Written exam of Condensed Matter Physics - February 6th 2023
Profs. S. Caprara and A. Polimeni

Exercise 1: Phonons.

Consider a monoatomic one-dimensional chain with total length $L = 30\,\text{cm}$. The phonon density of states of the chain is $D = 1.20 \times 10^{-4}\,\text{s}$, and the Debye model is assumed to be valid.

1. [3 points] Determine the velocity of sound v_s of the chain.

2. [2 points] Evaluate the number of atoms N of the chain knowing the Debye frequency $\omega_D = 8.38 \times 10^{12}\,\text{rad/s}$.

3. [4 points] Evaluate the spring constant K mimicking the nearest-neighbor interaction of the atoms in the chain (the mass of an atom forming the chain is $m = 7 \times 10^{-27}\,\text{kg}$).

4. [6 points] Evaluate the internal energy per unit length of the chain, u, at the two temperatures $T = 500\,\text{K}$ and $T = 1\,\text{K}$ [consider that $\int_0^{64} \text{d}x\, x/(e^x - 1) = 1.64$].

Exercise 2: Semiconductors.

Consider a three-dimensional intrinsic semiconductor with a simple cubic crystal structure and a lattice spacing $a = 0.575\,\text{nm}$. The conduction and valence band are well described by the expressions

$$\begin{cases} \varepsilon_c(\boldsymbol{k}) &= A - B\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right], \\ \varepsilon_v(\boldsymbol{k}) &= C + D\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right], \end{cases}$$

respectively, where $\boldsymbol{k} = (k_x, k_y, k_z)$ is the three-dimensional Bloch wave vector, $B = 0.325\,\text{eV}$, $C = -4.10\,\text{eV}$, and $D = 0.385\,\text{eV}$.

1. [4 points] Determine the numerical value of the parameter A, knowing that the gap energy is $E_g = 0.720\,\text{eV}$.

2. [5 points] Determine the numerical values of the masses of the electrons at the bottom of the conduction band, m_c, and of the holes at the top of the valence band, m_v.

3. [6 points] Assuming that the bands can be safely approximated by parabolic dispersions, with the electron and hole masses obtained in the previous point, determine the numerical values of the densities of electrons in the conduction band, n_c, and of holes in the valence band, p_v, at the temperature T such that the chemical potential is $0.004\,\text{eV}$ below the middle of the gap.

[Useful constants and conversion factors: the reduced Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J·s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\text{J·K}^{-1}$, the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\text{kg}$; $1\,\text{eV}$ corresponds to a temperature of $1.16 \times 10^4\,\text{K}$ or to an energy of $1.60 \times 10^{-19}\,\text{J}$].

Solution
Profs. S. Caprara and A. Polimeni

Exercise 1.

1. Within the Debye model, the density of states is $D = L/(\pi v_s)$. Thus $v_s = L/(\pi D) = 795.8\,\mathrm{m/s}$.

2. The number of atoms is given by $N = \int_0^{\omega_D} D\,\mathrm{d}\omega = D\omega_D = 10^9$.

3. The spring constant can be derived from $v_s = a\sqrt{K/m}$, where $a = L/N = 0.3\,\mathrm{nm}$. Thus, $K = m(v_s/a)^2 = 4.93 \times 10^{-2}\,\mathrm{N/m}$.

4. The Debye temperature is $\Theta_D = \hbar\omega_D/\kappa_B = 64\,\mathrm{K}$. Since $500\,K \gg \Theta_D$, $u(T = 500\,\mathrm{K}) \approx \kappa_B T/a = 2.3 \times 10^{-11}\,\mathrm{J/m}$. At $T = 1\,\mathrm{K}$, letting $\beta = (\kappa_B T)^{-1}$, we have

$$u = \int_0^{\omega_D} \mathrm{d}\omega\, \frac{D}{L}\frac{\hbar\omega}{\mathrm{e}^{\beta\hbar\omega} - 1} = \frac{(\kappa_B T)^2}{\pi\hbar v_s}\int_0^{\Theta_D/T} \mathrm{d}x\, \frac{x}{\mathrm{e}^x - 1} = \frac{(\kappa_B T)^2}{\pi\hbar v_s}\int_0^{64} \mathrm{d}x\, \frac{x}{\mathrm{e}^x - 1} = 1.64\frac{(\kappa_B T)^2}{\pi\hbar v_s} = 1.19 \times 10^{-15}\,\mathrm{J/m}.$$

Exercise 2.

1. The minimum of the conduction band and the maximum of the valence band are both evidently located at the $\Gamma = (0, 0, 0)$ point of the first Brillouin zone, where $\varepsilon_c(\Gamma) = A - 3B$ and $\varepsilon_v(\Gamma) = C + 3D$. Then, the gap energy is $E_g = \varepsilon_c(\Gamma) - \varepsilon_v(\Gamma) = A - C - 3(B + D)$, hence $A = E_g + C + 3(B + D) = -1.25\,\mathrm{eV}$.

2. Expanding the two bands near the Γ point we find

$$\begin{cases} \varepsilon_c(\boldsymbol{k}) \;\approx\; A - 3B + \frac{Ba^2}{2}\boldsymbol{k}^2, \\ \varepsilon_v(\boldsymbol{k}) \;\approx\; C + 3D - \frac{Da^2}{2}\boldsymbol{k}^2, \end{cases}$$

with $\boldsymbol{k}^2 = k_x^2 + k_y^2 + k_z^2$. Then, the masses of electrons and holes are

$$m_c = \frac{\hbar^2}{Ba^2} = 6.46 \times 10^{-31}\,\mathrm{kg} = 0.709\,m_0, \qquad m_v = \frac{\hbar^2}{Da^2} = 5.45 \times 10^{-31}\,\mathrm{kg} = 0.599\,m_0,$$

respectively.

3. In an intrinsic semiconductor $n_c = p_v = n_i$, where the number of intrinsic carriers is

$$n_i(T) = 2.5\left(\frac{m_c m_v}{m_0^2}\right)^{3/4}\left(\frac{T}{300\,\mathrm{K}}\right)^{3/2}\mathrm{e}^{-\frac{E_g}{2\kappa_B T}} \times 10^{25}\,\mathrm{m}^{-3},$$

and the chemical potential is

$$\mu_i(T) = \frac{1}{2}\left(\varepsilon_c + \varepsilon_v\right) + \frac{3}{4}\kappa_B T \ln\frac{m_v}{m_c},$$

where ε_c and ε_v are the energies of the bottom of the conduction band and of the top of the valence band, respectively. Since in our case $m_v/m_c = B/D$, the condition $\mu_i(T) = \frac{1}{2}\left(\varepsilon_c + \varepsilon_v\right) - \delta$, with $\delta = 0.004\,\mathrm{eV}$, gives

$$T = \frac{4\delta}{3\kappa_B \ln\frac{D}{B}} = 365\,\mathrm{K},$$

hence

$$n_c = p_v = n_i(T = 365\,\mathrm{K}) = 1.89 \times 10^{20}\,\mathrm{m}^{-3}.$$