Second mid-term test of Condensed Matter Physics - January 17th 2023
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Exercise 1: Tight binding.

Consider a one-dimensional lattice with lattice spacing $a = 0.6\,\text{nm}$. The lattice hosts a biatomic compound AB, and the A−B bonds in the crystal are alternately short and long, with length $a_\text{S} = a/3 = 0.2\,\text{nm}$ and $a_\text{L} = 2a/3 = 0.4\,\text{nm}$, respectively (see Fig. 1; NOTICE that the final solution does not depend on the specific values of a_S and a_L, as long as $a_\text{S} + a_\text{L} = a$). The outer orbitals of both A and B atoms are s orbitals, with atomic energies $\varepsilon_\text{A} = -5.0\,\text{eV}$ and $\varepsilon_\text{B} = -5.3\,\text{eV}$, respectively. Asssume that the electron states of the given lattice can be described within the tight-binding approach with attractive lattice potential, and that the transfer integral for short and long bonds are $\gamma_\text{S} = 0.3\,\text{eV}$ and $\gamma_\text{L} = 0.1\,\text{eV}$, respectively. All other transfer integrals, all overlap integrals and the β integrals can be neglected altogether. Indicate with $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$ the one-dimensional wave vector, and with b_A and b_B the coefficients of the linear combination of s orbitals of A and B atoms.

1. [5 points] Find the expressions of the dispersion laws for the conduction and valence band, respectively, $\varepsilon_c(k)$ and $\varepsilon_v(k)$.

2. [4 points] Calculate the numerical value of the velocity v_k of an electron in the valence band with with wave vector $k = \frac{\pi}{2a}$.

3. [6 points] Determine the numerical value of the band gap E_g that separates the conduction and valence band and its location within the first Brillouin zone.

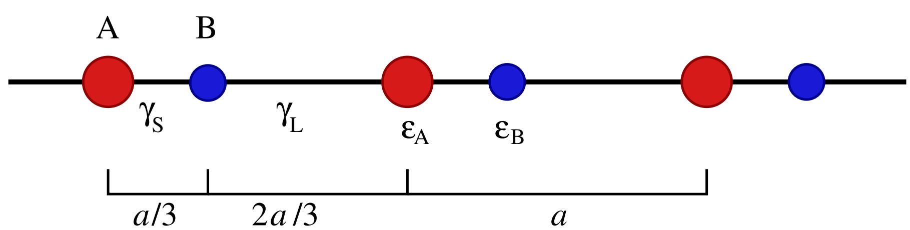

Fig. 1.

Exercise 2: Semiconductors.

Consider an intrinsic three-dimensional semiconductor, whose chemical potential μ_i stays in the middle of the gap independently of the temperature. At $T = 500\,\text{K}$ the density of electrons in the conduction band is $n_c = 1.27 \times 10^{14}\,\text{cm}^{-3}$, while at $T = 600\,\text{K}$ $n_c = 9.92 \times 10^{14}\,\text{cm}^{-3}$.

1. [6 points] Determine the numerical value of the band gap energy E_g.

2. [5 points] Determine the numerical value of the electron and hole effective masses, m_c and m_v, respectively.

3. [4 points] It is found that the conductivity of the semiconductor at $T = 500\,\text{K}$ is $\sigma = 20\,\Omega^{-1}\cdot\text{m}^{-1}$ and that the electron mobility $\widetilde{\mu}_e$ is four times greater than the hole mobility $\widetilde{\mu}_h$. Determine the electron and hole relaxation time (namely, the average time between two collisions), τ_e and τ_h, respectively.

[Useful constants and conversion factors: the reduced Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J}\cdot\text{s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\text{J}\cdot\text{K}^{-1}$, the elementary charge is $e = 1.60 \times 10^{-19}\,\text{C}$, 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
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Exercise 1.

1. We introduce the complex quantity

$$\Gamma_k \equiv \gamma_{\rm S} e^{{\rm i}ka_{\rm S}} + \gamma_{\rm L} e^{-{\rm i}ka_{\rm L}}.$$

Then, the tight-binding equations take the form of the 2×2 system of homogeneous equations

$$\begin{cases} [\varepsilon_{\rm A} - \varepsilon(k)] b_{\rm A} - \Gamma_k b_{\rm B} &= 0, \\ -\Gamma_k^* b_{\rm A} + [\varepsilon_{\rm B} - \varepsilon(k)] b_{\rm B} &= 0. \end{cases}$$

The systems admits non-trivial solutions if the energy $\varepsilon(k)$ is an eigenvalue of the linear problem,

$$\varepsilon_\pm(k) = \frac{\varepsilon_{\rm A} + \varepsilon_{\rm B}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\rm A} - \varepsilon_{\rm B}}{2}\right)^2 + |\Gamma_k|^2},$$

with

$$|\Gamma_k|^2 = \gamma_{\rm S}^2 + \gamma_{\rm L}^2 + 2\gamma_{\rm S}\gamma_{\rm L}\cos(ka),$$

where we used the fact that $a_{\rm S} + a_{\rm L} = a$. The conduction band is $\varepsilon_c(k) = \varepsilon_+(k)$ and the valence band is $\varepsilon_v(k) = \varepsilon_-(k)$.

2. The required velocity is

$$v_{k=\frac{\pi}{2a}} = \left.\frac{1}{\hbar}\frac{\partial \varepsilon_v}{\partial k}\right|_{k=\frac{\pi}{2a}} = \left.\frac{a\gamma_{\rm S}\gamma_{\rm L}\sin(ka)}{\hbar\sqrt{\left(\frac{\varepsilon_{\rm A}-\varepsilon_{\rm B}}{2}\right)^2 + |\Gamma_k|^2}}\right|_{k=\frac{\pi}{2a}} = \frac{a\gamma_{\rm S}\gamma_{\rm L}}{\hbar\sqrt{\left(\frac{\varepsilon_{\rm A}-\varepsilon_{\rm B}}{2}\right)^2 + \gamma_{\rm S}^2 + \gamma_{\rm L}^2}} = 7.81 \times 10^4\,{\rm m/s}.$$

3. $|\Gamma_k|^2$ is minimum at $k = \frac{\pi}{a}$, where $|\Gamma_k|^2 = (\gamma_{\rm S} - \gamma_{\rm L})^2$ and is maximum at $k = 0$, where $|\Gamma_k|^2 = (\gamma_{\rm S} + \gamma_{\rm L})^2$. Then, the band gap is located at $k = \frac{\pi}{a}$ and

$$E_g = 2\sqrt{\left(\frac{\varepsilon_{\rm A} - \varepsilon_{\rm B}}{2}\right)^2 + (\gamma_{\rm S} - \gamma_{\rm L})^2} = 0.5\,{\rm eV}.$$

Exercise 2.

1. The fact that the chemical potential μ_i is independent of the temperature indicates that $m_c = m_v$. Furthermore, since $\widetilde{\mu}_e = 4\widetilde{\mu}_h$ and the electron and hole masses are equal, we deduce that $\tau_e = 4\tau_h$. The ratio of the densities of electrons in the conduction band at the two given temperatures is

$$\frac{n_c(T = 500\,{\rm K})}{n_c(T = 600\,{\rm K})} = \left(\frac{5}{6}\right)^{3/2} e^{\frac{E_g}{2\kappa_B}\left(\frac{1}{600\,{\rm K}} - \frac{1}{500\,{\rm K}}\right)}.$$

The text assigns to this ratio the value 0.128, hence $E_g = 0.921\,{\rm eV}$.

2. From

$$n_c(T = 500\,{\rm K}) = 2.5\left(\frac{5}{3}\frac{m_c}{m_0}\right)^{3/2} e^{-\frac{0.921\,{\rm eV}}{2\kappa_B 500\,{\rm K}}}\,10^{19}\,{\rm cm}^{-3},$$

one finds $m_c = 0.220\,m_0$.

3. We know that $\sigma = en_i(\widetilde{\mu}_e + \widetilde{\mu}_h) = 5en_i\widetilde{\mu}_h = 5e^2 n_c\tau_h/m_c$. Then, one finds $\tau_h = 2.46 \times 10^{-13}\,{\rm s}$ and $\tau_e = 4\tau_h = 9.84 \times 10^{-13}\,{\rm s}$.