SOLUTIONS: ECE 656 Homework (Week 8)

Mark Lundstrom
Purdue University

1) The general expression for conductance,

$$G = \frac{2q^2}{h}\int \mathcal{T}(E)\,M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE,$$

can be written as

$$G = \frac{2q^2}{h}\langle\langle \mathcal{T}(E)\rangle\rangle\langle M(E)\rangle .$$

In the diffusive limit, for a 3D resistor

$$\sigma_{3D} = \frac{2q^2}{h}\langle\langle \lambda(E)\rangle\rangle\langle M(E)/A\rangle\frac{A}{L}.$$

Derive the general expressions for $\langle M(E)/A\rangle$ and for $\langle\langle \lambda(E)\rangle\rangle$ in terms of their energy-dependent quantities, $M(E)$ and $\lambda(E)$. HINT: Begin at the ballistic limit and determine $M(E)$ first.

Solution:

Begin in the ballistic limit, where $\mathcal{T} = 1$ and we have:

$$G = \int_{-\infty}^{+\infty}\frac{2q^2}{h}M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE = \frac{2q^2}{h}\langle M\rangle$$

$$\langle M\rangle = \int M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

Note that:

$$\int_{-\infty}^{+\infty}\left(-\frac{\partial f_0}{\partial E}\right)dE = -\int_{-\infty}^{+\infty}df_0 = -f_0(+\infty)+f_0(-\infty) = -0+1 = 1$$

so we can write:

$$\langle M\rangle = \frac{\int_{-\infty}^{+\infty}M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int_{-\infty}^{+\infty}\left(-\frac{\partial f_0}{\partial E}\right)dE}. \qquad \text{(i)}$$

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Equation (i) looks like an average. We interpret it as the average number of channels in the Fermi window.

Now include the transmission:

$$G = \frac{2q^2}{h}\int \mathcal{T}(E)\, M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$G = \frac{2q^2}{h}\frac{\int \mathcal{T}(E)\, M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\langle M\rangle}\langle M\rangle$$

so we define:

$$\langle\langle \mathcal{T}(E)\rangle\rangle = \frac{\int \mathcal{T}(E)\, M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

In the diffusive limit:

$$\left\langle\left\langle \frac{\lambda(E)}{L}\right\rangle\right\rangle = \frac{\int \frac{\lambda(E)}{L} M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

Multiple through by *L* to find

$$\langle\langle \lambda(E)\rangle\rangle = \frac{\int \lambda(E)\, M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE} \qquad \text{(ii)}$$

Writing (i) and (ii) on a per unit area basis, we find:

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$$\boxed{\begin{aligned}\langle M\rangle &= \frac{\int_{-\infty}^{+\infty}\left(M(E)/A\right)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int_{-\infty}^{+\infty}\left(-\frac{\partial f_0}{\partial E}\right)dE}\\ \langle\langle\lambda(E)\rangle\rangle &= \frac{\int\lambda(E)\left(M(E)/A\right)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int\left(M(E)/A\right)\left(-\frac{\partial f_0}{\partial E}\right)dE}\end{aligned}}$$

2) Begin this problem with the expression for the 2D conductivity:

$$\sigma_S = \frac{2q^2}{h}\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\,.$$

2a) Assume a constant mfp,

$$\lambda(E-E_C)=\lambda_0\,,$$

and work out an expression for the 2D mobility in terms of the mfp. Your results should be valid for any level of carrier degeneracy. Simplify your results for T = 0K and for non-degenerate conditions.

2b) Assume a "power law" mfp describe by

$$\lambda(E-E_C)=\lambda_0\left[\left(E-E_C/k_BT_L\right)\right]^r,$$

where "r" is a characteristic exponent that describes scattering. Repeat problem 2a) for this energy-dependent mfp.

Note: for T = 0 K, only one energy matters, so it is best just to write $\lambda(E)$ and not use the power law form.

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Solution:

Let's use the result in Lundstrom and Jeong, Appendix, p. 218, eqn. (A.30)

$$\sigma_S = \frac{2q^2}{h}\lambda_0 \frac{\sqrt{2m^* k_B T}}{\pi\hbar}\Gamma\left(r+\frac{3}{2}\right)\mathcal{F}_{r-1/2}\left(\eta_F\right)$$

2a) *r* = 0 energy independent mfp

$$\sigma_S = \frac{2q^2}{h}\lambda_0 \frac{\sqrt{2m^* k_B T}}{\pi\hbar}\Gamma\left(\frac{3}{2}\right)\mathcal{F}_{-1/2}\left(\eta_F\right) \equiv n_S q \mu_n \qquad \text{(i)}$$

$$n_S = \frac{m^* k_B T}{\pi\hbar^2}\mathcal{F}_0\left(\eta_F\right)$$

$$\mu_n = \frac{1}{n_S}\frac{2q}{h}\lambda_0 \frac{\sqrt{2m^* k_B T}}{\pi\hbar}\Gamma\left(\frac{3}{2}\right)\mathcal{F}_{-1/2}\left(\eta_F\right) = \frac{\frac{2q}{h}\lambda_0 \frac{\sqrt{2m^* k_B T}}{\pi\hbar}\Gamma\left(\frac{3}{2}\right)\mathcal{F}_{-1/2}\left(\eta_F\right)}{\frac{m^* k_B T}{\pi\hbar^2}\mathcal{F}_0\left(\eta_F\right)}$$

$$\mu_n = \frac{\frac{q}{\pi}\lambda_0\sqrt{\frac{2}{m^* k_B T}}\Gamma\left(\frac{3}{2}\right)}{}\frac{\mathcal{F}_{-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)} \qquad \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{2}$$

$$\mu_n = \frac{q\lambda_0\sqrt{\frac{2k_B T}{\pi m^*}}}{2k_B T}\frac{\mathcal{F}_{-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)} = \frac{\lambda_0 \upsilon_T}{2\left(k_B T/q\right)}\frac{\mathcal{F}_{-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)}$$

The result is:

$$\boxed{\mu_n = \frac{\left(\lambda_0 \upsilon_T/2\right)}{\left(k_B T/q\right)}\frac{\mathcal{F}_{-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)}}$$

For non-degenerate statistics, this simplifies to:

$$\boxed{\mu_n = \frac{\left(\lambda_0 \upsilon_T/2\right)}{\left(k_B T/q\right)}}$$

ECE 656 Homework (Week 8) (continued)

For degenerate statistics, is it best to begin again with:

$$\sigma_S = \frac{2q^2}{h} M_{2D}\left(E_F\right)\lambda\left(E_F\right) = nq\mu_n$$

$$\mu_n = \frac{1}{n_S}\frac{2q}{h} M_{2D}\left(E_F\right)\lambda\left(E_F\right) = \frac{1}{m^*/\left(\pi\hbar^2\right)\left(E_F - E_C\right)}\frac{2q}{h}\frac{\sqrt{2m^*\left(E_F - E_C\right)}}{\pi\hbar}\lambda\left(E_F\right)$$

$$\mu_n = \frac{1}{\left(E_F - E_C\right)/q}\frac{\sqrt{2\left(E_F - E_C\right)/m^*}}{\pi}\lambda\left(E_F\right)$$

$$\mu_n = \frac{1}{\left(E_F - E_C\right)/q}\frac{\left(2\upsilon_F/\pi\right)\lambda_F}{2} \qquad \left(\lambda_F = \lambda\left(E_F\right)\right)$$

$$\boxed{\mu_n = \frac{\left[\left(2\upsilon_F/\pi\right)\lambda_F\right]/2}{\left(E_F - E_C\right)/q}}$$

2b) energy dependent mfp

Use the result in Lundstrom and Jeong, Appendix, p. 218, eqn. (A.30)

$$\sigma_S = \frac{2q^2}{h}\lambda_0\frac{\sqrt{2m^* k_B T}}{\pi\hbar}\Gamma\left(r + 3/2\right)\mathcal{F}_{r-1/2}\left(\eta_F\right)$$

Repeating the derivation of part 2a), we find:

$$\mu_n = \frac{\frac{q}{\pi}\lambda_0\sqrt{\frac{2}{m^* k_B T}}\Gamma\left(r + 3/2\right)}{}\frac{\mathcal{F}_{r-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)}$$

$$\mu_n = \frac{\lambda_0\sqrt{\frac{2k_B T}{\pi m^*}}\frac{\Gamma\left(r + 3/2\right)}{\sqrt{\pi}}}{k_B T/q}\frac{\mathcal{F}_{r-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)}$$

$$\boxed{\mu_n = \frac{\left(\lambda_0\upsilon_T/2\right)}{k_B T/q}\frac{\Gamma\left(r + 3/2\right)}{\Gamma\left(3/2\right)}\frac{\mathcal{F}_{r-1/2}\left(\eta_F\right)}{\mathcal{F}_0\left(\eta_F\right)}}$$

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For non-degenerate statistics, this simplifies to:

$$\boxed{\mu_n = \frac{(\lambda_0 \upsilon_T/2)}{k_B T/q} \frac{\Gamma(r+3/2)}{\Gamma(3/2)}}$$

For degenerate statistics:

$$\boxed{\mu_n = \frac{[(2\upsilon_F/\pi)\lambda_F]/2}{(E_F - E_C)/q}}$$

3) In 3D, we relate the current density to the electric field by

$$\mathcal{E}_x = \rho_{3D} J_x \ ,$$

where $\mathcal{E}_x$ is the electric field in V/m and J_x is the current density in A/m^2. Write the corresponding equations in 1D and 2D and determine the units of ρ_{1D}, $\rho_{2D} = \rho_S$, and ρ_{3D}.

Solution:

For 1D, there is no current density, just current, so we have:

$$\mathcal{E}_x = \rho_{1D} I_x$$

in terms of units, we can write:

V/m = ( ) A

To make the units match, we must have: ( ) = V/(A-m) = **Ohms/m**

For 2D, the current density is in A/m:

$$\mathcal{E}_x = \rho_{2D} J_x$$

in terms of units, we can write:

V/m = ( ) A/m

To make the units match, we must have: ( ) = V/(A) = **Ohms**

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For 3D, the current density is in A/m²:

$$\mathcal{E}_x = \rho_{3D} J_x$$

in terms of units, we can write:

V/m = ( ) A/m²

To make the units match, we must have: ( ) = V-m/(A) = **Ohms-m**

4) Assume an n-channel MOSFET at T = 300 K with $n_S = 10^{13}$ cm^{-3}. Assume that only the lowest subband is occupied and compute $\langle M_{2D} \rangle$, the average number of modes in the Fermi window per micrometer of channel width.

Solution:

The first step is to determine the location of the Fermi level.

$$n_S = N_{2D} \mathcal{F}_0(\eta_F) = g_V \frac{m^* k_B T}{\pi \hbar^2} \ln\left(1 + e^{\eta_F}\right) \qquad \text{(i)}$$

For the first unprimed subband,

$$m^* = m_t = 0.19 m_0$$
$$g_V = 2$$

$$N_{2D} = g_V \frac{m^* k_B T}{\pi \hbar^2} = 2 \frac{0.19 \times 9.11 \times 10^{-31} \times 1.38 \times 10^{-23} \times 300}{3.14 \times \left(1.055 \times 10^{-34}\right)^2}$$

$$N_{2D} = 4.1 \times 10^{12} \text{ cm}^{-2}$$

$$n_S = N_{2D} \ln\left(1 + e^{\eta_F}\right) \rightarrow \eta_F = \ln\left(e^{n_S/N_{2D}} - 1\right) = \ln\left(e^{10/4.1} - 1\right)$$

$$\eta_F = 2.35$$

From slide 23 of Lecture 7, Fall 2011:

$$\langle M_{2D} \rangle = g_V \frac{\sqrt{2 m^* k_B T_L}}{\pi \hbar} \frac{\sqrt{\pi}}{2} \mathcal{F}_{-1/2}(\eta_F)$$

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Putting in numbers:

$$\langle M_{2D} \rangle = 2\frac{\sqrt{2\times 0.19\times 9.11\times 10^{-31}\times 1.38\times 10^{-23}\times 300}}{3.14\times 1.055\times 10^{-34}}\frac{\sqrt{3.14}}{2}\mathcal{F}_{-1/2}(2.35)$$

$$\langle M_{2D} \rangle = 2.025\times 10^{8}\times \mathcal{F}_{-1/2}(2.35) = 2.025\times 10^{8}\times 1.607 = 3.25\times 10^{8}\ \text{m}^{-1}$$

$$\boxed{\langle M_{2D} \rangle = 325\ \mu\text{m}^{-1}}$$

Consider an L = 22 nm technology with $W = L$ = 0.022 micrometers. We would have, $\langle M_{2D} \rangle = 7$, a fairly small number.

5) According to equ. (6.9) on p. 182 of *Advanced Semiconductor Fundamentals*, 2nd Ed., (R.F. Pierret, 2003) the mobility of electrons in Si for $N_D = 10^{14}\ \text{cm}^{-3}$ at $T = 300\ \text{K}$ is $1268\ \text{cm}^2/\text{V-s}$ and at $N_D = 10^{20}\ \text{cm}^{-3}$ it is $95\,\text{cm}^2/\text{V-s}$. Determine the average mean-free-path, $\langle\langle \lambda \rangle\rangle$ in both cases.

Solution:

The assumption is that we are dealing with a 3D semiconductor. The conductivity is written as:

$$\sigma = \frac{2q^2}{h}\lambda_0 \langle M_{3D}/A \rangle \qquad \text{(i)}$$

$$\langle M_{3D}/A \rangle = g_V \frac{m^* k_B T}{2\pi\hbar^2}\mathcal{F}_0(\eta_F) \qquad \text{(ii)}$$

What effective mass do we use in this expression?

Not the density of state effective mass

Not the conductivity effective mass

We should use the "distribution of modes" effective mass (See Jeong, et al., J. Appl. Phys., 107, 023707, 2010).

$$g_V m^* = m^*_{DOM} = 2m^*_t + 4\sqrt{m^*_t m^*_\ell} = 2.04 m_0 \qquad \text{(iii)}$$

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Before we can use (ii), however, we must determine η_F.

$$n = N_C \mathcal{F}_{1/2}(\eta_F)$$

$N_C = 1.03 \times 10^{19}\ \text{cm}^{-3}$ (Pierret, Adv. Semiconductor Fundamentals, p. 113)

Note that the effective DOS makes use of the density-of-states effective mass:

$$m^*_{DOS} = 6^{2/3}\left(m_\ell m_t^2\right)^{1/3} = 1.06 m_0,$$

which is quite different from the distribution of modes effective mass.

So now we have a **procedure:**

1) Given the carrier density, solve for η_F

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F)$$

2) Next, solve for the average number of channels in the Fermi window:

$$\langle M_{3D}/A \rangle = \frac{m^*_{DOM} k_B T}{2\pi\hbar^2} \mathcal{F}_0(\eta_F)$$

4) Then find the conductivity from the given data:

$$\sigma = n_0 q \mu_n$$

5) Finally, solve for the mean-free-path:

$$\lambda_0 = \frac{\sigma}{\left(2q^2/h\right)} \frac{1}{\langle M_{3D}/A \rangle}$$

Case i): $n_0 = N_D = 10^{14}\ \text{cm}^{-3}$ (non-degenerate)

$$\eta_F = \ln(n_0/N_C) = -11.5$$

$$\langle M_{3D}/A \rangle = \frac{m^*_{DOM} k_B T}{2\pi\hbar^2} \mathcal{F}_0(-11.5) = 1.07 \times 10^8\ \text{cm}^{-2}$$

$$\sigma = n_0 q \mu_n = 10^{14} \times 1.6 \times 10^{-19} \times 1268 = 2.03 \times 10^{-2}\ \text{S/cm}$$

$$\sigma = n_0 q \mu_n = 10^{14} \times 1.6 \times 10^{-19} \times 1268 = 2.03 \times 10^{-2}$$

$$\frac{\sigma}{\left(2q^2/h\right)} = 263$$

$$\lambda_0 = \frac{\sigma}{\left(2q^2/h\right)} \frac{1}{\langle M_{3D}/A \rangle} = 263 \times \frac{1}{1.07 \times 10^8} = 25\ \text{nm}$$

$$\boxed{\lambda_0 = 25\ \text{nm}}$$

ECE 656 Homework (Week 8) (continued)

Case ii): $n_0 = N_D = 10^{20}$ cm^{-3} (degenerate)

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F) \rightarrow 10^{20} = 1.03\times10^{19}\mathcal{F}_{1/2}(\eta_F) \rightarrow \eta_F = 5.34$$

$$\langle M_{3D}/A\rangle = \frac{m^*_{DOM}k_BT}{2\pi\hbar^2}\mathcal{F}_0(5.34) = 1.1\times10^{13}\ \mathcal{F}_0(5.34)\text{cm}^{-2} = 5.87\times10^{13}\ \text{cm}^{-2}$$

$$\sigma = n_0 q\mu_n = 10^{20}\times1.6\times10^{-19}\times95 = 1.52\times10^3$$

$$\frac{\sigma}{\left(2q^2/h\right)} = 1.97\times10^7$$

$$\lambda_0 = \frac{\sigma}{\left(2q^2/h\right)}\frac{1}{\langle M_{3D}/A\rangle} = 1.97\times10^7\times\frac{1}{5.87\times10^{13}} = 3.4\text{ nm}$$

$$\boxed{\lambda_0 = 3.4\text{ nm}}$$

6) We have asserted that $\Delta_n = 2k_BT_L$ for a non-degenerate, 3D semiconductor with parabolic energy bands and an energy-independent mean-free-path for backscattering. This means that the average energy at which current flows is $2k_BT_L$ above the bottom of the conduction band. Repeat the calculation, but this time assume power law scattering,

$$\lambda(E) = \lambda_0\left[(E-E_C)/(k_BT)\right]^r .$$

What is Δ_n in this case?

Solution:

$$\Delta_n = \frac{\int(E-E_C)\sigma'(E)dE}{\int\sigma'(E)dE}$$

$$\sigma'_n(E) = \frac{2q^2}{h}\frac{M(E)}{A}\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

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$$\Delta_n = \frac{\int (E-E_C)\frac{2q^2}{h}\frac{M(E)}{A}\lambda_0\left[(E-E_C)/k_BT\right]^r\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int \frac{2q^2}{h}\frac{M(E)}{A}\lambda_0\left[(E-E_C)/k_BT\right]^r\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

Most constants cancel (remember that $M \propto (E-E_C)$) and we find

$$\Delta_n = \frac{\int (E-E_C)^2\left[(E-E_C)/k_BT\right]^r\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int (E-E_C)\left[(E-E_C)/k_BT\right]^r\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

$$\eta = (E-E_C)/k_BT \qquad\qquad \eta_F = (E_F-E_C)/k_BT$$

$$\Delta_n = \frac{\int (k_BT)^2\eta^{2+r}\left(-\frac{\partial f_0}{\partial E}\right)k_BT\,d\eta}{\int k_BT\eta^{1+r}\left(-\frac{\partial f_0}{\partial E}\right)k_BT\,d\eta}$$

$$\Delta_n = k_BT\frac{\frac{\partial}{\partial\eta_F}\int\eta^{2+r}f_0\,d\eta}{\frac{\partial}{\partial\eta_F}\int\eta^{1+r}f_0\,d\eta} = k_BT\times\frac{\text{num}}{\text{dem}}$$

$$\text{num} = \frac{\partial}{\partial\eta_F}\int\eta^{2+r}f_0\,d\eta = \frac{\partial}{\partial\eta_F}\Gamma(3+r)\mathcal{F}_{2+r}(\eta_F) = \Gamma(3+r)\mathcal{F}_{1+r}(\eta_F)$$

$$\text{dem} = \frac{\partial}{\partial\eta_F}\int\eta^{1+r}f_0\,d\eta = \frac{\partial}{\partial\eta_F}\Gamma(2+r)\mathcal{F}_{1+r}(\eta_F) = \Gamma(2+r)\mathcal{F}_{r}(\eta_F)$$

Putting this together:

$$\Delta_n = k_BT\frac{\frac{\partial}{\partial\eta_F}\int\eta^{2+r}f_0\,d\eta}{\frac{\partial}{\partial\eta_F}\int\eta^{1+r}f_0\,d\eta} = k_BT\times\frac{\text{num}}{\text{dem}} = k_BT\frac{\Gamma(3+r)\mathcal{F}_{1+r}(\eta_F)}{\Gamma(2+r)\mathcal{F}_{r}(\eta_F)}$$

$$\boxed{\Delta_n = k_BT\frac{\Gamma(3+r)\mathcal{F}_{1+r}(\eta_F)}{\Gamma(2+r)\mathcal{F}_{r}(\eta_F)}}$$

ECE 656 Homework (Week 8) (continued)

For nondegenerate statistics, Fermi-Dirac integrals become exponentials and we find:

$$\boxed{\Delta_n = k_B T \frac{\Gamma(3+r)}{\Gamma(2+r)}}$$

For $r=0$ this gives $\Delta_n = 2k_B T$.

For ionized impurity scattering, $r=2$ and we find $\Delta_n = k_B T \frac{\Gamma(5)}{\Gamma(4)} = 4k_B T$.

7) Repeat prob. 6) in the strongly degenerate limit, and use the result to explain why the Seebeck coefficient of a metal approaches zero.

Solution:

Let's begin at:

$$\Delta_n = \frac{\int (E-E_C)^2 \left[(E-E_C)/k_B T\right]^r \left(-\frac{\partial f_0}{\partial E}\right) dE}{\int (E-E_C)\left[(E-E_C)/k_B T\right]^r \left(-\frac{\partial f_0}{\partial E}\right) dE} \tag{i}$$

$$\rightarrow \frac{(E_F-E_C)^2 \left[(E_F-E_C)/k_B T\right]^r}{(E_F-E_C)\left[(E_F-E_C)/k_B T\right]^r} = (E_F - E_C)$$

The Seebeck coefficient is

$$S_n = -\frac{(E_J - E_F)}{qT} \tag{ii}$$

$$E_J = E_C + \Delta_n = E_C + E_F - E_C = E_F$$

$E_J = E_F$. **Current flows at the Fermi level, so by (ii),** $S_n = 0$ **.**

ECE 656 Homework (Week 8) (continued)

8) In Lecture 10, Fall 2011, we worked out the approximate values of the four thermoelectric transport coefficients for lightly doped n-type Ge. For practical TE devices, the material would be doped so that $E_F \approx E_C$. Work out the four thermoelectric transport coefficients for n-type Ge doped at $N_D = 10^{19}$ cm^{-3}. You may assume that T = 300 K, that the dopants are fully ionized, and that the mean-free-path for backscattering, λ_0, is independent of energy.

Use the material parameters presented in Lecture 10, Fall 2011, but use a mobility of $\mu_n = 330\ \text{cm}^2/\text{V-s}$ (from http://www.ioffe.ru/SVA/NSM/Semicond/Ge/Figs/232.gif. You may assume **non-degenerate carrier statistics** (but realize that this assumption may not well-justified for $E_F \approx E_C$, which is the case here, so we will only obtain estimates). Work out approximate, numerical values for λ_0, ρ, S, π, and κ_e.

Solution:

Compute the thermal velocity:

$$\upsilon_T = \sqrt{\frac{2k_BT}{\pi m^*}} = 1.55\times 10^7 \text{ cm/s}$$

where we have used the **conductivity effective mass** of Ge: $m^* = 0.12 m_0$.

$$\frac{1}{m_c^*} \equiv \frac{1}{3}\left(\frac{1}{m_\ell^*} + \frac{2}{m_t^*}\right)$$

Now use the diffusion coefficient to determine the mean-free-path.

$$D_n = \frac{k_BT}{q}\mu_n = 8.6\,\text{cm}^2/\text{s} \qquad D_n = \frac{\upsilon_T \lambda_0}{2}\ \text{cm}^2/\text{s}$$

$$\lambda_0 = \frac{2D_n}{\upsilon_T} = 11.1\times 10^{-7}\,\text{cm} \qquad \boxed{\lambda_0 = 11.1\ \text{nm}}$$

$$\rho = 1/(n_0 q \mu_n) = 1/\left(10^{19}\times 1.6\times 10^{-19}\times 330\right) = 0.0019\ \Omega\text{-cm} \qquad \boxed{\rho = 0.0019\ \Omega\text{-cm}}$$

$$S = \left(\frac{k_B}{-q}\right)\left\{\frac{(E_c - E_F)}{k_BT} + \delta_n\right\}$$

$$(E_c - E_F)/k_BT \approx \ln(N_C/n_0) \qquad N_C = 1.04\times 10^{19}\ \ \text{cm}^{-3}$$

$$(E_c - E_F)/k_BT \approx \ln\left(\left(1.04\times 10^{19}\right)/10^{19}\right) = 3.9\times 10^{-2} \qquad \delta_n \approx 2$$

$$S = \left(\frac{k_B}{-q}\right)\left\{\frac{(E_c - E_F)}{k_BT} + \delta_n\right\} \approx -86\ \mu\text{V/K}\times\left\{3.92\times 10^{-2} + 2\right\} = -175\,\mu\text{V/K}$$

$$\boxed{S = -175\,\mu\text{V/K}}$$

ECE 656 Homework (Week 8) (continued)

$$\boxed{\pi = TS \approx -0.05\text{ V}}$$

$$\kappa_e = T\sigma\mathcal{L} = T\mathcal{L}/\rho \qquad \mathcal{L} \approx 2\left(k_B/q\right)^2$$

(We are using the factor of 2 because we assume nondegenerate carrier statistics.)

$$\kappa_e = \frac{T \times 2\left(k_B/q\right)^2}{\rho} = 0.24 \text{ W/m-K}$$

$$\boxed{\kappa_e = 0.24 \text{ W/m-K}}$$

9) Perhaps we should use Fermi-Dirac statistics for thermoelectric calculations when $E_F \approx E_c$. Repeat problem 8), but this time use Fermi-Dirac statistics to determine the approximate values of λ_0, ρ, S, π, and κ_e. You might find it useful to know that

$$\sigma_{3D} = \frac{2q^2}{h}\lambda_0\left(\frac{g_V m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0\left(\eta_F\right) \text{ and } S = -\left(\frac{k_B}{q}\right)\left\{\frac{2\mathcal{F}_1\left(\eta_F\right)}{\mathcal{F}_1\left(\eta_F\right)} - \eta_F\right\}$$

Solution:

The conductivity does not change from prob. 3):

$$\sigma_{3D} = 1/\rho = 1/0.0019 = 526 \text{ S/cm}$$

From: $\sigma_{3D} = \frac{2q^2}{h}\lambda_0\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0\left(\eta_F\right)$, we can solve for the MFP in terms of the conductivity:

$$\lambda_0 = \frac{\sigma_{3D}}{\left(\frac{2q^2}{h}\right)\left(g_V \frac{m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0\left(\eta_F\right)}$$

To proceed, we must find η_F using:

$$n_0 = 10^{19} = N_C \mathcal{F}_{1/2}\left(\eta_F\right) = 1.04\times10^{19}\mathcal{F}_{1/2}\left(\eta_F\right)$$

$$\eta_F = \mathcal{F}_{1/2}^{-1}\left(\frac{10^{19}}{1.04\times10^{19}}\right) = \mathcal{F}_{1/2}^{-1}\left(0.962\right) = 0.297$$

(computed with the iPhone app or with the nanoHUB tool: http://nanohub.org/resources/11396)

ECE 656 Homework (Week 8) (continued)

$$\lambda_0 = \frac{\sigma_{3D}}{\left(\frac{2q^2}{h}\right)\left(g_V \frac{m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0(\eta_F)} = \frac{5.26\times10^4 \ \text{S/m}}{\left(7.71\times10^{-5}\right)\left(6.37\times10^{16}\right)\mathcal{F}_0\left(0.297\right)} = 0.13\times10^{-7}\,\text{m}$$

where we used the "distribution of modes effective mass," $m^* = 1.18 m_0$. For a discussion of distribution of modes (DOM) effective mass, see:

> Changwook Jeong, Raseong Kim, Mathieu Luisier, Supriyo Datta, and Mark Lundstrom, "On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Transport Coefficients," *J. Appl. Phys.*, Vol. 107, 023707, 2010.

$\boxed{\lambda_0 = 13\ \text{nm}}$ a bit longer than for MB statistics

$\boxed{\rho = 0.0019\ \Omega\text{-cm}}$ same as before

$$S = -\left(\frac{k_B}{q}\right)\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F\right\} = -86\times10^{-6}\left\{\frac{2\mathcal{F}_1(0.297)}{\mathcal{F}_0(0.297)} - 0.297\right\} = -186\,\mu\text{V/K}$$

$\boxed{S = -186\ \mu\text{V/K}}$

$\boxed{\pi = TS \approx -0.06\ \text{V}}$

$$\kappa_e = T\sigma\mathcal{L} = T\mathcal{L}/\rho \qquad \mathcal{L} \approx \frac{\pi^2}{3}\left(k_B/q\right)^2$$

(We are using the fully degenerate Lorenz number, for simplicity.)

$$\kappa_e = \frac{T\times\frac{\pi^2}{3}\left(k_B/q\right)^2}{\rho} = 0.40 \ \ \text{W-m/K}$$

$\boxed{\kappa_e = 0.40 \ \ \text{W-m/K}}$

ECE 656 Homework (Week 8) (continued)

10) We have discussed two different electronic thermal conductivities – one measured under short circuit conditions, κ_0, and one measured under open circuit conditions, κ_e. The two are related according to:

$$\kappa_e = \kappa_0 - T\sigma S^2$$

Using the estimated TE transport coefficients for Ge doped such that $E_F \approx E_C$ (from prob. 9) find the numerical value of the ratio, κ_0 / κ_e.

Solution:

The relation between the two electronic thermal conductivities is:

$$\kappa_e = \kappa_0 - T\sigma S^2$$

$$\kappa_0 = \kappa_e + T\sigma S^2$$

Use numbers from problem 4)

$$\kappa_e = 0.40 \text{ W-m/K}$$

$$\sigma = 1/\rho = 1/0.0019 = 526 \text{ S/cm} = 5.26\times 10^4 \text{ S/m}$$

$$S = -186\ \mu\text{V/K} = -1.86\times 10^{-4} \text{ V/K}$$

$$\kappa_0 = \kappa_e + T\sigma S^2 = 0.40 + 300\times 5.26\times 10^4 \times \left(1.86\times 10^{-4}\right)^2 = 0.40 + 0.55$$

$$\kappa_0 = 0.95 \text{ W-m/K}$$

$$\boxed{\frac{\kappa_0}{\kappa_e} = 2.38}$$

11) Using the results of prob. 9), estimate the thermoelectric FOM, ZT for n-type Ge at T = 300 K. You may assume that $\kappa_L = 58$ W/m-K.

ECE 656 Homework (Week 8) (continued)

Solution:

$$\kappa_e = 0.40 \quad \text{W-m/K}$$

$$\sigma = 1/\rho = 1/0.0019 = 526 \text{ S/cm} = 5.26\times10^4 \quad \text{S/m}$$

$$S = -186\ \mu\text{V/K} = \text{-}1.86\times10^{-4} \quad \text{V/K}$$

$$ZT = \frac{\left(1.86\times10^{-4}\right)^2 5.24\times10^4\times300}{0.40+58} = 0.01 \qquad \boxed{ZT = 0.01}$$

12) This problem concerns the Peltier coefficient for a 3D semiconductor with parabolic energy bands. Assuming that the mfp, λ_0 is independent of energy and show that the Peltier coefficient is:

$$\pi_{3D} = TS_{3D} = \left(\frac{k_B T}{-q}\right)\left(\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F\right).$$

Solution:

Begin with:

$$\pi = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)\sigma'(E)\,dE}{\int \sigma'(E)\,dE}$$

$$\sigma'(E) = \frac{2q^2}{h}\lambda(E)\big(M(E)/A\big)\left(-\frac{\partial f_0}{\partial E}\right)$$

$$\pi = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)\sigma'(E)\,dE}{\int \sigma'(E)\,dE} = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)\frac{2q^2}{h}\lambda(E)\big(M(E)/A\big)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int \frac{2q^2}{h}\lambda(E)\big(M(E)/A\big)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

Cancel out constants:

ECE 656 Homework (Week 8) (continued)

$$\pi = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)(E-E_C)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int (E-E_C)\left(-\frac{\partial f_0}{\partial E}\right)dE} = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_C+E_C-E_F)(E-E_C)\left(-\frac{\partial f_0}{\partial E}\right)dE}{\int (E-E_C)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

Now change variables:

$$\eta = \frac{(E-E_C)}{k_BT} \qquad \eta_F = \frac{(E_F-E_C)}{k_BT} \qquad dE = k_BTd\eta$$

$$\pi = -\frac{k_BT}{q}\frac{\int_{-\infty}^{+\infty}(\eta^2-\eta_F\eta)\left(-\frac{\partial f_0}{\partial E}\right)d\eta}{\int \eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta} = -\frac{k_BT}{q}\left\{\frac{\int_{-\infty}^{+\infty}\eta^2\left(-\frac{\partial f_0}{\partial E}\right)d\eta - \eta_F\int_{-\infty}^{+\infty}\eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta}{\int \eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta}\right\}$$

$$\pi = -\frac{k_BT}{q}\left\{\frac{\frac{\partial}{\partial\eta_F}\int_{-\infty}^{+\infty}\eta^2 f_0\,d\eta - \eta_F\frac{\partial}{\partial\eta_F}\int_{-\infty}^{+\infty}\eta f_0\,d\eta}{\frac{\partial}{\partial\eta_F}\int \eta f_0\,d\eta}\right\} \qquad \text{(i)}$$

The denominator is:

$$\text{den} = \frac{\partial}{\partial\eta_F}\int \eta f_0\,d\eta = \frac{\partial}{\partial\eta_F}\Gamma(1)\mathcal{F}_1(\eta_F) = \mathcal{F}_0(\eta_F) \qquad \text{(ii)}$$

The numerator is:

$$\text{num} = \frac{\partial}{\partial\eta_F}\int_{-\infty}^{+\infty}\eta^2 f_0\,d\eta - \eta_F\frac{\partial}{\partial\eta_F}\int_{-\infty}^{+\infty}\eta f_0\,d\eta = \frac{\partial}{\partial\eta_F}\Gamma(3)\mathcal{F}_2(\eta_F) - \eta_F\frac{\partial}{\partial\eta_F}\Gamma(2)\mathcal{F}_1(\eta_F)$$

$$\text{num} = \Gamma(3)\mathcal{F}_1(\eta_F) - \eta_F\Gamma(2)\mathcal{F}_0(\eta_F) \qquad \text{(iii)}$$

ECE 656 Homework (Week 8) (continued)

Now use (ii) and (iii) in (i) to find:

$$\pi = -\frac{k_B T}{q}\left\{\frac{\Gamma(3)\mathcal{F}_1(\eta_F) - \eta_F \Gamma(2)\mathcal{F}_0(\eta_F)}{\mathcal{F}_0(\eta_F)}\right\} = -\frac{k_B T}{q}\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F\right\}$$

$$\boxed{\pi = -\frac{k_B T}{q}\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F\right\}}$$

13) The expression for the short circuit (electronic) thermal conductivity is:

$$\kappa_0 = \int_{-\infty}^{+\infty} \frac{(E - E_F)^2}{q^2 T} \sigma'(E)\, dE$$

where $\sigma'(E)$, the differential conductivity, is given by

$$\sigma'(E) = \frac{2q^2}{h}\lambda(E)\big(M(E)/A\big)\left(-\frac{\partial f_0}{\partial E}\right).$$

Evaluate this expression assuming that the Fermi level is located above the middle of the gap, so that only the conduction band need be considered. You may assume that the mean-free-path for backscattering is independent of energy, $\lambda(E) = \lambda_0$, and parabolic energy bands so that in 3D:

$$M(E)/A = \frac{m^*}{2\pi\hbar^2}(E - E_C) H(E - E_C),$$

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

Your answer should be expressed in terms of Fermi-Dirac integrals. For a tutorial on Fermi-Dirac integrals see: "Notes on Fermi-Dirac Integrals, 3rd Ed." http://nanohub.org/resources/5475/

Your final answer should be an expression for the short-circuit thermal conductivity of 3D electrons in a semiconductor with parabolic energy bands in terms of the normalized Fermi energy, $\eta_F = (E_F - E_C)/k_B T_L$.

ECE 656 Homework (Week 8) (continued)

Solution:

$$\kappa_0 = \int_{-\infty}^{+\infty} \frac{(E - E_F)^2}{q^2 T} \sigma'(E)\, dE$$

Substituting in for the differential conductivity, we find:

$$\kappa_0 = \int_{-\infty}^{+\infty} \frac{(E - E_F)^2}{q^2 T} \frac{2q^2}{h} \lambda_0 \left(M(E)/A \right) \left(-\frac{\partial f_0}{\partial E} \right) dE\,,$$

and then for the number of channels:

$$\kappa_0 = \int_{-\infty}^{+\infty} \frac{(E - E_F)^2}{q^2 T} \frac{2q^2}{h} \lambda_0 \left(\frac{m^*}{2\pi\hbar^2} (E - E_C) \right) \left(-\frac{\partial f_0}{\partial E} \right) dE\,.$$

Pull the constants out front:

$$\kappa_0 = \left[\frac{1}{q^2 T} \left(\frac{2q^2}{h} \right) \lambda_0 \left(\frac{m^*}{2\pi\hbar^2} \right) \right] \times \int_{-\infty}^{+\infty} (E - E_F)^2 (E - E_C) \left(-\frac{\partial f_0}{\partial E} \right) dE\,. \qquad \text{(i)}$$

Work on the integral first:

$$\kappa_0 = \left[\frac{1}{q^2 T} \left(\frac{2q^2}{h} \right) \lambda_0 \left(\frac{m^*}{2\pi\hbar^2} \right) \right] \times I \qquad \text{(ii)}$$

$$I = \int_{-\infty}^{+\infty} (E - E_F)^2 (E - E_C) \left(-\frac{\partial f_0}{\partial E} \right) dE\,.$$

Add and subtract, E_C:

$$I = \int_{-\infty}^{+\infty} (E - E_C + E_C - E_F)^2 (E - E_C) \left(-\frac{\partial f_0}{\partial E} \right) dE\,.$$

Now change variables:

$$\eta = \frac{(E - E_C)}{k_B T} \qquad \eta_F = \frac{(E_F - E_C)}{k_B T} \qquad dE = k_B T d\eta$$

ECE 656 Homework (Week 8) (continued)

$$I=\left(k_BT\right)^4\int_{-\infty}^{+\infty}\left(\eta-\eta_F\right)^2\eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta$$

$$I=\left(k_BT\right)^4\int_{-\infty}^{+\infty}\left(\eta^2-2\eta_F\eta+\eta_F^2\right)\eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta$$

$$I=\left(k_BT\right)^4\left[\int_{-\infty}^{+\infty}\eta^3\left(-\frac{\partial f_0}{\partial E}\right)d\eta-2\eta_F\int_{-\infty}^{+\infty}\eta^2\left(-\frac{\partial f_0}{\partial E}\right)d\eta+\eta_F^2\int_{-\infty}^{+\infty}\eta\left(-\frac{\partial f_0}{\partial E}\right)d\eta\right]$$

$$I=\left(k_BT\right)^4\left[\frac{\partial}{\partial E_F}\int_{-\infty}^{+\infty}\eta^3 f_0\,d\eta-2\eta_F\frac{\partial}{\partial E_F}\int_{-\infty}^{+\infty}\eta^2 f_0\,d\eta+\eta_F^2\frac{\partial}{\partial E_F}\int_{-\infty}^{+\infty}\eta f_0\,d\eta\right]$$

$$I=\left(k_BT\right)^3\left[\frac{\partial}{\partial \eta_F}\int_{-\infty}^{+\infty}\eta^3 f_0\,d\eta-2\eta_F\frac{\partial}{\partial \eta_F}\int_{-\infty}^{+\infty}\eta^2 f_0\,d\eta+\eta_F^2\frac{\partial}{\partial \eta_F}\int_{-\infty}^{+\infty}\eta f_0\,d\eta\right]$$

$$I=\left(k_BT\right)^3\left[\frac{\partial}{\partial \eta_F}\Gamma(4)\mathcal{F}_3(\eta_F)-2\eta_F\frac{\partial}{\partial \eta_F}\Gamma(3)\mathcal{F}_2(\eta_F)+\eta_F^2\frac{\partial}{\partial \eta_F}\Gamma(2)\mathcal{F}_1(\eta_F)\right]$$

$$I=\left(k_BT\right)^3\left[6\mathcal{F}_2(\eta_F)-4\eta_F\mathcal{F}_1(\eta_F)+\eta_F^2\mathcal{F}_0(\eta_F)\right].$$

Now insert this result in (ii) above to find:

$$\kappa_0=\left[\frac{1}{q^2T}\left(\frac{2q^2}{h}\right)\lambda_0\left(\frac{m^*}{2\pi\hbar^2}\right)\right]\times\left(k_BT\right)^3\left[6\mathcal{F}_2(\eta_F)-4\eta_F\mathcal{F}_1(\eta_F)+\eta_F^2\mathcal{F}_0(\eta_F)\right]$$

$$\boxed{\kappa_0=\left[T\left(\frac{k_B}{q}\right)^2\left(\frac{2q^2}{h}\right)\lambda_0\left(\frac{m^*k_BT}{2\pi\hbar^2}\right)\right]\times\left\{6\mathcal{F}_2(\eta_F)-4\eta_F\mathcal{F}_1(\eta_F)+\eta_F^2\mathcal{F}_0(\eta_F)\right\}}$$

Please see the Appendix of *Near-Equilibrium Transport: Fundamentals and Applications*, by Lundstrom and Jeong, for a list transport coefficients worked out for 1D, 2D, and 3D conductors. This is eqn. (A34).

Additional exercise for those who are interested:

Assume that the mean-free-path is energy-dependent according to

$$\lambda(E)=\lambda_0\left[\left(E-E_C\right)/k_BT\right]^r .$$

Work out the analytical expression and explain physically why $r>0$ increases the magnitude of the Seebeck coefficient.

ECE 656 Homework (Week 8) (continued)

14) An appreciation of the coupled current equations is necessary when experimentally characterizing electronic materials. The basic equations are:

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx} \text{ V/m} \qquad \text{(i)}$$

$$J_{Qx} = \pi J_x - \left(\kappa_e + \kappa_L\right)\frac{dT}{dx} \text{ W/m}^2 \qquad \text{(ii)}$$

To measure the resistivity of the sample, we force a current, J_x, and measure the resulting voltage. In the first case, we are careful to maintain isothermal conditions, and in the second case, we are careful to maintain adiabatic (zero heat current) conditions. Answer the following questions.

14a) If we divide the measured voltage by the injected current, what "isothermal resistivity" do we measure. (First case.)

14b) If we divide the measured voltage by the injected current, what "adiabatic resistivity" do we measure. (Second case.)

14c) Using numbers for lightly doped Ge at room temperature (from Lecture 10, Fall 2011), compare the numerical values of the two measured "resistivities."

Solution:
14a)

For isothermal conditions, (i) gives:

$$\mathcal{E}_x = \rho J_x \text{ V/m}$$

$$\frac{\mathcal{E}_x}{J_x} = \rho \ \frac{\text{V/m}}{\text{A/m}^2} = \rho \quad \Omega\text{-m} \qquad \boxed{\left.\frac{\mathcal{E}_x}{J_x}\right|_{dT/dx=0} = \rho \quad \Omega\text{-m}}$$

ECE 656 Homework (Week 8) (continued)

Solution:
14b)

For adiabatic conditions, (ii) gives:

$$J_{Qx} = \pi J_x - \left(\kappa_e + \kappa_L\right)\frac{dT}{dx} \;=0$$

$$\frac{dT}{dx} = \frac{\pi J_x}{\left(\kappa_e + \kappa_L\right)}$$

Insert this in (i)

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx} = \rho J_x + S\frac{\pi J_x}{\left(\kappa_e + \kappa_L\right)} = \left(\rho + \frac{S\pi}{\left(\kappa_e + \kappa_L\right)}\right)J_x = \rho\left(1 + \frac{S\pi\sigma}{\left(\kappa_e + \kappa_L\right)}\right)J_x$$

$$\mathcal{E}_x = \rho\left(1 + ZT\right)J_x$$

$$\boxed{\left.\frac{\mathcal{E}_x}{J_x}\right|_{J_Q=0} = \rho\left(1+ZT\right) \quad \Omega\text{-m}}$$

So we measure something a little different (much different if we are measuring a good thermoelectric material).

Solution:
14c)

Need to compute ZT for this case:

$$ZT = \frac{S^2\sigma T}{\kappa_L + \kappa_e}$$

Use numbers from Lecture 10, Fall 2011

$$\rho_n = 2 \quad \Omega\text{-cm} = 0.02 \;\; \Omega\text{-m}$$

$$S_n = -970 \quad \mu\text{V/K}$$

$$\kappa_e = 2.2\times10^{-4} \quad \text{W/m-K}$$

$$\kappa_L = 58 \text{ W/m-K} >> \kappa_n$$

$$ZT = \frac{S^2\sigma T}{\kappa_L + \kappa_e} \approx \frac{S^2 T}{\rho\kappa_L} = \frac{\left(9.7\times10^{-4}\right)^2 300}{0.02\times58} = 2.4\times10^{-3}$$

$$\boxed{\left.\frac{\mathcal{E}_x}{J_x}\right|_{J_Q=0} = \rho\left(1+ZT\right) = 2\left(1+0.002\right) \approx 2 \quad \Omega\text{-cm}}$$

ECE 656 Homework (Week 8) (continued)

In this case the difference is very small, but consider what would happen if we were measuring a good thermoelectric material, such as Bi_2Te_3 with $ZT \approx 1$.

15) We have seen a lot of equations so far, but the course is not about memorizing equations. With a solid understanding of the physical concepts, only a few equations are needed. On one sheet (front only, font size 12) summarize the key equations describing near-equilibrium transport. The point is not to write down every equation, the point is to identify the few, really important results from which you can derive anything else you need.

Solution:

Landauer expression: $$I = \frac{2q}{h}\int \mathcal{T}(E) M(E)(f_1 - f_2)\, dE$$

Bulk current expression: $$J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} - S_n \sigma_n \frac{dT}{dx}$$

The coupled current equations (3D):

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx}$$

$$J_{Qx} = \pi J_x - (\kappa_e + \kappa_L)\frac{dT}{dx}$$

The transport coefficients (3D):

$$\sigma'(E) = \frac{2q^2}{h}\lambda(E)\big(M(E)/A\big)\left(-\frac{\partial f_0}{\partial E}\right) \quad \sigma = \int_{-\infty}^{+\infty} \sigma'(E)\, dE = \frac{2q^2}{h}\langle M_{el}/A\rangle \langle\langle \lambda_{el}\rangle\rangle = n_0 q \mu_n$$

$$S = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E - E_F)\sigma'(E)\, dE}{\int \sigma'(E)\, dE} = -\left(\frac{k_B}{q}\right)\left(\frac{E_J - E_F}{k_B T}\right) \qquad \pi = TS$$

$$\kappa_e = \kappa_0 - T\sigma S^2 = T\sigma\mathcal{L} \qquad \kappa_0 = \frac{1}{q^2 T}\int_{-\infty}^{+\infty}(E - E_F)^2 \sigma'(E)\, dE$$

ECE 656 Homework (Week 8) (continued)

Modes:

$$M(E) = \frac{h}{4}\left\langle \upsilon_x^+ \right\rangle D(E) \qquad \text{1D: } \left\langle \upsilon_x^+ \right\rangle = \upsilon \qquad \text{2D: } \left\langle \upsilon_x^+ \right\rangle = \frac{2}{\pi}\upsilon \qquad \text{3D: } \left\langle \upsilon_x^+ \right\rangle = \frac{\upsilon}{2}$$

Transmission:

$$\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

Diffusion coefficient:

$$D_n = \frac{\left\langle \upsilon_x^+ \right\rangle \left\langle\left\langle \lambda \right\rangle\right\rangle}{2}$$

Power law scattering for mean-free-path: $\lambda(E) = \lambda_0\left[\left(E - E_C\right)/k_B T\right]^r$

$$ZT = \frac{S^2 \sigma\, T}{\kappa_L + \kappa_e}$$