UNIVERSITY OF STRASBOURG

Problem Set 3

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Exercise 1 : Occupation of dopant levels

Consider a non-degenerate doped semiconductor. The density n_d of neutral (non ionized) donor is described by

$$n_\mathrm{d} = \frac{N_\mathrm{d}}{1 + \frac{1}{g_\mathrm{d}} \exp\left[(\epsilon_\mathrm{d} - \mu)/k_\mathrm{B}T\right]},$$

where ϵ_d is the energy level of the dopant and g_d its degeneracy (often equal to 2). N_d is the density of dopants.

a) Derive the formula above using the general expression

$$\langle n \rangle = \frac{\sum_j N_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}{\sum_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}$$

for the mean number of particles in a system from sums over all states j of the system, with E_j and N_j the energy and particle number in state j.

We will use that

$$N_j = \begin{cases} 0 \\ 1 \end{cases} \quad \Longrightarrow g_d \qquad\qquad E_j = \begin{cases} 0 = \sum_j N_j \epsilon_d \\ \epsilon_d \end{cases}$$

$$\begin{aligned} \langle n \rangle &= \frac{\sum_j N_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}{\sum_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]} \\ &= \frac{0 + g_d e^{-\beta(\epsilon_d - \mu)}}{1 + g_d e^{-\beta(\epsilon_d - \mu)}} \\ &= \frac{1}{1 + \frac{1}{g_d} e^{\beta(\epsilon_d - \mu)}} \end{aligned}$$

This is for one level, so we have to multiply by N_d, thus,

$$n_d = N_d \langle n \rangle = \frac{N_\mathrm{d}}{1 + \frac{1}{g_\mathrm{d}} \exp\left[(\epsilon_\mathrm{d} - \mu)/k_\mathrm{B}T\right]}$$

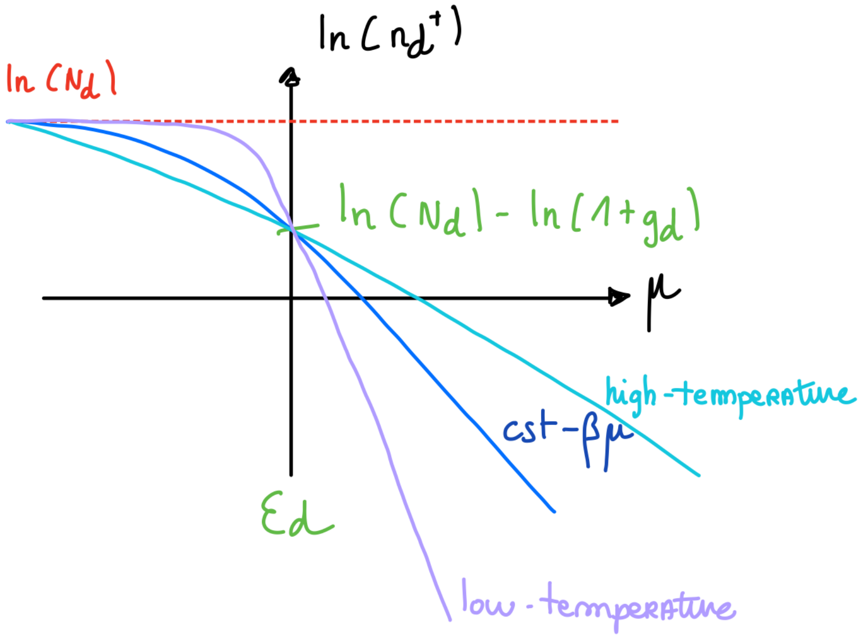
b) Give the expression for the density of ionized donors n_d^+.

$$\begin{aligned} n_d^+ &= N_d - n_d \\ &= N_d \left(1 - \frac{1}{1 + \frac{1}{g_\mathrm{d}} \exp\left[(\epsilon_\mathrm{d} - \mu)/k_\mathrm{B}T\right]}\right) \\ &= \frac{N_d}{1 + g_d \exp\left[-(\epsilon_\mathrm{d} - \mu)/k_\mathrm{B}T\right]} \end{aligned}$$

c) Draw a qualitative sketch of the behavior of $\ln n_\mathrm{d}^+$ as a function of the chemical potential μ, for two different temperatures T_1 and T_2. Pay attention in particular to the limiting case $|\epsilon_\mathrm{d} - \mu| \gg k_\mathrm{B}T$ and $|\epsilon_\mathrm{d} - \mu| \ll k_\mathrm{B}T$.

$$\ln\left(n_d^+\right) = \ln(N_d) - \ln\left(1 + g_d e^{-\beta(\epsilon_d - \mu)}\right)$$

$$\begin{cases} \lim\limits_{\mu\to-\infty} (n_d^+) = \ln(N_d) - g_d e^{-\beta(\epsilon_d-\mu)} \\ \lim\limits_{\mu\to+\infty} (n_d^+) \simeq \ln(N_d) - \ln(g_d) + \beta(\epsilon_d - \mu) \end{cases}$$



d) Respond to the same questions as in **a)**, **b)**, **c)**, but for the case of doping with acceptors (with degeneracy g_a of acceptor level), where the density n_a of not ionized acceptor atoms is given by

$$n_\mathrm{a} = \frac{N_\mathrm{a}}{1 + g_\mathrm{a} \exp\left[(\mu - \epsilon_\mathrm{a})/k_\mathrm{B}T\right]}.$$

Acceptor density N_a. We are gonna use

$$\langle n \rangle = \frac{\sum_j N_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}{\sum_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}$$

$$N_j = \begin{cases} 0 \\ 1 \end{cases} \implies g_a \qquad\qquad E_j = \begin{cases} 0 \\ \epsilon_a \end{cases}$$

$$\begin{aligned} \langle n \rangle &= \frac{\sum_j N_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]}{\sum_j \exp\left[-(E_j - \mu N_j)/k_\mathrm{B}T\right]} \\ &= \frac{0 + g_a e^{-\beta(\epsilon_a - \mu)}}{1 + g_d e^{-\beta(\epsilon_a - \mu)}} \\ &= \frac{1}{1 + \frac{1}{g_a} e^{\beta(\epsilon_a - \mu)}} \end{aligned}$$

And we know that

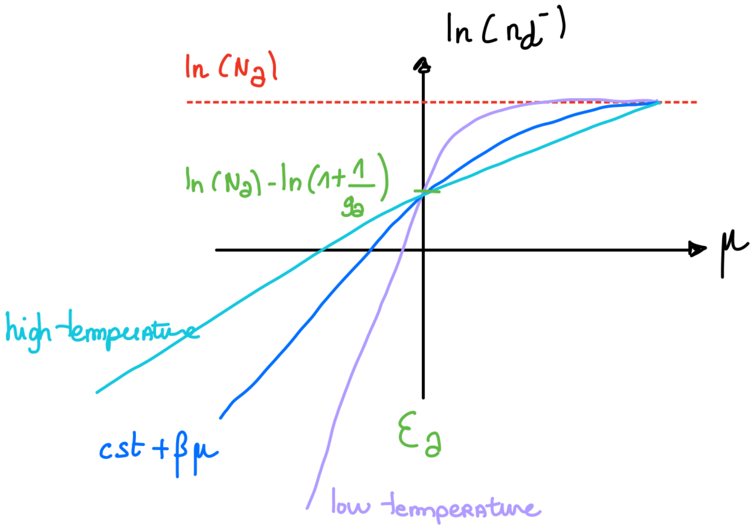
$$n_a^- = N_a \langle n \rangle \qquad\qquad n_a = N_a(1 - \langle n \rangle)$$

Where n_a is the non-ionized density and n_a^- is the ionized density. This is swapped from the previous case, because an acceptor level is ionized when it is filled.

$$n_a = \frac{N_\mathrm{a}}{1 + g_\mathrm{a} \exp\left[(\mu - \epsilon_\mathrm{a})/k_\mathrm{B}T\right]} \qquad\qquad n_a^- \frac{N_a}{1 + \frac{1}{g_a} e^{(\epsilon_a - \mu)/k_B T}}$$

$$\ln\left(n_d^-\right) = \ln(N_a) - \ln\left(1 + \frac{1}{g_a} e^{\beta(\epsilon_a - \mu)}\right)$$

$$\begin{cases} \lim\limits_{\mu \to +\infty} (n_d^-) = \ln(N_a) - \dfrac{1}{g_a} e^{-\beta(\mu - \epsilon_a)} \\ \lim\limits_{\mu \to -\infty} (n_d^-) \simeq \ln(N_a) + \ln(g_a) + \beta(\mu - \epsilon_a) \end{cases}$$



Exercise 2 : Electrons in the conduction band of a doped semiconductor

We study the density of electrons in the conduction band of an n-doped semiconductor (only donors, no acceptors).

a) Write the detailed expressions (in term of an energy integral) for the densities n_c of electrons in the conduction band, and p_v of holes in the valence band.

$$n_c = \int_{\epsilon_c}^{\infty} \mathrm{d}\epsilon g_c(\epsilon)\frac{1}{e^{\beta(\epsilon-\mu)}+1}, \quad p_v = \int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon)\left(1-\frac{1}{e^{\beta(\epsilon-\mu)}+1}\right) = \int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon)\frac{1}{e^{-\beta(\epsilon-\mu)}+1}$$

What will change is the value of this chemical potential, but it is the same formula as in the intrinsic case.

b) Suppose that the chemical potential μ is far away (several $k_\mathrm{B}T$) from both the conduction and the valence band edges ϵ_c and ϵ_v and write simplified approximate expression for n_c and p_v.

$$\begin{cases} \epsilon_c - \mu \gg k_B T \\ \mu - \epsilon_v \gg k_B T \end{cases}$$

And so we can approximate n_c and p_v as Boltzmann distributions,

$$\begin{cases} n_c \approx \int_{\epsilon_c}^{\infty} \mathrm{d}\epsilon g_c(\epsilon)e^{-\beta(\epsilon-\mu)} = e^{-\beta(\epsilon_c-\mu)}\int_{\epsilon_c}^{\infty} \mathrm{d}\epsilon g_c(\epsilon)e^{-\beta(\epsilon-\epsilon_c)} = e^{-\beta(\epsilon_c-\mu)}N_c(T) \\ p_v \approx \int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon)e^{\beta(\epsilon-\mu)} = e^{-\beta(\mu-\epsilon_v)}\int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon)e^{\beta(\epsilon-\epsilon_v)} = e^{-\beta(\mu-\epsilon_v)}P_v(T) \end{cases}$$

c) Assume that all donors levels are ionized (due to high enough temperature). Use charge conservation to determine the chemical potential and explicit expression for n_c and p_v. *Hint : use the resuts of the intrinsic case n_i and μ_i as a starting point for these considerations.*

$$n_c + n_a^- = p_v + n_d^+$$

Since we are in the high-temperature limit, we can simplify n_a^- as N_a and n_d^+ as N_d. As said in the problem sheet, $N_a = 0$, thus,

$$n_c = p_v + N_d$$

$$n_c p_v = e^{-\beta(\epsilon_c - \epsilon_v)} N_c(T) P_v(T)$$

The chemical potential disappeared, but it was the only difference from the intrinsic case, meaning this quantity is independent of the doping. Thus we can still write,

$$n_c p_v = n_i^2$$

So now we have two equations,

$$\begin{cases} n_c - p_v = N_d \\ n_c p_v = n_i^2 \end{cases}$$

Thus,

$$n_c = \frac{N_d + \sqrt{N_a^2 + 4n_i^2}}{2} \qquad p_v = \frac{\sqrt{N_a^2 + 4n_i^2} - N_d}{2}$$

$$\begin{cases} n_c = N_c(T) e^{-\beta(\epsilon_c - \mu + \mu_i - \mu_i)} = n_i e^{-\beta(\mu_i - \mu)} \\ p_v = P_v(T) e^{-\beta(\mu - \epsilon_v + \mu_i - \mu_i)} = n_i e^{-\beta(\mu - \mu_i)} \end{cases}$$

Thus,

$$\begin{aligned} N_d = n_c - p_v &= n_i \left[e^{\beta(\mu - \mu_i)} - e^{-\beta(\mu - \mu_i)} \right] \\ &= 2n_i \sinh[\beta(\mu - \mu_i)] \end{aligned}$$

And now we can solve for the chemical potential,

$$\mu = \mu_i + k_B T \sinh^{-1}\left(\frac{N_d}{2n_i}\right)$$

d) Give n_c, p_v and μ for the case $N_\mathrm{d} \gg n_\mathrm{i}$ (predominantly extrinsic behavior) and for the opposite case $N_\mathrm{d} \ll n_\mathrm{i}$ (predominantly intrinsic behavior). What is the transition temperature between the two regimes ?

- $N_d \gg n_i$:

$$\mu = \mu_i + k_B T \ln\left(\frac{N_d}{n_i}\right)$$

$$n_c = \frac{N_d}{2}\left(1 + \sqrt{1 + 4\left(\frac{n_i}{N_d}\right)^2}\right) \approx N_d\left(1 + \left(\frac{n_i}{N_d}\right)^2\right)$$

Thus,

$$p_v \approx N_d \left(\frac{n_i}{N_d}\right)^2$$

- $N_d \ll n_i$:

$$\mu = \mu_i + k_B T \frac{N_d}{2n_i}$$

$$n_c = n_i \left(\frac{N_d}{2n_i} + \sqrt{1 + \left(\frac{N_d}{2n_i} \right)^2} \right) \approx n_i \left(\frac{N_d}{2n_i} + 1 + \frac{1}{2} \left(\frac{N_d}{2n_i} \right)^2 \right) \approx n_i + \frac{N_d}{2}$$

Thus,

$$p_v \approx n_i - \frac{N_d}{2}$$

We look for the temperature at which $N_i = N_d$,

$$-\frac{E_g}{2k_B T} = \ln\left(\frac{N_d}{\sqrt{N_c P_v}} \right)$$

So we get,

$$T = -\frac{E_g}{2k_B \ln\left(\frac{N_d}{\sqrt{N_c P_v}} \right)}$$

e) Consider now the low-temperature case with predominantly extrinsic behavior, and when not all donors are ionized. Below which temperature is this regime expected to occur ? Find the asymptotic behavior of n_c and μ in the regime of very low temperatures.

We can assume that $p_v = 0$.

$$n_c = n_d^+$$

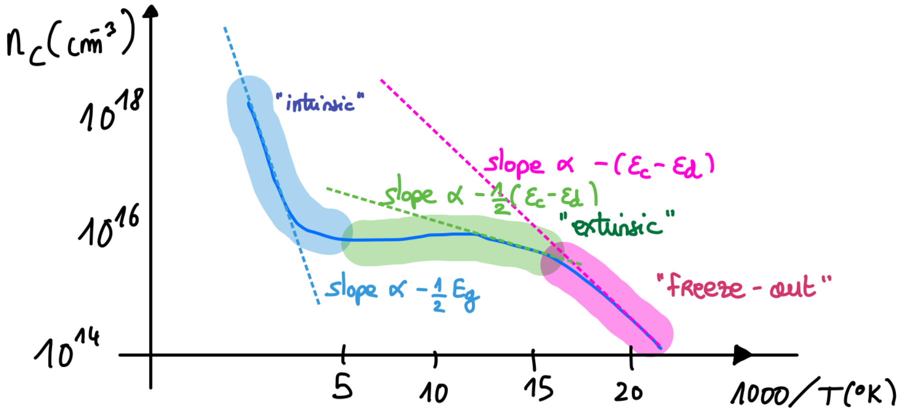
$$n_c = N_c e^{\beta(\mu - \epsilon_c)} = \frac{N_d}{1 + g_d e^{\beta(\mu - \epsilon_d)}} \approx \frac{N_d}{g_d} e^{-\beta(\mu - \epsilon_d)}$$

$$e^{2\beta\mu} = \frac{N_d}{N_c g_d} e^{\beta(\epsilon_d + \epsilon_c)}$$

And so,

$$\mu = \frac{\epsilon_d + \epsilon_c}{2} + \frac{k_B T}{2} \ln\left(\frac{N_d}{N_c g_d} \right)$$

$$n_c = \sqrt{\frac{N_c N_d}{g_d}} e^{-\beta(\epsilon_c - \epsilon_d)/2}$$


$n_c\,(cm^{-3})$
10^{18}
10^{16}
10^{14}
"intrinsic"
slope $\propto -\frac{1}{2}E_g$
slope $\propto -\frac{1}{2}(\varepsilon_c-\varepsilon_d)$
"extrinsic"
slope $\propto -(\varepsilon_c-\varepsilon_d)$
"freeze-out"
5
10
15
20
1000/T(°K)

Exercise 3 : At which energy are most of the carrier ?

The electron density in the conduction band (the hole density in the valence band) is given by an integral over contributions from different energies. These contributions are given by the product of an increasing density of states with a decreasing occupation probability when the energy moves away from the band edge. The maximum contribution to the electron (hole) density occurs at a finite energy above (below) the conductance (valence) band edge.

a) Use the Boltzmann approximation to determine to determine the energy $E_{\mathrm{max,c}}$ at which the contribution to the density of electron in the conduction band assumes its maximum value.

$$E_{\max} = \epsilon_c + a k_B T$$

Using Boltzmann approximation we know that

$$n_c \approx \int_{\epsilon_c}^{+\infty} \mathrm{d}\epsilon \; g(\epsilon) e^{-\beta(\epsilon-\mu)} \implies \mathrm{d}n_c = \mathrm{d}\epsilon \; g(\epsilon) e^{-\beta(\epsilon-\mu)}$$

$$\implies \frac{\mathrm{d}n_c}{\mathrm{d}\epsilon} = g(\epsilon) e^{-\beta(\epsilon-\mu)} = \mathrm{d}(\epsilon)$$

$$\frac{\mathrm{d}(\mathrm{d}(\epsilon))}{\mathrm{d}\epsilon} = 0 \implies \frac{K}{2\sqrt{\epsilon-\epsilon_c}} e^{-\beta(\epsilon-\mu)} - \beta g(\epsilon)) e^{-\beta(\epsilon-\mu)} = 0$$

$$\frac{K}{2\sqrt{\epsilon-\epsilon_c}} e^{-\beta(\epsilon-\mu)} - K\beta\sqrt{\epsilon-\epsilon_c} e^{-\beta(\epsilon-\mu)} = 0$$

Thus,

$$\frac{1}{2\sqrt{\epsilon-\epsilon_c}} - \beta\sqrt{\epsilon-\epsilon_c} = 0$$

$$\beta(\epsilon-\epsilon_c) - \frac{1}{2} = 0$$

$$\epsilon = \epsilon_c + \frac{1}{2} k_B T$$

b) Determine in the same way the energy $E_{\mathrm{max,v}}$ where the contribution to the density of holes in the valence band is maximum.

Hint : The following expression can be used for the densities of states in the conduction and valence band :

$$g_{\mathrm{c}}(\epsilon) = \frac{(m_{\mathrm{c}}^*)^{3/2}}{\pi^2\hbar^3}\sqrt{2(\epsilon - \epsilon_{\mathrm{c}})}$$

$$g_{\mathrm{v}}(\epsilon) = \frac{(m_{\mathrm{v}}^*)^{3/2}}{\pi^2\hbar^3}\sqrt{2(\epsilon_{\mathrm{v}} - \epsilon)}$$

It is the same idea as before,

$$\epsilon_{\mathrm{max}} = \epsilon_v - \frac{1}{2}k_B T$$