SOLUTIONS: ECE 656 Homework 1: Week 1

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To complete this HW assignment, you will need a basic familiarity with Fermi-Dirac integrals. A good reference is the following.

R. Kim and M. Lundstrom, "Notes on Fermi-Dirac Integrals," 3rd Ed., https://www.nanohub.org/resources/5475

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

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

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:

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

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

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

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

$$I_1 = W\frac{\sqrt{2m^*}}{\pi\hbar}\int_{0}^{\infty}\frac{(k_BT\eta)^{1/2}}{1+e^{\eta-\eta_F}}(k_BT) d\eta$$

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

Now we can recognize the FD integral of order ½:

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

so the result becomes

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

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

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

and then work out the integral

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

but it is easier to recognize that "non-degenerate" means $E_F << E$ or $\eta_F << 0$ and that

$$\mathcal{F}_{1/2}\left(\eta_F\right) \rightarrow \exp\left(\eta_F\right) \quad \text{for } \eta_F << 0$$

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

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

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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

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

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

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

Finally, using the differentiation property of FD integrals, $\partial\mathcal{F}_j/\partial\eta_F = \mathcal{F}_{j-1}$, we find

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

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.

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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:

$$n_L/n_L^{MB} = \mathcal{F}_{-1/2}(\eta_F)\ /\exp(\eta_F) = \mathcal{F}_{-1/2}(-10)\ /\exp(-10) = 4.54\times10^{-5}/4.54\times10^{-5} = 1$$

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

$$n/n^{MB} = \mathcal{F}_{+1/2}(\eta_F)\ /\exp(\eta_F) = \mathcal{F}_{+1/2}(-10)\ /\exp(-10) = 4.54\times10^{-5}/4.54\times10^{-5} = 1$$

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

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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:

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

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

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

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

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e) eta_F = +10:

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

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

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

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

We see that the carrier density computed with Fermi-Dirac statistics is equal to the carrier density computed with Maxwell-Boltzmann (nondegenerate) carrier statistics when the semiconductor is nondegenerate, but it is a small fraction of the carrier density computed with Maxwell-Boltzmann statistics when the semiconductor is degenerate. We also see that the influence of FD statistics is stronger in 1D than in 3D.

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:

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

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

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

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

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

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

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

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

Assuming Maxwell-Boltzmann statistics, we find a Fermi level that is just a little above E_C, but for Fermi-Dirac statistics, we see that the Fermi level is $10k_BT$ above E_C. This is a significant difference, and might be important for some problems. For example, in this case, the Fermi level is well above the bottom of the band where conduction band non-parabolicity may be important.