Homework # 12

Exercise 1 – Tight-binding method for single atomic s-level

Let us consider a tight-binding model for a single band which comes from an atomic s-level with energy E_s. As proved explicitly in the lectures, assuming that only nearest-neighbours (n.n.) separations give non-zero overlap integrals, we have the following expression for the band dispersion:

$$E(\boldsymbol{k}) = E_s - \beta - \sum_{\text{n.n.}} \gamma(\boldsymbol{R}) \cos(\boldsymbol{k} \cdot \boldsymbol{R}) \tag{1}$$

1. Find the electron dispersion relation for a simple cubic Bravais lattice with lattice parameter a. Use the fact that, due to the cubic symmetry of the lattice, the overlap integral, $\gamma(\boldsymbol{R})$, is the same for every $\boldsymbol{R}$ that is nearest-neighbour: $\gamma(\boldsymbol{R}) = \gamma$.

2. Knowing that the average velocity of an electron with crystal wavevector $\boldsymbol{k}^*$ is given by[1]:

$$\boldsymbol{v}(\boldsymbol{k}^*) = \frac{1}{\hbar} \frac{\partial E(\boldsymbol{k})}{\partial \boldsymbol{k}}\Big|_{\boldsymbol{k}=\boldsymbol{k}^*} \equiv \frac{1}{\hbar} \Big(\frac{\partial E(\boldsymbol{k})}{\partial k_x}\Big|_{k_x=k_x^*}, \frac{\partial E(\boldsymbol{k})}{\partial k_y}\Big|_{k_y=k_y^*}, \frac{\partial E(\boldsymbol{k})}{\partial k_z}\Big|_{k_z=k_z^*} \Big) \tag{2}$$

   find in which points $\boldsymbol{k}^*$ of the Brillouin zone the average velocity is zero.

3. Compute the effective mass m_i^* along the direction i ($i = x, y, z$) at the band minimum, i.e. at $\Gamma = (0, 0, 0)$, knowing that

$$\frac{1}{m_i^\star} = \frac{1}{\hbar^2} \frac{\partial^2 E(\boldsymbol{k})}{\partial k_i^2}. \tag{3}$$

   Show that it is isotropic, i.e. $m_x^* = m_y^* = m_z^*$.

   What is the minimum value of γ such that m_i^* is smaller than the free electron mass? Estimate its value in case $a = 2$ Å.

4. Do a qualitative draw of the dispersion of the band along the direction in the Brillouin zone specified by: $-\frac{\pi}{a} < k_x < \frac{\pi}{a}$, $k_y = 0$, $k_z = 0$.
   Find the bandwidth (that is the spanned energy range) of the band along this direction?

Exercise 2 - Intrinsic Semiconductors

As we learnt from the lectures, in the parabolic band approximation the electron and hole densities of a semiconductor can be written as:

$$n_c(T, \mu) = \frac{1}{4} \left(\frac{2 m_c k_B T}{\pi \hbar^2} \right)^{3/2} e^{-\frac{\varepsilon_c - \mu}{k_B T}}, \tag{4}$$

$$p_v(T, \mu) = \frac{1}{4} \left(\frac{2 m_v k_B T}{\pi \hbar^2} \right)^{3/2} e^{-\frac{\mu - \varepsilon_v}{k_B T}}. \tag{5}$$

Here, T is the temperature, μ is the chemical potential, ε_c and m_c are the energy and the effective mass of electrons at the bottom of the conduction band, while ε_v and m_v are the energy and the effective mass of holes at the top of the valence band. Answer to the following questions:

[1] The proof is given, for example, in the Appendix E of the Ashcroft and Mermin, *Solid state physics*.

1. What is the relation between $n_c(T, \mu)$ and $p_v(T, \mu)$ for an intrinsic semiconductor?

2. Use the relation obtained in the previous point to find the expression for the chemical potential μ as a function of T, m_c, m_v, ε_c, and ε_v.

3. What is the value of the chemical potential at $T = 0\,\mathrm{K}$?
   Estimate the shift in chemical potential $\Delta\mu$ from $T = 0\,\mathrm{K}$ to $T = 300\,\mathrm{K}$ in the case of GaAs. Is it positive or negative? How does it compare with the band gap of GaAs?
   (*Hint: In GaAs, the effective masses are* $m_c/m = 0.063$ *and* $m_v/m = 0.51$*, and the energy gap is* $E_g = 1.43\,\mathrm{eV}$.)

4. Consider a crystal of silicon in which the number of impurities is so small that their contribution to the carrier densities is negligible (in this situation the semiconductor is "intrinsic"). Knowing that the band gap of Si is 1.12 eV, calculate the intrinsic carrier density of electrons and holes at room temperature.
   [Hint: In Si the effective mass at the bottom of the conduction band is $m_c/m = 0.3$ *and the effective mass at the top of valence band is* $m_v/m = 0.55$*. Remember also that silicon has six equivalent conduction band minima inside the Brillouin zone.]*