NAME:______________________________ **PUID:** ______________________________

ECE 656 Exam 3 SOLUTIONS: Fall 2017
December 12, 2017

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This is a closed book exam. You may use a calculator and the formula sheet at the end of this exam. **Only the Texas Instruments TI-30X IIS scientific calculator is allowed.**

There are four equally weighted questions. To receive full credit, you must **show your work** (scratch paper is attached).

The exam is designed to be taken in 75 minutes.

Be sure to fill in your name and Purdue student ID at the top of the page.

DO NOT open the exam until told to do so, and stop working immediately when time is called.

The last two pages, which list equations may be removed, if you wish.

100 points possible, 25 per question

1) 25 points	2a) 5 points	3a) 5 points	4a) 10 points
2.5pts each	2b) 5 points	3b) 10 points	4b) 5 points
	2c) 10 points	3c) 5 points	4c) 10 points
	2d) 5 points	3d) 5 points	

------------------------ Course policy ------------------------

I understand that if I am caught cheating in this exam, I will earn an F for the course and be reported to the Dean of Students.

Read and understood: ______________________________
signature

1a) When we write the recombination term in the various balance equations as $R_\phi = \left(n_\phi - n_\phi^0\right) / \langle \tau_\phi \rangle$, sometimes a term corresponding to n_ϕ appears and a term corresponding to its equilibrium value, n_ϕ^0, **does not appear**. When does it **not** appear?

a) Under steady-state conditions.
b) Under spatially uniform conditions.
c) When the balance equation corresponds to a moment higher than 2.
d) When the balance equation corresponds to a moment higher than 3.
e) When the quantity in the balance equation is a flux.

1b) When we write a drift-diffusion equation in the form, $J_{nj} = nq\mu_n \mathcal{E}_j + (2/3)\mu_n \partial W / \partial x_j$, what assumption are we making?

a) Non-degenerate carrier statistics.
b) The temperature does not vary with position.
c) The electron temperature is equal to the lattice temperature.
d) The kinetic energy is equally distributed between the three degrees of freedom.
e) Only that the BTE is valid.

1c) What does moment equation does $\phi(\vec{p}) = \upsilon_x \left(p^2/2m^*\right)$ give us?

a) The carrier continuity equation.
b) The carrier flux equation.
c) The carrier energy balance equation.
d) The carrier energy flux equation.
e) The carrier energy squared continuity equation.

1d) When simulating $\left(\vec{r}(t), \vec{p}(t)\right)$, in phase space by the Monte Carlo approach, which of the following is true?

a) $\vec{r}(t)$ is continuous and $\vec{p}(t)$ is continuous.
b) $\vec{r}(t)$ is discontinuous and $\vec{p}(t)$ is continuous.
c) $\vec{r}(t)$ is continuous and $\vec{p}(t)$ is discontinuous.
d) $\vec{r}(t)$ is discontinuous and $\vec{p}(t)$ is discontinuous.
e) None of the above

1e) What is "self scattering" in a Monte Carlo simulation?

a) A many body effect in which an electron interacts with itself.
b) An electron-electron scattering event in which an electron scatters from another electron.
c) An electron-electron scattering event in which an electron scatters from the entire plasma of all the electrons.
d) A mathematical technique that simplifies the computation of free-flight times.
e) A mathematical technique that simplifies the computation of the final scattering state.

1f) In practice, one commonly extends the near-equilibrium drift-diffusion equation to high-fields by replacing the mobility and diffusion coefficients by electric field dependent quantities, as in $J_{nx} = nq\mu_n(\mathcal{E})\mathcal{E}_x + qD_n(\mathcal{E})\,dn/dx$. What assumption is necessary to write the DD equation in this form?

a) Parabolic energy bands.
b) Non-degenerate carrier statistics.
c) The microscopic relaxation time approximation.
d) That the energy relaxation time is shorter than the momentum relaxation time.
e) That the shape of the distribution at the particular location, whatever it is, depends only on the electric field at that location.

1g) In the classic description of the velocity vs. electric field characteristic in bulk Si, $\upsilon_d = \mu_{n0}\mathcal{E}\Big/\sqrt{1+\left(\mathcal{E}/\mathcal{E}_C\right)^2}$, approximately what is the magnitude of $\mathcal{E}_C$?

a) $\approx 0.1\,\mathrm{kV/cm}$.
b) $\approx 1\,\mathrm{kV/cm}$.
c) $\approx 10\,\mathrm{kV/cm}$.
d) $\approx 100\,\mathrm{kV/cm}$.
e) $\approx 1000\,\mathrm{kV/cm}$.

1h) What is meant by the term, "non-local" semiclassical transport.

a) Transport that cannot be described by a DD equation with a field-dependent mobility and diffusion coefficient.
b) Steady-state transport in an electric field that varies more rapidly in space than the energy relaxation length, where T_e is the electron temperature.
c) Transient transport in an electric field that varies more rapidly in time than the energy relaxation time.
d) All of the above.
e) None of the above.

1i) Under what conditions does velocity overshoot occur for a rapidly varying electric field?
a) When transport is ballistic.
b) When transport is quasi-ballistic.
c) When the momentum relaxation time is much shorter than the energy relaxation time.
d) When the momentum relaxation time is much longer than the energy relaxation time.
e) When the momentum relaxation time is nearly equal to the energy relaxation time.

1j) Which of the following is true about a ballistic device with two, ideal Landauer contacts at different voltages?

a) The distribution function in the device is a Fermi-Dirac distribution with the average Fermi level of the two contacts.
b) The distribution function in the device is a Fermi-Dirac distribution with the Fermi level of the contact with the more positive potential.
c) The distribution function in the device is a Fermi-Dirac distribution with the Fermi level of the contact with the more negative potential.
d) **Each state in the device is in equilibrium with one of the two contacts.**
e) Each state in the device is in equilibrium with both the two contacts

2) Monte Carlo simulations of high-field transport in bulk silicon with an electric field of 100,000 V/cm show the following results for the average velocity and kinetic energy:

$$\upsilon_d = \langle \upsilon \rangle = 1.04 \times 10^7 \text{ cm/s}$$

$$u = \langle KE \rangle = 0.364 \text{ eV}$$

For this problem, you may assume a simple parabolic band with an effective mass of $m^* = m_C^* = 0.26 m_0$.

2a) Estimate the average momentum relaxation time, $\langle \tau_m \rangle$. **A numerical answer is required.**

Solution:

$$\mu_n = \langle \upsilon \rangle / \mathcal{E} = 104 \text{ cm}^2/\text{V-s}$$

$$\mu_n = \frac{q\langle \tau_m \rangle}{m_c^*},$$

where m_c^* is the conductivity effective mass. Use MKS units for the calculation:

$$\langle \tau_m \rangle = \frac{q}{\mu_n m_c^*} = \frac{\mu_n m_c^*}{q} = \frac{104 \times 10^{-4} \times 0.26 \times 9.11 \times 10^{-31}}{1.6 \times 10^{-19}} 1.54 \times 10^{-14}$$

$$\boxed{\langle \tau_m \rangle = 1.54 \times 10^{-14} \text{ s}}$$

2b) Estimate the average energy relaxation time, $\langle \tau_E \rangle$. **A numerical answer is required.**

Solution:

From the energy balance equation:

$$J_x \mathcal{E}_x = nq\langle \upsilon \rangle \mathcal{E}_x = \frac{n(u-u_0)}{\langle \tau_E \rangle}$$

$$\langle \tau_E \rangle = \frac{(u-u_0)}{q\langle \upsilon \rangle \mathcal{E}_x}$$

$$\frac{u_0}{q} = 1.5\frac{k_B T_L}{q} = 0.039$$

$$\langle \tau_E \rangle = \frac{(u-u_0)}{q\langle \upsilon \rangle \mathcal{E}_x} = \frac{(0.364-0.039)}{1.04 \times 10^7 \times 10^5} = 0.313 \times 10^{-12}$$

$$\boxed{\langle \tau_E \rangle = 0.3 \text{ ps}}$$

2c) Estimate the **drift** energy in electron volts. **A numerical answer is required.**

Solution:

$$E_{dr} = \frac{1}{2} m^* \upsilon_d^2 = 0.5(0.26)(9.11\times10^{-31})(1.04\times10^{5})^2 = 1.28\times10^{-21}\text{ J}$$

$$E_{dr}(\text{eV}) = \frac{1.28\times10^{-21}}{q} = 8.01\times10^{-3}\text{ eV}$$

$$\boxed{E_{dr}(\text{eV}) = 8.01\times10^{-3}\text{ eV}}$$

2d) Estimate the **thermal** energy in electron volts. **A numerical answer is required.**

Solution:

From the formula sheet: $u = \frac{1}{2} m^* \upsilon_d^2 + \frac{3}{2} k_B T_e$

$$\frac{3}{2} k_B T_e = u - \frac{1}{2} m^* \upsilon_d^2 = 0.364 - 0.008 = 0.356$$

$$\boxed{\frac{3}{2} k_B T_e = 0.356\text{ eV}}$$

Virtually all of the energy is thermal energy.

3) When deriving the momentum balance equation in 3D, a tensor,

$$W_{ij} = \frac{1}{\Omega}\sum_{\vec{p}} \frac{\upsilon_i p_j}{2} f(\vec{r},\vec{p},t)$$

occurs. This question is about the diagonal component of the tensor, W_{xx}. You may assume a simple, parabolic energy band and spatial variation in the x-direction only.

3a) Use the balance equation prescription to obtain an expression for the x-directed flux associated with W_{xx}.

Solution:

$$\boxed{F_{\phi x} \equiv \frac{1}{\Omega}\sum_{p}\left(\frac{1}{2}m^*\upsilon_x^2\right)\upsilon_x f(x,\vec{p},t) = F_{W_{xx}}}.$$

$F_{W_{xx}}$ is a flux of the quantity, W_{xx}. It can also be written as

$$F_{W_{xx}} \equiv \frac{1}{\Omega}\sum_{p}\left(\frac{1}{2}m^*\upsilon_x^2\right)\upsilon_x f = n\frac{1}{2}m^*\langle\upsilon_x^3\rangle$$

3b) Use the balance equation prescription to obtain an expression for the "generation rate" associated with W_{xx}.

Solution:

$$G_\phi = -q\mathcal{E}_x\left\{\frac{1}{\Omega}\sum_p \frac{\partial\phi}{\partial p_x} f\right\}$$

The term inside the sum is

$$\frac{\partial\phi}{\partial p_x} = \frac{\partial\left(\frac{1}{2}m^*\upsilon_x^2\right)}{\partial p_x} = \frac{1}{2m^*}\frac{\partial\left(p_x^2\right)}{\partial p_x} = \upsilon_x$$

so we find

$$\boxed{G_\phi = -q\mathcal{E}_i\left\{\frac{1}{\Omega}\sum_{\vec{p}}\upsilon_x f\right\} = J_{nx}\mathcal{E}_x}$$

3c) Write down an expression for the “recombination rate” associated with W_{xx}.

Solution:

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{W_{xx} - W_{xx}^0}{\langle \tau_{W_{xx}} \rangle} \qquad W_{xx}^0 = n_0 \frac{k_B T_L}{2}$$

3d) Write down the total balance equation for W_{xx}, **and explain** what would need to be done in order to solve this equation in combination with the first balance equation (the continuity equation) and the second balance equation (the momentum balance equation).

Solution:

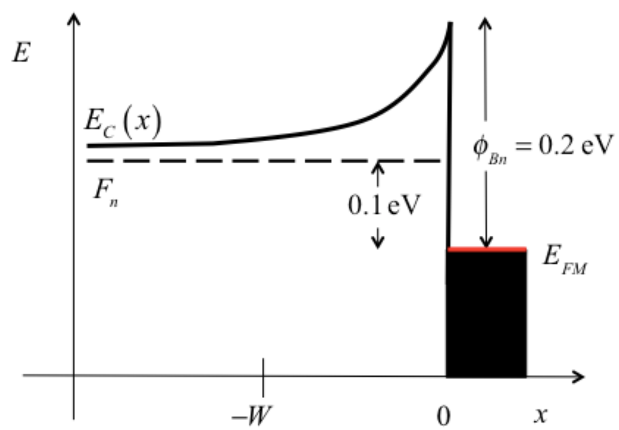
$$\frac{\partial W_{xx}}{\partial t} = -\frac{d}{dx}\left(F_{W_{xx}}\right) + J_{nx}\mathcal{E}_x - \frac{W_{xx} - W_{xx}^0}{\langle \tau_{W_{xx}} \rangle}$$

To solve this equation, we would need to terminate the hierarchy and develop an approximation for $F_{W_{xx}}$ in terms of the quantities in the previous balance equations.

We would also need to develop an expression for the relaxation time, $\langle \tau_{W_{xx}} \rangle$.

4) This problem concerns the **ballistic** Schottky barrier diode shown in the figure below. Note that it is forward biased. Assume that the semiconductor is silicon with an effective density of states of $N_C = 3.23\times10^{19}$ cm^{-3} and that the temperature is 300 K. The quantity, F_n, is the electron quasi-Fermi level (elecrochemical potential) in the semiconductor and E_{FM} is the Fermi level in the metal. Not shown on the left is an ideal contact in equilibrium.

Answer the following questions. **Numerical answers are required.**



4a) At the metal-semiconductor junction, what is the density of ballistic electrons in the semiconductor with **positive** velocities, $n^+(x=0^-)$?

Solution:

In a bulk, diffusive semiconductor,

$$n = N_C e^{(F_n - E_C)/k_BT}$$

At $x = 0^-$ only the positive velocity states are filled by the contact at the left. Half of the states have positive velocities, so

$$n^+(x=0^-) = \frac{N_C}{2} e^{(F_n - E_C)/k_BT} = \frac{3.23\times10^{19}}{2} e^{-0.1/0.026} = 3.45\times10^{17}\ \text{cm}^{-3}$$

$$\boxed{n^+(x=0^-) = 3.45\times10^{17}\ \text{cm}^{-3}}$$

The non-degenerate assumption we are making is clearly OK.

4b) At the metal-semiconductor junction, what is the density of ballistic electrons in the semiconductor with **negative** velocities, $n^{-}\left(x=0^{-}\right)$?

Solution:

In a bulk, diffusive semiconductor,

$$n = N_C e^{\left(F_n - E_C\right)/k_B T}$$

At $x=0^{-}$ only the negative velocity states are filled by the contact at the right. Half of the states have negative velocities, so

$$n^{-}\left(x=0^{-}\right) = \frac{N_C}{2} e^{\left(E_{FM}-E_C\right)/k_B T} = \frac{3.23\times10^{19}}{2} e^{-0.2/0.026} = 7.37\times10^{15}\ \text{cm}^{-3}$$

$$\boxed{n^{-}\left(x=0^{-}\right) = 7.37\times10^{15}\ \text{cm}^{-3}}$$

The non-degenerate assumption we are making is clearly OK.

4c) What is the current density in Amperes per cm2? You will need an effective mass for this question; you may assume a simple parabolic band with an effective mass of $m^{*} = m_C^{*} = 0.26 m_0$.

Solution:

$$J_n = q\upsilon_T\left[n^{+}\left(0^{-}\right) - n^{-}\left(0^{-}\right)\right]$$

From the formula sheet: $\left\langle \upsilon_x^{+} \right\rangle = \upsilon_T = \sqrt{2k_B T/\pi m^{*}} \quad \left(\eta_F << 0\right)$

$$\upsilon_T = \sqrt{\frac{2k_B T}{\pi m^{*}}} = \sqrt{\frac{2\left(1.38\times10^{-23}\right)300}{3.14\left(0.26\right)\left(9.11\times10^{-31}\right)}} = 1.06\times10^{5}\ \text{m/s}$$

$$J_n = q\upsilon_T\left[n^{+}\left(0^{-}\right) - n^{-}\left(0^{-}\right)\right] = 1.6\times10^{19}\left(1.06\times10^{7}\right)\left[3.45\times10^{17} - 7.37\times10^{15}\right]\ \text{A/cm}^2$$

$$\boxed{J_n = 5.73\times10^{5}\ \text{A/cm}^2}$$

ECE-656 Key Equations (Weeks 1-15)

Physical constants:

$\hbar = 1.055\times10^{-34}$ [J-s] $m_0 = 9.109\times10^{-31}$ [kg]

$k_B = 1.380\times10^{-23}$ [J/K] $q = 1.602\times10^{-19}$ [C] $\varepsilon_0 = 8.854\times10^{-14}$ [F/cm]

Density of states in k-space:

1D: $N_k = 2\times(L/2\pi) = L/\pi$ 2D: $N_k = 2\times(A/4\pi^2) = A/2\pi^2$ 3D:
$N_k = 2\times(\Omega/8\pi^2) = \Omega/4\pi^3$

Density of states in energy (parabolic bands, per length, area, or volume):

$$D_{1D}(E) = \frac{g_v}{\pi\hbar}\sqrt{\frac{2m^*}{(E-\varepsilon_1)}} \qquad D_{2D}(E) = g_V\frac{m^*}{\pi\hbar^2} \qquad D_{3D}(E) = g_v\frac{m^*\sqrt{2m^*(E-E_C)}}{\pi^2\hbar^3}$$

Fermi function and Fermi-Dirac Integrals / Bose-Einstein function

$$f_0(E) = \frac{1}{1+e^{(E-E_F)/k_BT}} \qquad N_0 = \frac{1}{e^{\hbar\omega_0/k_BT}-1}$$

$$\mathcal{F}_j(\eta_F) = \frac{1}{\Gamma(j+1)}\int_0^\infty \frac{\eta^j d\eta}{1+e^{\eta-\eta_F}} \qquad \mathcal{F}_j(\eta_F) \to e^{\eta_F} \quad \eta_F << 0 \qquad \frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}$$

$\Gamma(n) = (n-1)!$ (n an integer) $\Gamma(1/2) = \sqrt{\pi}$ $\Gamma(p+1) = p\Gamma(p)$

Scattering:

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{\vec{p}\,',\vec{p}}\right|^2 \delta(E'-E-\Delta E) \qquad H_{\vec{p}\,',\vec{p}} = \frac{1}{\Omega}\int_{-\infty}^{+\infty} e^{-i\vec{p}\,'\bullet r/\hbar} U_S(\vec{r}) e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

$$\frac{1}{\tau(\vec{p})} == \sum_{\vec{p}\,',\uparrow} S(\vec{p},\vec{p}\,') \qquad \frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}\,',\uparrow} S(\vec{p},\vec{p}\,')\frac{\Delta p_z}{p_{z0}} \qquad \frac{1}{\tau_E(\vec{p})} = \sum_{\vec{p}\,',\uparrow} S(\vec{p},\vec{p}\,')\frac{\Delta E}{E_0}$$

ADP: $|K_q|^2 = q^2 D_A^2$ ODP: $|K_q|^2 = D_0^2$ PZ: $|K_q|^2 = (ee_{PZ}/\kappa_S\varepsilon_0)^2$ POP: $|K_\beta|^2 = \dfrac{\rho e^2\omega_0^2}{q^2\kappa_0\varepsilon_0}\left(\dfrac{\kappa_0}{\kappa_\infty}-1\right)$

$$S(\vec{p},\vec{p}\,') = \frac{\pi}{\Omega\rho\,\omega}|K_q|^2\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\delta(\vec{p}\,'-\vec{p}\mp\hbar\vec{q})\delta(E'-E\mp\hbar\omega)$$

$$\delta(\vec{p}\,'-\vec{p}\mp\hbar\vec{q})\delta(E'-E\mp\hbar\omega_\beta) \to \frac{1}{\hbar\upsilon q}\delta\left(\pm\cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega_q}{\upsilon q}\right)$$

$$\frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \frac{2\pi}{\hbar}\left(\frac{D_A^2 k_B T}{c_l}\right)\frac{D_{3D}(E)}{2} \text{ (ADP)} \qquad L_D = \sqrt{\frac{\kappa_S\varepsilon_0 k_B T}{q^2 n_0}}$$

$$\frac{1}{\tau} = \frac{1}{\tau_m} = \frac{2\pi}{\hbar}\left(\frac{\hbar D_O^2}{2\rho\omega_0}\right)\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right)\frac{D_{3D}(E\pm\hbar\omega_0)}{2} \qquad N_0 = \frac{1}{e^{\hbar\omega_o/k_BT}-1} \text{ (ODP)}$$

Boltzmann Transport Equation:

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \left.\frac{df}{dt}\right|_{coll} \qquad \vec{F}_e = -q\vec{\mathcal{E}} - q\vec{\upsilon} \times \vec{B} \qquad \left.\frac{df}{dt}\right|_{coll} = -\frac{\left(f - f_S\right)}{\tau_m} = -\frac{\delta f}{\tau_m} \text{ (RTA)}$$

With a small B-field, the resulting 2D current equation is $\vec{J}_n = \sigma_S \vec{\mathcal{E}} - \sigma_S \mu_H \left(\vec{\mathcal{E}} \times \vec{B}\right)$

$\left(\omega_c \tau_m << 1\right)$

$$\mu_H = \mu_n r_H \qquad r_H \equiv \left\langle\left\langle \tau_m^2 \right\rangle\right\rangle \big/ \left\langle\left\langle \tau_m \right\rangle\right\rangle^2 \quad \left\langle\left\langle \bullet \right\rangle\right\rangle \equiv \left\langle (\bullet) E \right\rangle \big/ \left\langle E \right\rangle$$

Isothermal Near-Equilibrium Transport: Summary of Landauer Approach

$I = \frac{2q}{h}\int \mathcal{T}(E) M(E)\left(f_1 - f_2\right) dE$ → small bias, isothermal: $f_1(E) - f_2(E) = \left(-\frac{\partial f_0}{\partial E}\right)(qV)$

Linear response (also called low bias, near-equilibrium):

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

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

$$R_{ball} = \frac{1}{M\left(E_F\right)} \frac{h}{2q^2} = \frac{12.8\,\mathrm{k}\Omega}{M}$$

Modes / channels (general):

$$M(E) \equiv \frac{h}{4}\left\langle \upsilon_x^+(E) \right\rangle D_{1D}(E) \qquad \left\langle \upsilon_x^+(E) \right\rangle = \upsilon(E)$$

$$M(E) = W M_{2D} \equiv W \frac{h}{4}\left\langle \upsilon_x^+(E) \right\rangle D_{2D}(E) \qquad \left\langle \upsilon_x^+(E) \right\rangle = \frac{2}{\pi}\upsilon(E)$$

$$M(E) = A M_{3D} \equiv A \frac{h}{4}\left\langle \upsilon_x^+(E) \right\rangle D_{3D}(E) \qquad \left\langle \upsilon_x^+(E) \right\rangle = \frac{1}{2}\upsilon(E)$$

Modes (Parabolic bands): $\left(E(k) = E_C + \hbar^2 k^2 / 2m^*\right)$

$$M(E) = M_{1\mathrm{D}}(E) = g_v$$

$$M(E) = W\, M_{2\mathrm{D}}(E) = g_v W \frac{\sqrt{2m^*\left(E - E_C\right)}}{\pi\hbar}$$

$$M(E) = A\, M_{3\mathrm{D}}(E) = g_v A \frac{m^*}{2\pi\hbar^2}\left(E - E_C\right)$$

Modes (graphene):

$$M(E) = W\, 2|E| / \pi\hbar\upsilon_F$$

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

Mean-free-path for backscattering:

1D: $\lambda(E) = 2\upsilon(E)\tau_m(E)$ 2D: $\lambda(E) = \frac{\pi}{2}\upsilon(E)\tau_m(E)$ 3D: $\lambda(E) = \frac{4}{3}\upsilon(E)\tau_m(E)$

Diffusion coefficient: $D_n = \langle \upsilon_x^+ \rangle \langle\langle \lambda \rangle\rangle / 2$ $D_n = \upsilon_T \lambda_0 / 2$ $D_n(E) = \langle \upsilon_x^+(E) \rangle \lambda(E)/2$

Uni-directional thermal velocity: $\langle \upsilon_x^+ \rangle = \upsilon_T = \sqrt{2k_BT/\pi m^*}$ $(\eta_F << 0)$

Thermoelectric transport:

Coupled current equations (diffusive): $J_x = \sigma \mathcal{E}_x - \sigma S\, dT/dx$ $J_x^Q = T\sigma S \mathcal{E}_x - \kappa_0\, dT/dx$

Coupled current equations (inverted): $\mathcal{E}_x = \rho J_x + S\frac{dT_L}{dx}$ $J_x^Q = \pi J_x - \kappa_e \frac{dT}{dx}$

Transport coefficients:

$$\sigma = \int \sigma'(E)\, dE = \frac{2q^2}{h}\langle M \rangle \langle\langle \lambda \rangle\rangle \qquad \sigma'(E) = \frac{2q^2}{h}\lambda(E)\frac{M(E)}{A}\left(-\frac{\partial f_0}{\partial E}\right) \qquad \langle M \rangle = \int M(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

$$S = -\frac{k_B}{q}\int \left(\frac{E-E_F}{k_BT}\right)\sigma'(E)\,dE \Big/ \int \sigma'(E)\,dE = -\left(\frac{k_B}{q}\right)\left\langle \frac{E-E_F}{k_BT} \right\rangle = \left(\frac{k_B}{-q}\right)\left\{\frac{(E_C - E_F)}{k_BT} + \frac{\Delta_n}{k_BT}\right\}$$

$\pi = T_L S$ (**Kelvin Relation**)

$$\kappa_0 = T\left(\frac{k_B}{q}\right)^2 \int \left(\frac{E-E_F}{k_BT}\right)^2 \sigma'(E)\,dE = \kappa_0 = \sigma T\left(\frac{k_B}{q}\right)^2 \left\{\left(\frac{E-E_F}{k_BT}\right)^2\right\}_{\text{ave}} \quad \kappa_e = \kappa_0 - \pi S \sigma$$

$$\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q}\right)^2 \left\{\left\langle \left(\frac{E-E_F}{k_BT}\right)^2 \right\rangle - \left\langle \left(\frac{E-E_F}{k_BT}\right) \right\rangle^2 \right\} T = LT$$

(**Weidemann-Franz "Law"**)

$2\left(\frac{k_B}{q}\right)^2 < L < \frac{\pi^2}{3}\left(\frac{k_B}{q}\right)^2$ (parabolic bands with energy-independent scattering)

Thermoelectric material Figure of Merit: $zT = \frac{S^2 \sigma T}{\kappa}$

Lattice thermal conductivity: $\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h}\int \lambda_{ph}(\hbar\omega)\frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)$

General balance equation

$$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

Prescription:

$$n_\phi(\vec{r},t) = \frac{1}{\Omega}\sum_{\vec{p}} \phi(\vec{p}) f\left(\vec{r},\vec{p},t\right) \qquad \vec{F}_\phi \equiv \frac{1}{\Omega}\sum_{\vec{p}} \phi\left(\vec{p}\right)\vec{\upsilon} f\left(\vec{r},\vec{p},t\right)$$

$$G_\phi = -q\vec{\mathcal{E}} \bullet \left\{\frac{1}{\Omega}\sum_{\vec{p}} \vec{\nabla}_p \phi f\right\} \qquad R_\phi \equiv \frac{n_\phi - n_\phi^0}{\left\langle \tau_\phi \right\rangle}$$

Current equation:

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{d\left(nu_{xx}\right)}{dx} \qquad u = \frac{1}{2}m^* \upsilon_d^2 + \frac{3}{2}k_B T_e$$

$$\upsilon_{SAT} \approx \sqrt{\frac{\hbar\omega_0}{m^*}}$$