Homework # 11

Exercise 1 – The Fermi-Dirac distribution

Fermi–Dirac statistics applies to identical and indistinguishable particles with half-integer spin (1/2, 3/2, etc.), called fermions, in thermodynamic equilibrium. For the case of negligible interaction between particles, the system can be described in terms of single-particle energy states.
The probability $n(\varepsilon)$ that a state with energy ε can be occupied by an electron is given by the *Fermi-Dirac* distribution function:

$$n(\varepsilon) = \frac{1}{1 + e^{(\varepsilon-\mu)/k_\mathrm{B}T}},$$

where μ is the chemical potential. For the system with a band gap, μ lies somewhere in between the top of valence band ε_v and and the bottom of conduction band ε_c, respectively.

1. Sketch a drawing of $n(\varepsilon)$ as a function of the energy (*e.g.* $\mu = 2$ eV), at $T = 0$ and $T = 1200\,\mathrm{K}$.
   What is the probability that a state at $\varepsilon = \mu$ is occupied?
   What is the probability that a state at $\varepsilon = 2\mu$ is empty?

2. If the highest occupied state of a semiconductor is at $\varepsilon_\mathrm{v} = 12\,\mathrm{eV}$ and its band gap is $E_g = 1.1\,\mathrm{eV}$, where is the chemical potential located, assuming that the probability of a state being filled at the valence band edge is equal to the probability of a state being empty at the conduction band edge?

3. In the classical limit $\varepsilon - \mu \gg k_\mathrm{B}T$, the *Fermi-Dirac* distribution tends to the *Maxwell-Boltzmann* distribution $n(\varepsilon) = e^{-(\varepsilon-\mu)/k_\mathrm{B}T}$. What is the minimal energy from which the two distributions will differ by less than 1/100? (*Hint: call* $x := e^{(\varepsilon-\mu)/k_\mathrm{B}T}$)

Exercise 2 – Effective masses and band gap

Gallium arsenide (GaAs) is a III-V direct band gap semiconductor with a zinc blende crystal structure. Among many other applications, it is an important semiconductor material for high-cost, high-efficiency solar cells and is used for single-crystalline thin-film solar cells, for instance.

Semiconductors such as GaAs have two valence bands that are degenerate at Γ and that differ only in their curvature. In the parabolic approximation, their band dispersions can be written as:

$$\epsilon_{hh}(k) = \epsilon_\mathrm{v} - \frac{\hbar^2 k^2}{2m_{hh}} \qquad \text{and} \qquad \epsilon_{lh}(k) = \epsilon_\mathrm{v} - \frac{\hbar^2 k^2}{2m_{lh}},$$

where the band with smaller curvature is called *heavy-hole band* since the corresponding effective mass $m_{hh} = 0.45m$ is larger, while the other one is called *light-hole band* and has a smaller effective mass $m_{lh} = 0.082m$.

1. In the cartoon of Fig. 1, knowing that the effective mass follows $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$, identify which is the light and which is the heavy valence band in the band structure. What is the maximum energy ε_v of the valence band?

2. In the lectures, we saw that the density of states for a single parabolic band can be written as:
$$g_v(\varepsilon) = \frac{m_v^{3/2}}{\pi^2\hbar^3}\sqrt{2(\varepsilon_v - \varepsilon)}.$$
In this case, we have *two* degenerate states contributing to the density of states, that simply sum up to yield the total density of states of valence electrons. Show that the latter can be written as the density of states of a *single* parabolic band with an effective mass of:
$$m_v = \left(m_{hh}^{3/2} + m_{lh}^{3/2}\right)^{2/3}.$$
Compute the m_v for GaAs.

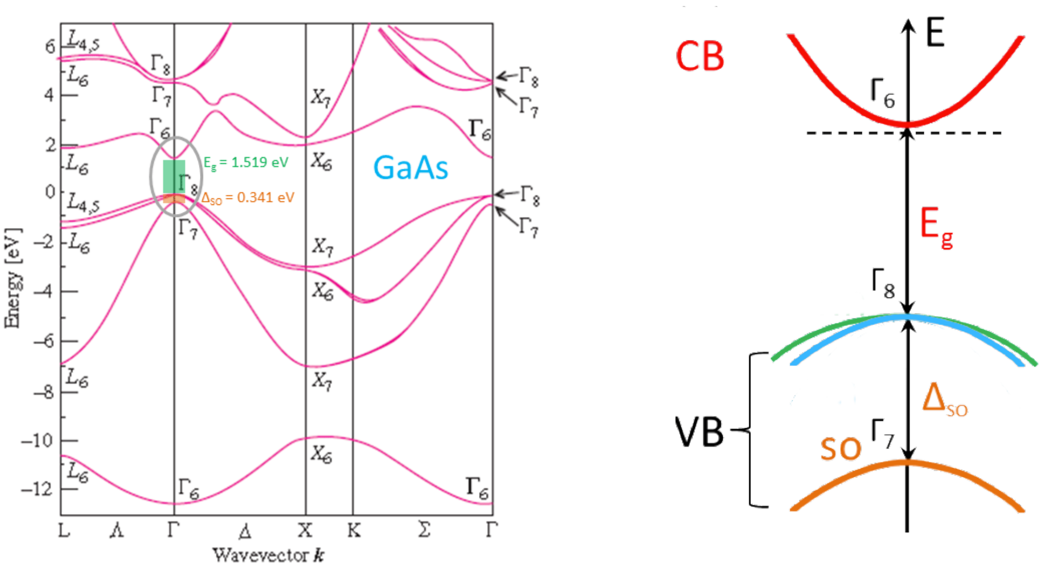

Figure 1: *Band structure of GaAs and its cartoon representation around* Γ.

The band gaps of some crystalline compounds at room temperature $T = 300$K are reported in the following tables:

Compound	E_g [eV]
C (diamond)	5.50
GaN (LED)	3.44
GaP	2.26
Na	0.00
GaAs	1.42
Si	1.12
Ge	0.67

3. In the system with a band gap, electrons in the valence band can jump to empty states of the conduction band by absorbing photons with energy $\geq E_g$. [1]
Based on this observation, and assuming all gaps to be direct, which of the systems above is transparent to the human eye? (*Hint: remember that visible light corresponds to a wavelength of* $0.4 - 0.7\,\mu$m).
Which color do you expect GaP will exhibit?

[1] Useful number: $hc \approx 1.24\,(\text{eV}\cdot\mu\text{m})$

Which compound, transparent to our sight, would be opaque to the *Sara Longwing* butterfly whose visual range is from 310 nm to 650 nm?