Series - Electronic and optical semiconductor devices

Series 6 - Semiconductor statistics and Hall effect in compensated semiconductors

Exercise 1 - Degenerate bulk semiconductor - Sommerfeld expansion

1- $N_c = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}$ $\qquad$ Si, $m_{e,l}^* = 0.916\ m_0$

GaAs, $m_e^* = 0.067\ m_0$

$$N_c(Si) = 2\left[\frac{2\pi \times 0.916 \times 9.1\times10^{-31} \times 1.38\times10^{-23} \times 300}{(6.64\times10^{-34})^2}\right]^{3/2} \sim 2.18\times10^{25}\ m^{-3}$$

i.e. $2.18\times10^{19}\ cm^{-3}$

$N_c(GaAs) \sim 4.31\times10^{17}\ cm^{-3}$

2- We consider (1.4) limited to its first two terms.

$$\int_{-\infty}^{+\infty} \rho_c(E) f_n(E)\, dE \approx \int_{-\infty}^{\mu} \rho_c(E)\, dE + \frac{\pi^2}{6}(k_B T)^2 \rho_c'(\mu)$$

Knowing that $\rho_c(E) = 0$ for energies $E < E_c$, we get the following relationship:

$$n = \int_{E_c}^{\mu} \rho_c(E)\, dE + \frac{\pi^2}{6}(k_B T)^2 \rho_c'(\mu)$$

i.e. $$n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} \underbrace{\int_{E_c}^{\mu} (E-E_c)^{1/2} dE}_{I} + \frac{\pi^2}{6}(k_B T)^2 \times \left.\frac{d\rho_c(E)}{dE}\right|_{E=\mu}$$

$$I = \left[\frac{2}{3}(E-E_c)^{3/2}\right]_{E_c}^{\mu} = \frac{2}{3}(\mu - E_c)^{3/2}$$

$$\left.\frac{d\rho_c(E)}{dE}\right|_{E=\mu} = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} \times \frac{1}{2}(\mu - E_c)^{-1/2}$$

so that $$n = \frac{1}{3\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(\mu - E_c)^{3/2} + \frac{1}{24}(k_B T)^2\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(\mu - E_c)^{-1/2}$$

Since $N_c = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}$, we obtain after some simplifications:

$$\boxed{n = \frac{4}{3\sqrt{\pi}} N_c \left(\frac{\mu - E_c}{k_B T}\right)^{3/2}\left[1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\mu - E_c}\right)^2\right]} \quad (1.5)$$

with $A = \frac{4}{3\sqrt{\pi}}$ and $B = \frac{\pi^2}{8}$

3- As $N_C \propto (k_B T)^{3/2}$ and in the highly degenerate case $\mu - E_C >> k_B T$, the free carrier density will reduce to

$$\boxed{n \approx \frac{8}{3\sqrt{\pi}}\left(\frac{2\pi m_e^*}{h^2}\right)^{3/2}(\mu - E_c)^{3/2} = \frac{1}{3\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(\mu - E_c)^{3/2}}$$

It is thus seen that the free carrier density becomes independent of the temperature, i.e. the semiconductor exhibits a transition toward a metallic behavior. However we should not speak of a metal here since the involved densities are not comparable. Indeed, if $\mu - E_c \approx 5 k_B T$ (at $T = 300\,K$) then $n \approx 1.74 \times 10^{20}\ cm^{-3}$ in the case of silicon which is at least two orders of magnitude lower than in a metal ($n \sim$ a few $10^{22}\ cm^{-3}$).

4- See graph

Additional information on the effective density of states

$$n = \int_{-\infty}^{+\infty} \rho_C(E) f_n(E)\, dE$$

3D case $\quad n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\int_{E_c}^{+\infty}(E - E_c)^{1/2} \times \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}\, dE$

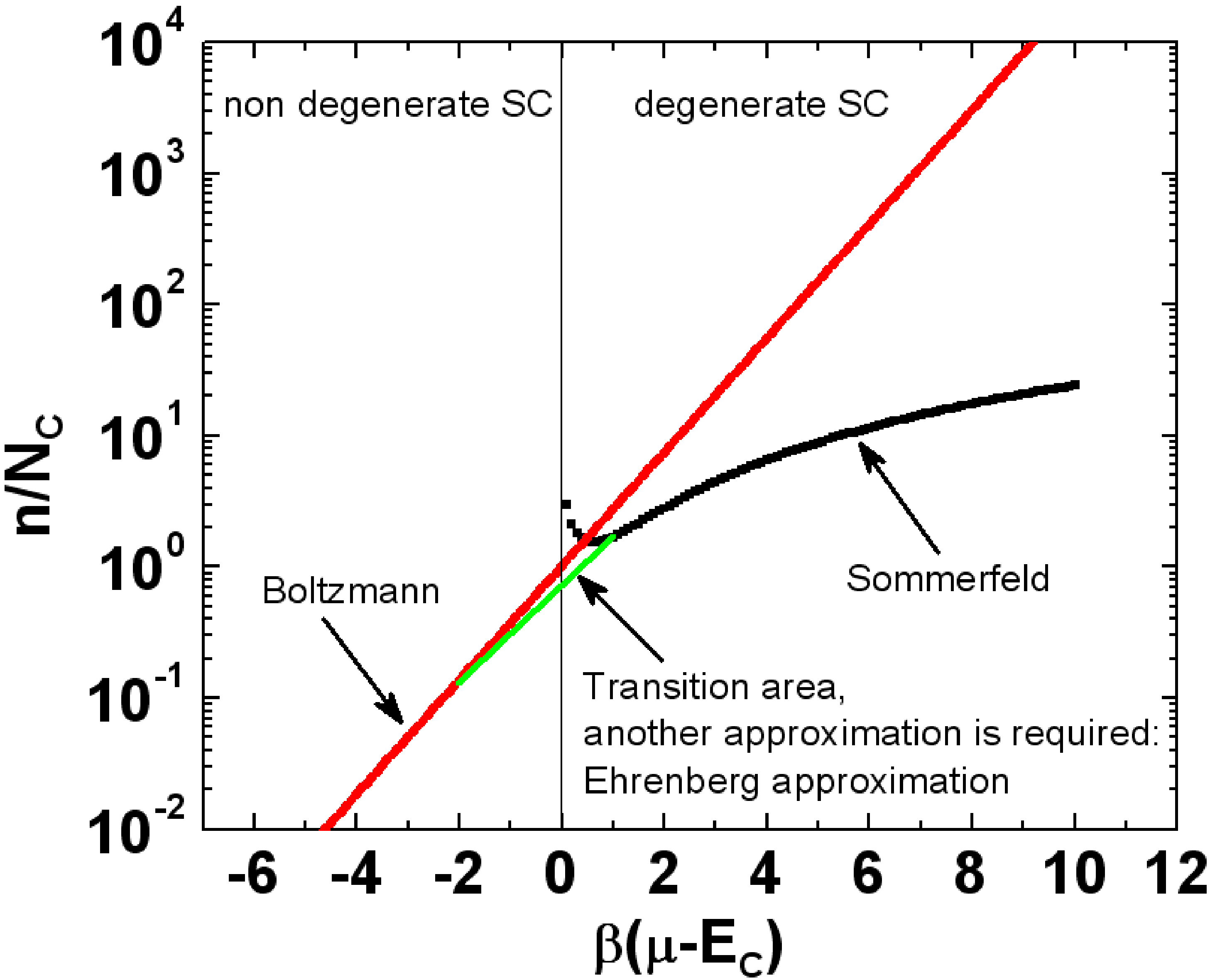
Boltzmann approximation $\rightarrow f_n(E) \sim \exp\left[-\frac{(E - E_F)}{k_B T}\right]$

$\hookrightarrow$ valid when the Fermi level lies deeply enough in the band gap so that $(E - E_F) >> k_B T$

$$n = \int_{E_c}^{+\infty} \rho_C(E) \exp\left[-(E - E_F)/k_B T\right] dE$$

$$n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\int_{E_c}^{+\infty}(E - E_c)^{1/2}\exp\left[-(E - E_F)/k_B T\right] dE$$

i.e. $n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\exp\left[-(E_c - E_F)/k_B T\right]\underbrace{\int_{E_c}^{+\infty}(E - E_c)^{1/2}\exp\left[-(E - E_c)/k_B T\right] dE}_{I'}$



non degenerate SC
degenerate SC
Boltzmann
Sommerfeld
Transition area,
another approximation is required:
Ehrenberg approximation
n/N_C
$\beta(\mu-E_C)$
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
-6
-4
-2
0
2
4
6
8
10
12

Evaluation of I'

$$I' = \int_{E_c}^{+\infty} (E-E_c)^{1/2} \exp[-\beta(E-E_c)]\, dE \quad \text{and } \beta = \frac{1}{k_B T}$$

Change of variable #1, $x = E - E_c$

$$\Rightarrow I' = \int_0^{+\infty} x^{1/2} \exp(-\beta x)\, dx$$

Change of variable #2, $x^{1/2} = X$

$$dX = \frac{1}{2} x^{-1/2} dx \Rightarrow dx = 2x^{1/2} dX = 2X\, dX$$

$$I' = \int_0^{+\infty} 2X^2 \exp(-\beta X^2)\, dX$$

Note that integral of the form $I_n = \int_0^{+\infty} x^n e^{-ax^2} dx$ are related through the formulas $I_{n+2} = \frac{n+1}{2a} I_n$ $(n \in \mathbb{N})$ and $I_0 = \frac{1}{2}\sqrt{\frac{\pi}{a}}$, $I_1 = \frac{1}{2a}$

As a consequence $I' = 2I_2 = 2 \times \frac{1}{2\beta} I_0$ so that $I' = \frac{\beta^{-3/2}}{2}\sqrt{\pi}$

which leads to $N_c = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} \times \frac{(k_B T)^{3/2}}{2}\sqrt{\pi}$

$$\Rightarrow \boxed{N_c = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \quad \text{and} \quad n = N_c \exp\left[-\frac{(E_c - E_F)}{k_B T}\right]}$$

This last expression is valid as long as E_F is far from $E_c \Rightarrow E_c - E_F > k_B T$ (cf. Question 4 - exercise 1).

The denomination "effective density of states" means that the occupied bands behave like two discrete levels with a concentration N_c and N_V in the semiconductor with respect to the Fermi level (approximation valid for slightly doped semiconductors only). However, one should not identify these two quantities (N_c and N_V) to the total number of states available in each band. It is a prefactor with a characteristic value allowing estimating beyond which doping level a semiconductor will be degenerate.

Exercise 1 - Maxwell-Boltzmann velocity distribution function

1- The most probable velocity for electrons corresponds to the maximum of the velocity distribution function $F(v)$, i.e. $v_{th_{max}}$ is such that $\frac{dF(v)}{dv} = 0$.

Therefore we have $\frac{d}{dv}\left(v^2 e^{-m^* v^2/2k_BT}\right) = 0$

i.e. $2v e^{-m^* v^2/2k_BT} - \frac{m^* v^3}{k_BT} e^{-m^* v^2/2k_BT} = 0$

which leads to $2v\left(1 - \frac{m^* v^2}{2k_BT}\right) = 0$

As v is necessarily different from zero, we obtain $\boxed{v_{th_{max}} = \left(\frac{2k_BT}{m^*}\right)^{1/2}}$

2- The root mean square velocity is linked to the mean thermal energy through the relation $\frac{1}{2} m^* v_{rms}^2 = \frac{3}{2} k_BT$, where the mean thermal energy is equal to $\frac{k_BT}{2}$ per degree of freedom so that we get $\boxed{v_{rm} = \left(\frac{3k_BT}{m^*}\right)^{1/2}}$

Alternatively, the mathematical approach is:

$$v_{rms}^2 = \int_0^{+\infty} v^2 F(v)\,dv \Big/ \underbrace{\int_0^{+\infty} F(v)\,dv}_{=1}$$

$= 1$ as $F(v)$ is a normalized distribution function.

i.e. $v_{rms}^2 = 4\pi\left(\frac{m^*}{2\pi k_BT}\right)^{3/2} \int_0^{+\infty} v^4 e^{-m^* v^2/2k_BT}\,dv$

Knowing that integrals of the form $I_n = \int_0^{+\infty} x^n e^{-ax^2}\,dx$ are related through the formulas $I_{n+2} = \frac{n+1}{2a} I_n$ ($n \in \mathbb{N}$) where $I_0 = \frac{1}{2}\sqrt{\frac{\pi}{a}}$ and $I_1 = \frac{1}{2a}$

we thus obtain $I_4 = \frac{3}{8a^2}\sqrt{\frac{\pi}{a}}$ where in our case $a = \frac{m^*}{2k_BT}$ so that

$I_4 = \frac{3\sqrt{\pi}}{8}\left(\frac{2k_BT}{m^*}\right)^{5/2}$ which leads to $v_{rms}^2 = 4\pi \times \frac{3\sqrt{\pi}}{8}\left(\frac{m^*}{2\pi k_BT}\right)^{3/2} \cdot \left(\frac{2k_BT}{m^*}\right)^{5/2}$

i.e. $v_{rms}^2 = \frac{3}{2}\pi^{3/2} \cdot \pi^{-3/2}\left(\frac{m^*}{2k_BT}\right)^{3/2} \cdot \left(\frac{2k_BT}{m^*}\right)^{5/2} \Rightarrow \boxed{v_{rms} = \left(\frac{3k_BT}{m^*}\right)^{1/2}}$

3- The mean velocity is given by: $\bar{v}_{th} = \dfrac{\int_0^{+\infty} v F(v)\,dv}{\int_0^{+\infty} F(v)\,dv}$

which leads to $\bar{v}_{th} = 4\pi\left(\dfrac{m^*}{2\pi k_B T}\right)^{3/2} \underbrace{\int_0^{+\infty} v^3 e^{-m^* v^2/2k_B T}\,dv}_{I_3}$

$I_3 = \dfrac{1}{a} I_1 = \dfrac{1}{2a^2}$ with $a = \dfrac{m^*}{2k_B T}$

Then $I_3 = \dfrac{1}{2} \times 4\left(\dfrac{k_B T}{m^*}\right)^2$ so that we get $\bar{v}_{th} = 8\pi\left(\dfrac{m^*}{2\pi k_B T}\right)^{3/2}\left(\dfrac{k_B T}{m^*}\right)^2$

i.e. $\boxed{\bar{v}_{th} = \left(\dfrac{8 k_B T}{\pi m^*}\right)^{1/2}}$

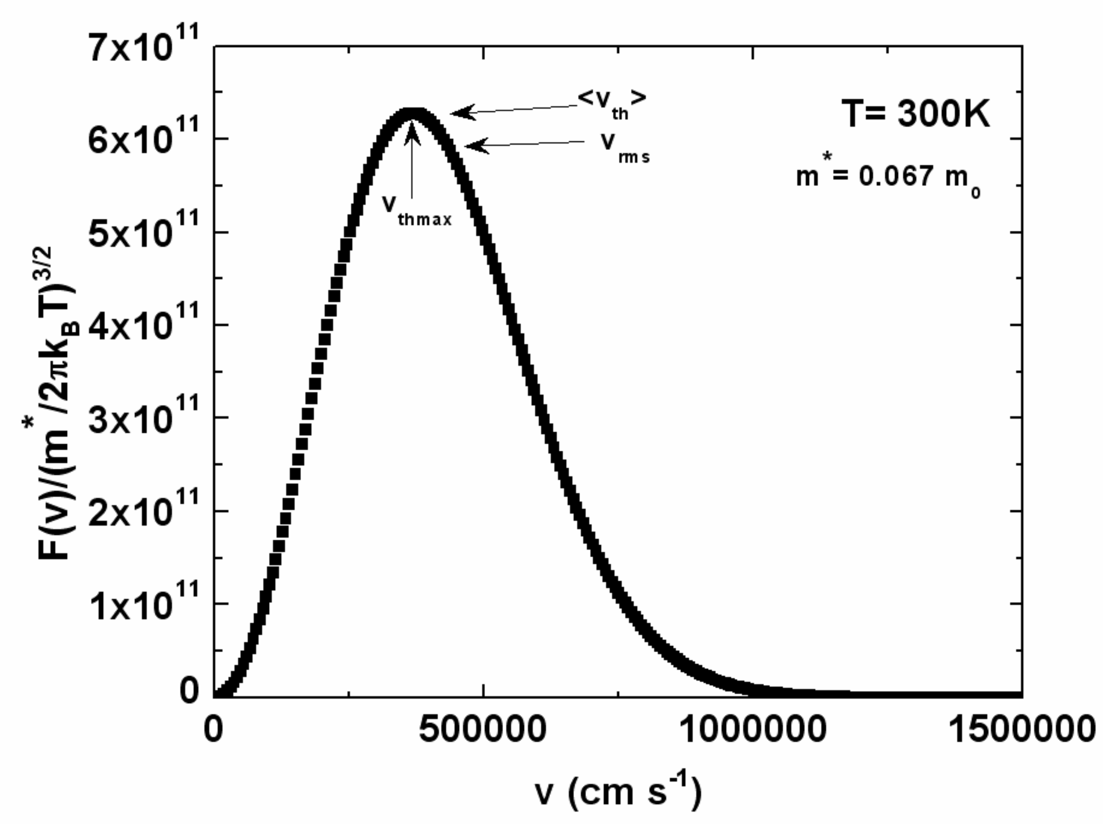
Finally, we thus have $v_{rms} > \bar{v}_{th} > v_{th_{max}}$ (cf. figure showing the velocity distribution function of electrons in GaAs at $T = 300K$)

4- $|\vec{E}| = 1 \times 10^5\ V.cm^{-1}$

$|\vec{v}_{d_n}(Si)| = 1.35 \times 10^8\ cm.s^{-1}$ and $|\vec{v}_{d_n}(GaAs)| = 8 \times 10^8\ cm.s^{-1}$

$v_{rms}(Si) \approx 1.22 \times 10^7\ cm.s^{-1}$ and $v_{rms}(GaAs) \approx 4.51 \times 10^7\ cm.s^{-1}$

It is seen that in this specific case the drift velocity $|\vec{v}_{d_n}|$ exceeds v_{rms} by more than one order of magnitude. Obviously such a situation is clearly a physical nonsense as for high fields, electrons reach their saturation velocity, the excess energy being released to the atomic lattice through the emission of optical phonons (cf. lecture).



7x10^11
6x10^11
5x10^11
4x10^11
3x10^11
2x10^11
1x10^11
0
F(v)/(m*/2πk_B T)^3/2
0
500000
1000000
1500000
v (cm s^-1)
<v_th>
v_rms
v_thmax
T= 300K
m* = 0.067 m_0

Exercise 3 - Generalization of the statistics of donor levels

1- First, we can establish the relationship giving the number density of electrons n_d bound to donor sites: $n_d = N_d \langle n \rangle$ where $\langle n \rangle$ corresponds to the mean number of electrons in the levels at thermal equilibrium.

The donor level can be occupied in the following way:

(a) empty level, $N_j = 0$, $E_j = 0$, $g_j^{-1} = 1$ ↳ 1 configuration is associated with this level!

(b) singly occupied level, $N_j = 1$, $E_j = \varepsilon_d$, $g_j^{-1} = 2$ because the donor level can be occupied by an e^- of spin ↑ or ↓

(c) doubly occupied level, $N_j = 2$, $E_j = 2\varepsilon_d + \Delta$, $g_j^{-1} = 1$

As a result we get: $$\langle n \rangle = \frac{2e^{-\beta(\varepsilon_d-\mu)} + 2e^{-\beta(2\varepsilon_d+\Delta-2\mu)}}{1+2e^{-\beta(\varepsilon_d-\mu)} + e^{-\beta(2\varepsilon_d+\Delta-2\mu)}}$$

i.e. $$\langle n \rangle = \frac{2\cancel{e^{-\beta(\varepsilon_d-\mu)}}}{2\cancel{e^{-\beta(\varepsilon_d-\mu)}}} \; \frac{1+e^{-\beta(\varepsilon_d+\Delta-\mu)}}{\frac{1}{2}e^{\beta(\varepsilon_d-\mu)} + 1 + \frac{1}{2}e^{-\beta(\varepsilon_d+\Delta-\mu)}}$$

and finally $$\boxed{n_d = \frac{N_d\left(1+e^{-\beta(\varepsilon_d+\Delta-\mu)}\right)}{\frac{1}{2}e^{\beta(\varepsilon_d-\mu)} + 1 + \frac{1}{2}e^{-\beta(\varepsilon_d+\Delta-\mu)}}} \qquad (4.2)$$

2- As $\Delta \to +\infty$, $e^{-\beta(\varepsilon_d+\Delta-\mu)} \to 0$ so that eq. (4.2) is reduced to

$$\boxed{n_d = \frac{N_d}{\frac{1}{2}e^{\beta(\varepsilon_d-\mu)}+1}} \qquad (4.3)$$

3- As $\Delta \to 0$, (4.2) can be simplified in the following way:

$$\boxed{n_d = \frac{1+e^{-\beta(\varepsilon_d-\mu)}}{\frac{1}{2}e^{\beta(\varepsilon_d-\mu)} + 1 + \frac{1}{2}e^{-\beta(\varepsilon_d-\mu)}} N_d}$$

By putting $x = \beta(\varepsilon_d - \mu)$, we get $n_d = 2N_d \dfrac{1+e^{-x}}{2+e^{x}+e^{-x}}$

As $e^{x}+e^{-x}+2 = (e^{x}+1)(e^{-x}+1)$, we then obtain

$$n_d = 2\,\frac{\cancel{(1+e^{-x})}}{\cancel{(1+e^{-x})}} \times \frac{1}{1+e^{x}}\,N_d$$

i.e. $n_d = 2N_d\,\underbrace{[1+e^{\beta(\varepsilon_d-\mu)}]^{-1}}$ Fermi-Dirac distribution

and finally $\boxed{n_d = \underset{\smile}{2}N_d f_{FD}(\varepsilon_d)}$

factor indicating that the donor levels can be occupied by $2e^-$ of opposite spin.

4- We still have the relationship $n_d = N_d \langle n \rangle$. However, each donor level will introduce many bound electronic orbitals of energy ε_i. As a consequence in (4.3) ε_d must be replaced with the ε_i. If we consider a system where donor levels possess two orbitals, we get from (4.3) (in fact from (4.1)) $n_d = N_d\left[\dfrac{2e^{-\beta(\varepsilon_1-\mu)}+2e^{-\beta(\varepsilon_2-\mu)}}{1+2e^{-\beta(\varepsilon_1-\mu)}+2e^{-\beta(\varepsilon_2-\mu)}}\right]$

$$\text{i.e. } n_d = 2N_d\,\frac{\sum_{i=1}^{2} e^{-\beta(\varepsilon_i-\mu)}}{2\sum_{i=1}^{2} e^{-\beta(\varepsilon_i-\mu)}} \times \frac{1}{\frac{1}{2}\left(\sum_{i=1}^{2} e^{-\beta(\varepsilon_i-\mu)}\right)^{-1}+1}$$

and finally $$n_d = N_d\,\frac{1}{\frac{1}{2}\left(\sum_{i=1}^{2} e^{-\beta(\varepsilon_i-\mu)}\right)^{-1}+1}$$

Such an equation can be extended to a larger number of orbitals which finally leads to (4.4).