conventional unit cell (highlighted in Fig. 1) are $a = 0.15\,\mathrm{nm}$ and $b = 0.20\,\mathrm{nm}$.

1. Neglecting all overlap integrals, write the expression of the energy band dispersion $E(k_x, k_y)$ in the tight-binding approximation, considering the contributions from the first, second, and third neighbours only (for the site 0, taken as the origin, these are indicated in Fig. 1 by the labels 1, 2, and 3, respectively). The values of the transfer integrals $\gamma_i \equiv \gamma(\boldsymbol{R}_i) = -\int \mathrm{d}\boldsymbol{r}\, \phi_s(\boldsymbol{r})\Delta U(\boldsymbol{r})\phi_s(\boldsymbol{r} - \boldsymbol{R}_i)$ are $\gamma_1 = 0.75\,\mathrm{eV}$, $\gamma_2 = 0.25\,\mathrm{eV}$, and $\gamma_3 = 0.15\,\mathrm{eV}$, for the first, second, and third neighbours, respectively. Indicate with E_s the energy level of the atomic s orbital and let $\beta = \gamma(\boldsymbol{R} = 0)$. [The numerical values of these two parameters are not needed to answer the following question].

2. Evaluate the elements of the electron effective mass tensor, m_{xx}, m_{yy}, and $m_{xy} = m_{yx}$ (in kg) at the Γ point of the first Brillouin zone ($k_x = 0, k_y = 0$).

3. Determine the electron density n (in m^{-2}).

[Note that $1\,\mathrm{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$, and the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$. The free electron mass is $m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$].

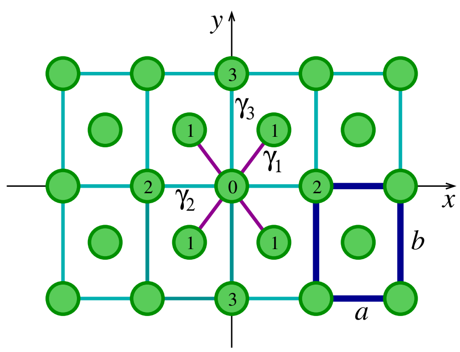

Fig. 1.

Exercise 2: Semiconductors.

Consider an intrinsic semiconductor that can be described as a two band system, with effective mass of the electrons in the conduction band $m_c = 0.2\,m_0$ and effective mass of the holes in the valence band $m_v = 0.5\,m_0$, where $m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$ is the free electron mass.

1. Knowing that the density of intrinsic carriers at a temperature $T = 300\,\mathrm{K}$ is $n_i = 7 \times 10^{17}\,\mathrm{m}^{-3}$, determine the value of the band gap E_g (in eV).

2. Assuming the origin of the energies at the top of the valence band, ε_v, so that $\varepsilon_v = 0$ and the bottom of the conduction band is $\varepsilon_c = E_g$, determine the value of the chemical potential μ_i (in eV), at $T = 300\,\mathrm{K}$.

3. To increase the density of electrons in the conduction band, the semiconductor is doped with donors. Assuming that the donors are fully ionized at $T = 300\,\mathrm{K}$, determine the density of donors N_d that is needed to increase the density of electrons in the conduction band n_c by a factor 10^3 with respect to the intrinsic case considered before. What is now the density of holes in the valence band p_v?

[Note that $1\,\mathrm{eV}$ corresponds to a temperature of $1.16 \times 10^4\,\mathrm{K}$ or to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$, the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$, and the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$].

Solution of the mid-term assessment test
Prof. S. Caprara

Exercise 1.

1. We have

$$E(k_x,k_y)=E_s-\beta-\sum_{i=1,2,3}\sum_{\boldsymbol{R}_i}\gamma(\boldsymbol{R}_i)\,\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{R}_i},$$

where $\boldsymbol{R}_1=(\pm\frac{1}{2}a,\pm\frac{1}{2}b)$; $\boldsymbol{R}_2=(\pm a,0)$; $\boldsymbol{R}_2=(0,\pm b)$; $\boldsymbol{k}=(k_x,k_y)$. Then

$$E(k_x,k_y)=E_s-\beta-4\gamma_1\cos\left(\frac{1}{2}k_xa\right)\cos\left(\frac{1}{2}k_yb\right)-2\gamma_2\cos(k_xa)-2\gamma_3\cos(k_yb).$$

2. Expanding near the Γ point we find

$$E(k_x,k_y)\approx E_s-\beta-4\gamma_1-2\gamma_2-2\gamma_3+\frac{1}{2}(\gamma_1+2\gamma_2)a^2k_x^2+\frac{1}{2}(\gamma_1+2\gamma_3)b^2k_y^2,$$

hence the effective mass tensor is diagonal, $m_{xy}=m_{yx}=0$, and

$$m_{xx}=\frac{\hbar^2}{(\gamma_1+2\gamma_2)a^2}=2.47\times10^{-30}\,\mathrm{kg}=2.71\,m_0,\qquad m_{yy}=\frac{\hbar^2}{(\gamma_1+2\gamma_3)b^2}=1.65\times10^{-30}\,\mathrm{kg}=1.81\,m_0.$$

3. There are two atoms in the conventional unit cell, each contributing one electron, hence

$$n=\frac{2}{ab}=6.67\times10^{19}\,\mathrm{m}^{-2}.$$

Exercise 2.

1. We have $\kappa_BT=4.14\times10^{-21}$ J$=2.58\times10^{-2}$ eV. Since

$$n_i=\frac{1}{4}\left(\frac{2\kappa_BT}{\pi\hbar^2}\right)^{3/2}(m_cm_v)^{3/4}\,\mathrm{e}^{-E_g/2\kappa_BT},$$

we find

$$E_g=2\kappa_BT\log\left[\frac{1}{4n_i}\left(\frac{2\kappa_BT}{\pi\hbar^2}\right)^{3/2}(m_cm_v)^{3/4}\right]=0.812\,\mathrm{eV}.$$

2. The chemical potential is

$$\mu_i=\frac{1}{2}E_g+\frac{3}{4}\kappa_BT\log\frac{m_v}{m_c}=0.424\,\mathrm{eV}.$$

3. If the donors are fully ionized

$$N_d\approx n_c=10^3\,n_i=7\times10^{20}\,\mathrm{m}^{-3}.$$

Then, according to the law of mass action,

$$p_v=\frac{n_i^2}{n_c}=10^{-3}\,n_i=7\times10^{14}\,\mathrm{m}^{-3}$$

is reduced by a factor 10^3 with respect to the intrinsic case.