

SOLUTIONS: ECE 656 Homework 1: Week 1

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- 1) Working out Fermi-Dirac integrals just takes some practice. For practice, work out the integral

$$I_1 = \int_{-\infty}^{\infty} M(E) f_0(E) dE$$

where

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

and

$$M(E) = W \frac{\sqrt{2m^*(E-E_C)}}{\pi \hbar} H(E-E_C)$$

where

$H(E-E_C)$ is the unit step function.

Solution:

$$I_1 = \int_{E_C}^{\infty} W \frac{\sqrt{2m^*(E-E_C)}}{\pi \hbar} \frac{1}{1 + e^{(E-E_F)/k_B T}} dE$$

Note that the unit step function in $M(E)$ makes the lower limit of the integral E_C .

$$I_1 = W \frac{\sqrt{2m^*}}{\pi \hbar} \int_{E_C}^{\infty} \frac{(E-E_C)^{1/2}}{1 + e^{(E-E_F)/k_B T}} dE$$

Now make the change in variables, $\eta = (E-E_C)/k_B T$ and $\eta_F = (E_F-E_C)/k_B T$ to find:

$$I_1 = W \frac{\sqrt{2m^*}}{\pi \hbar} \int_0^{\infty} \frac{(k_B T \eta)^{1/2}}{1 + e^{\eta - \eta_F}} (k_B T) d\eta$$

ECE 656 Homework 1: Week 1 (continued)

$$I_1 = W \frac{\sqrt{2m^*}}{\pi \hbar} (k_B T)^{3/2} \int_0^\infty \frac{\eta^{1/2}}{1 + e^{\eta - \eta_F}} d\eta$$

Now we can recognize the FD integral of order $1/2$:

$$\int_0^\infty \frac{\eta^{1/2}}{1 + e^{\eta - \eta_F}} d\eta = \frac{\sqrt{\pi}}{2} \mathcal{F}_{1/2}(\eta_F)$$

so the result becomes

$$I_1 = W \frac{\sqrt{m^*/2\pi}}{\hbar} (k_B T)^{3/2} \mathcal{F}_{1/2}(\eta_F),$$

which is the final answer.

2) For more practice, work out the integral in 1) assuming non-degenerate carrier statistics.

Solution:

We could approximate the Fermi function as

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}} \approx e^{(E_F - E)/k_B T}$$

and then work out the integral

$$I_1 = \int_{E_C}^\infty W \frac{\sqrt{2m^*(E - E_C)}}{\pi \hbar} \frac{1}{1 + e^{(E - E_F)/k_B T}} dE \approx \int_{E_C}^\infty W \frac{\sqrt{2m^*(E - E_C)}}{\pi \hbar} e^{(E_F - E)/k_B T} dE$$

but it is easier to recognize that “non-degenerate” means $E_F \ll E$ or $\eta_F \ll 0$ and that

$$\mathcal{F}_{1/2}(\eta_F) \rightarrow \exp(\eta_F) \text{ for } \eta_F \ll 0$$

so we can use the result of prob. 1) and write the answer as

$$I_1 \approx W \frac{\sqrt{m^*/2\pi}}{\hbar} (k_B T)^{3/2} \exp(\eta_F)$$

ECE 656 Homework 1: Week 1 (continued)

3) For still more practice, work out this integral:

$$I_2 = \int_{E_C}^{\infty} M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE ,$$

where $M(E)$ is as given in problem 1).

Solution:

From the form of the Fermi function, we see that

$$\left(-\frac{\partial f_0}{\partial E} \right) = \left(+\frac{\partial f_0}{\partial E_F} \right)$$

so the integral becomes

$$I_2 = \int_{E_C}^{\infty} M(E) \left(+\frac{\partial f_0}{\partial E_F} \right) dE .$$

Since we are integrating with respect to energy, not Fermi energy, we can move the derivative outside of the integral to write

$$I_2 = \frac{\partial}{\partial E_F} \int_{E_C}^{\infty} M(E) f_0(E) dE = \frac{1}{k_B T} \frac{\partial}{\partial (E_F / k_B T)} \int_{E_C}^{\infty} M(E) f_0(E) dE = \frac{1}{k_B T} \frac{\partial}{\partial \eta_F} \int_{E_C}^{\infty} M(E) f_0(E) dE$$

The integral can be recognized as the one we worked out in prob. 1), so

$$I_2 = \frac{1}{k_B T} \frac{\partial}{\partial \eta_F} I_1 = \frac{1}{k_B T} \frac{\partial}{\partial \eta_F} \left\{ W \frac{\sqrt{m^* / 2\pi}}{\hbar} (k_B T)^{3/2} \mathcal{F}_{1/2}(\eta_F) \right\} = W \frac{\sqrt{m^* k_B T / 2\pi}}{\hbar} \frac{\partial}{\partial \eta_F} \mathcal{F}_{1/2}(\eta_F)$$

Finally, using the differentiation property of FD integrals, we find

$$\boxed{I_2 = W \frac{\sqrt{m^* k_B T / 2\pi}}{\hbar} \mathcal{F}_{-1/2}(\eta_F)}$$

The trick of replacing $-\partial f_0 / \partial E$ with $+\partial f_0 / \partial E_F$ and then moving the derivative outside of the integral is very useful in evaluating FD integrals.

ECE 656 Homework 1: Week 1 (continued)

- 4) It is important to understand when Fermi-Dirac statistics must be used and when non-degenerate (Maxwell-Boltzmann) statistics are good enough. The electron density in 1D is

$$n_L = N_{1D} \mathcal{F}_{-1/2}(\eta_F) \text{ cm}^{-1},$$

where N_{1D} is the 1D effective density of states and $\eta_F = (E_F - E_C)/k_B T$. In 3D,

$$n = N_{3D} \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}.$$

For Maxwell Boltzmann statistics

$$n_L^{MB} = N_{1D} \exp(\eta_F) \text{ cm}^{-1}$$

$$n^{MB} = N_{3D} \exp(\eta_F) \text{ cm}^{-3}.$$

Compute the ratios, n_L/n_L^{MB} and n/n^{MB} for each of the following cases:

- a) $\eta_F = -10$
- b) $\eta_F = -3$
- c) $\eta_F = 0$
- d) $\eta_F = 3$
- e) $\eta_F = 10$

Note that there is a Fermi-Dirac integral calculator available on nanoHUB.org. An iPhone app is also available.

Solution:

The iPhone app is called: "FD Integral"

The nanoHUB.org app is at: nanohub.org/resources/11396

a) $\eta_F = -10$:

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{-1/2}(-10) / \exp(-10) = 4.54 \times 10^{-5} / 4.54 \times 10^{-5} = 1$$

$$\boxed{n_L/n_L^{MB} = \mathcal{F}_{-1/2}(-10) / \exp(-10) = 1}$$

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{+1/2}(-10) / \exp(-10) = 4.54 \times 10^{-5} / 4.54 \times 10^{-5} = 1$$

$$\boxed{n/n^{MB} = \mathcal{F}_{+1/2}(-10) / \exp(10) = 1}$$

ECE 656 Homework 1: Week 1 (continued)**b) eta_F = -3:**

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{-1/2}(-3) / \exp(-3) = 4.81 \times 10^{-2} / 4.98 \times 10^{-2} = 0.97$$

$$\boxed{n_L/n_L^{MB} = \mathcal{F}_{-1/2}(-3) / \exp(-3) = 0.97}$$

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{+1/2}(-3) / \exp(-3) = 4.89 \times 10^{-2} / 4.98 \times 10^{-2} = 0.98$$

$$\boxed{n/n^{MB} = \mathcal{F}_{+1/2}(-3) / \exp(-3) = 0.98}$$

c) eta_F = 0:

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{-1/2}(0) / \exp(0) = 6.05 \times 10^{-1} / 1 = 0.61$$

$$\boxed{n_L/n_L^{MB} = \mathcal{F}_{-1/2}(-3) / \exp(-3) = 0.61}$$

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{+1/2}(0) / \exp(0) = 7.65 \times 10^{-1} / 1 = 0.77$$

$$\boxed{n/n^{MB} = \mathcal{F}_{+1/2}(-3) / \exp(-3) = 0.77}$$

d) eta_F = +3:

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{-1/2}(3) / \exp(3) = 1.85 \times 10^0 / 2.01 \times 10^1 = 0.092$$

$$\boxed{n_L/n_L^{MB} = \mathcal{F}_{-1/2}(3) / \exp(3) = 0.092}$$

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{+1/2}(3) / \exp(3) = 4.49 \times 10^0 / 2.01 \times 10^1 = 0.22$$

$$\boxed{n/n^{MB} = \mathcal{F}_{+1/2}(-3) / \exp(-3) = 0.22}$$

ECE 656 Homework 1: Week 1 (continued)**e) $\eta_F = +3$:**

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{-1/2}(10) / \exp(10) = 3.55 \times 10^0 / 2.20 \times 10^4 = 1.610 \times 10^{-4}$$

$$\boxed{n_L/n_L^{MB} = \mathcal{F}_{-1/2}(10) / \exp(10) = 1.61 \times 10^{-4}}$$

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F) / \exp(\eta_F) = \mathcal{F}_{+1/2}(10) / \exp(10) = 2.41 \times 10^1 / 2.20 \times 10^4 = 1.10 \times 10^{-3}$$

$$\boxed{n/n^{MB} = \mathcal{F}_{+1/2}(10) / \exp(10) = 1.10 \times 10^{-3}}$$

- 5) Consider GaAs at room temperature doped such that $n = 10^{19} \text{ cm}^{-3}$. The electron density is related to the position of the Fermi level according to

$$n = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}$$

where

$$N_C = 4.21 \times 10^{17} \text{ cm}^{-3}.$$

Determine the position of the Fermi level relative to the bottom of the conduction band, E_C .

- a) assuming Maxwell-Boltzmann carrier statistics
- b) NOT assuming Maxwell-Boltzmann carrier statistics

Solution:

$$\text{a) } n = N_C \mathcal{F}_{1/2}(\eta_F) \rightarrow n = N_C \exp(\eta_F) \text{ cm}^{-3}$$

$$\eta_F = \frac{E_F - E_C}{k_B T} = \ln\left(\frac{n}{N_C}\right) = \ln\left(\frac{10^{19}}{4.21 \times 10^{17}}\right) = 3.17$$

$$E_F = E_C + 3.17 \times 0.026 \text{ eV} = E_C + 0.082 \text{ eV}$$

$$\boxed{E_F = E_C + 0.082 \text{ eV}}$$

ECE 656 Homework 1: Week 1 (continued)

$$\text{b) } n = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}$$

$$\eta_F = \mathcal{F}_{1/2}^{-1}(n/N_C) = \mathcal{F}_{1/2}^{-1}(10^{19}/4.21 \times 10^{17}) = \mathcal{F}_{1/2}^{-1}(23.75) = 9.91$$

$$E_F = E_C + 9.91 \times 0.026 \text{ eV} = E_C + 0.26 \text{ eV}$$

$$\boxed{E_F = E_C + 0.26 \text{ eV}}$$