

ECE-656 Key Equations (Weeks 1-12)

Physical constants:

$$\begin{aligned} \hbar &= 1.055 \times 10^{-34} \text{ [J-s]} & m_0 &= 9.109 \times 10^{-31} \text{ [kg]} & \epsilon_0 &= 8.854 \times 10^{-14} \text{ [F/cm]} \\ k_B &= 1.380 \times 10^{-23} \text{ [J/K]} & k_B &= 8.625 \times 10^{-5} \text{ [eV/K]} & q &= 1.602 \times 10^{-19} \text{ [C]} \end{aligned}$$

Density of states in k-space:

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

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

$$D_{1D}(E) = \frac{g_v}{\pi\hbar} \sqrt{\frac{2m^*}{(E - \epsilon_1)}} \quad D_{2D}(E) = g_v \frac{m^*}{\pi\hbar^2} \quad D_{3D}(E) = g_v \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2\hbar^3}$$

Fermi function and Fermi-Dirac Integrals:

$$\begin{aligned} f_0(E) &= \frac{1}{1 + e^{(E-E_F)/k_B T}} \\ \mathcal{F}_j(\eta_F) &= \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j d\eta}{1 + e^{\eta - \eta_F}} & \mathcal{F}_j(\eta_F) &\rightarrow e^\eta \quad \eta_F \ll 0 & \frac{d\mathcal{F}_j}{d\eta_F} &= \mathcal{F}_{j-1} \\ \Gamma(n) &= (n-1)! \quad (n \text{ an integer}) & \Gamma(1/2) &= \sqrt{\pi} & \Gamma(p+1) &= p\Gamma(p) \end{aligned}$$

Scattering:

$$\begin{aligned} S(\vec{p}, \vec{p}') &= \frac{2\pi}{\hbar} \left| H_{\vec{p}', \vec{p}} \right|^2 \delta(E' - E - \Delta E) & H_{\vec{p}', \vec{p}} &= \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}' \cdot \vec{r}/\hbar} U_S(\vec{r}) e^{i\vec{p} \cdot \vec{r}/\hbar} d\vec{r} \\ \frac{1}{\tau(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') & \frac{1}{\tau_m(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') \frac{\Delta p_z}{p_{z0}} & \frac{1}{\tau_E(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') \frac{\Delta E}{E_0} \\ \text{ADP: } |K_\beta|^2 &= \beta^2 D_A^2 & \text{ODP: } |K_\beta|^2 &= D_0^2 & \text{PZ: } |K_\beta|^2 &= (qe_{PZ}/\kappa_s \epsilon_0)^2 & \text{POP: } |K_\beta|^2 &= \frac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \epsilon_0} \left(\frac{\kappa_0}{\kappa_\infty} - 1 \right) \\ S(\vec{p}, \vec{p}') &= \frac{\pi}{\Omega \rho \omega} |K_\beta|^2 \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}} \delta(E' - E \mp \hbar\omega) \\ \delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}} \delta(E' - E \mp \hbar\omega_\beta) &\rightarrow \frac{1}{\hbar v \beta} \delta \left(\pm \cos \theta + \frac{\hbar \beta}{2p} \mp \frac{\omega_\beta}{v \beta} \right) \\ \frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} &= \frac{2\pi}{\hbar} \left(\frac{D_A^2 k_B T}{c_l} \right) \frac{D_{3D}(E)}{2} \quad (\text{ADP}) & L_D &= \sqrt{\frac{\kappa_s \epsilon_0 k_B T}{q^2 n_0}} \\ \frac{1}{\tau} = \frac{1}{\tau_m} = \frac{2\pi}{\hbar} \left(\frac{\hbar D_O^2}{2\rho \omega_0} \right) \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \frac{D_{3D}(E \pm \hbar\omega_0)}{2} & N_0 &= \frac{1}{e^{\hbar\omega_0/k_B T} - 1} \quad (\text{ODP}) \end{aligned}$$

Landauer expressions for current:

$$I = \frac{2q}{h} \int T(E) M(E) (f_1 - f_2) dE \quad I = \left\{ \frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \right\} V \quad (\text{near-equilibrium})$$

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

Distribution of Modes:

$$M_{1D}(E) = \frac{h}{4} \langle v_x^+ \rangle D_{1D}(E) \quad M_{2D}(E) W = W \frac{h}{4} \langle v_x^+ \rangle D_{2D}(E) \quad M_{3D}(E) A = A \frac{h}{4} \langle v_x^+ \rangle D_{3D}(E)$$

$$\text{Transmission: } T(E) = \lambda(E) / (\lambda(E) + L) \quad \text{Diffusion coefficient: } D_n = \langle v_x^+ \rangle \langle \langle \lambda \rangle \rangle / 2$$

$$\text{Uni-directional thermal velocity: } \langle v_x^+ \rangle = v_T = \sqrt{2k_B T / \pi m^*} \quad (\eta_F \ll 0)$$

Mean-free-path for backscattering:

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

$$\text{(Diffusive) Coupled current equations: } J_x = \sigma \mathcal{E}_x - \sigma S dT/dx \quad J_x^q = T \sigma S \mathcal{E}_x - \kappa_0 dT/dx$$

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

Transport coefficients:

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

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

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

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

$$\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q} \right)^2 \left\{ \left\langle \left(\frac{E - E_F}{k_B T} \right)^2 \right\rangle - \left\langle \left(\frac{E - E_F}{k_B T} \right) \right\rangle^2 \right\} T = LT \quad (\text{Weidemann-Franz "Law"})$$

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

$$\text{Mobility: } \mu_n \equiv \frac{1}{n_s} \frac{2q}{h} \int \lambda(E) M_{2D}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

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

Equation of motion in k-space: $d(\hbar\vec{k})/dt = \vec{F}_e$

Boltzmann Transport Equation (BTE): $\frac{\partial f}{\partial t} + \vec{v} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C}f$

Collision integral:

$$\hat{C}f(\vec{r}, \vec{p}, t) = \sum_{p'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') [1 - f(\vec{p})] - \sum_{p'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) [1 - f(\vec{p}')]$$

Relaxation Time Approximation: $\hat{C}f = - (f(\vec{p}) - f_0(\vec{p})) / \tau_m$

$$\sigma = n q \mu_n \quad \mu_n = \frac{q \langle \langle \tau_m \rangle \rangle}{m^*} \quad \langle \langle \tau_m \rangle \rangle = \frac{\langle E \tau_m(E) \rangle}{\langle E \rangle} \quad D_n = \langle v_x^2 \tau_m \rangle$$

$$\vec{J}_n = \sigma_s \vec{\mathcal{E}} - \sigma_s \mu_H (\vec{\mathcal{E}} \times \vec{B}) \quad \mu_H = \mu_n r_H \quad r_H \equiv \langle \langle \tau_m^2 \rangle \rangle / \langle \langle \tau_m \rangle \rangle^2 \quad \omega_c = \frac{qB}{m^*}$$

$$R_C = \frac{\sqrt{\rho_C \rho_{SD}}}{W} \coth(L_C / L_T)$$