SOLUTIONS: ECE 656 Homework (Week 9)
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1) We have asserted that $\Delta_n = 2k_BT$ 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 $2k_BT$ 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:

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

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

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

Most constants cancel (remember that $M \propto (E-E_C)$ in 3D) and we find

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

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

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

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

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

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

Putting this together:

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

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

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 $\Delta_n = 2k_B T$, as expected.

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

2) Repeat prob. 1) 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:

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

but assume $\left(-\partial f_0/\partial E\right) = \delta(E_F)$ to find:

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$$\Delta_n = \frac{(E_F - E_C)^2\left[(E_F - E_C)/k_BT\right]^r}{(E_F - E_C)\left[(E_F - E_C)/k_BT\right]^r} = (E_F - E_C)$$

$$\boxed{\Delta_n = (E_F - E_C)}$$

The Seebeck coefficient is

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

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

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

3) For practical TE devices, the semiconductor is doped so that $E_F \approx E_C$. Work out the four thermoelectric transport coefficients for n-type Ge doped at $N_D = 10^{19}\ \text{cm}^{-3}$. 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 following material parameters:

$T = 300\ \text{K}$

$N_C = 1.04 \times 10^{19}\ \ \text{cm}^{-3}$

$\mu_n = 330\ \text{cm}^2/\text{V-s}$

$m^* = 0.12 m_0$

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: $m^* = 0.12 m_0$.

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Recall that the definition of conductivity effective mass for Si and Ge is:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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4) Perhaps we should use Fermi-Dirac statistics for thermoelectric calculations when $E_F \approx E_c$. Repeat problem 3), 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
$\sigma_{3D} = \frac{2q^2}{h}\lambda_0\left(\frac{g_V m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0(\eta_F)$ and $S = -\left(\frac{k_B}{q}\right)\left\{\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_1(\eta_F)} - \eta_F\right\}$

Solution:

The conductivity does not change from prob. 3):

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

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

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

To proceed, we must find η_F using:

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

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

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

$$\lambda_0 = \frac{\sigma_{3D}}{\left(\frac{2q^2}{h}\right)\left(g_V \frac{m^* k_B T}{2\pi\hbar^2}\right)\mathcal{F}_0(\eta_F)} = \frac{5.26\times 10^4 \text{ S/m}}{\left(7.71\times 10^{-5}\right)\left(6.37\times 10^{16}\right)\mathcal{F}_0(0.297)} = 0.13\times 10^{-7}\text{ m}$$

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.

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$\boxed{\lambda_0 = 13 \text{ nm}}$ 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.)

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

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

5) 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. 4) find the numerical value of the ratio, κ_0/κ_e.

Solution:

The relation between the two electronic thermal conductivities is:

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

or

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

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Use numbers from problem 4)

$$\kappa_e = 0.40 \text{ W-m/K}$$
$$\sigma = 1/\rho = 1/0.0019 = 526 \text{ S/cm} = 5.26\times10^4 \text{ S/m}$$
$$S = -186\ \mu\text{V/K} = -1.86\times10^{-4} \text{ V/K}$$
$$\kappa_0 = \kappa_e + T\sigma S^2 = 0.40 + 300\times5.26\times10^4\times\left(1.86\times10^{-4}\right)^2 = 0.40+0.55$$
$$\kappa_0 = 0.95 \text{ W-m/K}$$

$$\boxed{\frac{\kappa_0}{\kappa_e} = 2.4}$$

6) Using the results of prob. 4), estimate the thermoelectric material FOM, zT for n-type Ge at T = 300 K. You may assume that $\kappa_L = 58 \text{ W/m-K}$.

Solution:

$$\kappa_e = 0.40 \text{ W-m/K}$$
$$\sigma = 1/\rho = 1/0.0019 = 526 \text{ S/cm} = 5.26\times10^4 \text{ S/m}$$
$$S = -186\ \mu\text{V/K} = -1.86\times10^{-4} \text{ V/K}$$

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

We need $ZT \approx 1$ to build good thermoelectric devices, so Ge is not a good thermoelectric material.

7) 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:

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

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Solution:

Begin with:

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

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

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

Cancel out constants:

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

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:

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

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The numerator is:

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

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

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

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

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

8) 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. 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, $\eta_F = (E_F - E_C)/k_B T_L$.

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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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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.

9a) If we divide the measured voltage by the injected current, what "isothermal resistivity" do we measure. (First case.)

9b) If we divide the measured voltage by the injected current, what "adiabatic resistivity" do we measure. (Second case.)

9c) Using numbers for lightly doped Ge at room temperature:

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

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

Solution: 9a)

For isothermal conditions, (i) gives:

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

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

Solution: 9b)

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)

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

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

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

ECE 656 Homework Solutions (Week 9) (continued)

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

Solution: 9c)

Need to compute zT for this case:

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

Use the following numbers:

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

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

$$\kappa_e = 2.2 \times 10^{-4} \quad \text{W/m-K}$$

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

$$zT = \frac{S^2 \sigma T}{\kappa_L + \kappa_e} \approx \frac{S^2 T}{\rho \kappa_L} = \frac{\left(9.7 \times 10^{-4}\right)^2 300}{0.02 \times 58} = 2.4 \times 10^{-3}$$

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

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 $ZT \approx 1$.

10) 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.

ECE 656 Homework Solutions (Week 9) (continued)

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 in inverted form (3D):

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx} \qquad J_{Qx} = \pi J_x - (\kappa_e + \kappa_L)\frac{dT}{dx}$$

The transport coefficients (3D):

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

$$S = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)\sigma'(E)dE}{\int \sigma'(E)dE} = -\left(\frac{k_B}{q}\right)\left(\frac{E_J - E_F}{k_BT}\right) \qquad \pi = TS$$

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

Modes:

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

Transmission: $\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E)+L}$ **Diffusion coefficient:** $D_n = \frac{\langle v_x^+\rangle\langle\langle\lambda\rangle\rangle}{2}$

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

Material figure of merit: $zT = \frac{S^2\sigma T}{\kappa_L + \kappa_e}$