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

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

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

$$\frac{1}{\tau} = \frac{1}{\tau_{abs}}+\frac{1}{\tau_{ems}} = \frac{2\pi}{\hbar}\left(\frac{D_A^2k_BT}{c_l}\right)\frac{D_{3D}(E)}{2}\ \text{(ADP)} \qquad L_D = \sqrt{\frac{\kappa_S\varepsilon_0k_BT}{q^2n_0}}$$

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

Boltzmann Transport Equation:

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

With a small B-field, the resulting 2D current equation is $\vec{J}_n = \sigma_S \vec{\mathcal{E}} - \sigma_S \mu_H (\vec{\mathcal{E}} \times \vec{B}) \qquad (\omega_c \tau_m << 1)$

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

Isothermal Near-Equilibrium Transport: Summary of Landauer Approach

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

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

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

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

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

Modes / channels (general):

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

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

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

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

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

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

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

Modes (graphene):

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

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

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: $\langle \upsilon_x^+ \rangle = \upsilon_T = \sqrt{2k_B T / \pi m^*}$ $(\eta_F << 0)$

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:

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

$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T} \right) \sigma'(E) dE \Big/ \int \sigma'(E) dE = -\left(\frac{k_B}{q} \right) \left\langle \frac{E - E_F}{k_B T} \right\rangle = \left(\frac{k_B}{-q} \right) \left\{ \frac{(E_C - E_F)}{k_B T} + \frac{\Delta_n}{k_B T} \right\}$$

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

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

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

(**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:

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

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