

Week 13 Summary: Near-equilibrium Transport: Landauer vs. Moments

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review: coupled charge and heat currents

electrical current:

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

heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

heat current (lattice):

$$q_x = -\kappa_L \left(\frac{dT}{dx} \right)$$

$$\sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle$$

$$S = - \left(\frac{k_B}{q} \right) \left(\frac{E_J - E_F}{k_B T} \right) \quad \pi = TS$$

$$\kappa_0 = \frac{\pi^2 k_B^2 T}{3h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle$$

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

$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \langle M_{ph}/A \rangle \langle \langle \lambda_{ph} \rangle \rangle$$

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2

parabolic bands, power law scattering

$$\sigma = \frac{2q^2}{h} \left\langle M_{el}/A \right\rangle \left\langle \left\langle \lambda_{el} \right\rangle \right\rangle = \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right) \Gamma(r+2) \mathcal{F}_r(\eta_F)$$

$$S = - \left(\frac{k_B}{q} \right) \left(\frac{E_J - E_F}{k_B T} \right) = - \left(\frac{k_B}{q} \right) \left(\frac{(r+2) \mathcal{F}_{r+1}(\eta_F)}{\mathcal{F}_r(\eta_F)} - \eta_F \right) \quad \pi = TS$$

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

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non-degenerate

$$\sigma = \frac{2q^2}{h} \left\langle M_{el}/A \right\rangle \left\langle \left\langle \lambda_{el} \right\rangle \right\rangle = \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right) \Gamma(r+2) e^{\eta_F}$$

$$S = - \left(\frac{k_B}{q} \right) \left(\frac{E_J - E_F}{k_B T} \right) = - \left(\frac{k_B}{q} \right) ((r+2) - \eta_F) \quad \pi = TS$$

$$\kappa_e = T \left(\frac{k_B}{q} \right)^2 \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right) \times \Gamma(r+3) e^{\eta_F}$$

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non-degenerate: conductivity

$$\sigma = \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right) \Gamma(r+2) e^{\eta_F}$$

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3} = N_C e^{\eta_F} \quad e^{\eta_F} = \frac{n_0}{N_C} \quad N_C = \frac{1}{4} \left(\frac{2m^* k_B T}{\pi\hbar^2} \right)^{3/2}$$

$$\sigma = n_0 q \left\{ \frac{v_T \lambda_0 \Gamma(r+2)}{2 k_B T / q} \right\} = n_0 q \mu_n$$

$$\sigma = n_0 q \mu_n$$

$$\mu_n = \frac{v_T \lambda_0 \Gamma(r+2)}{2 k_B T / q} = \frac{v_T \langle\langle \lambda \rangle\rangle}{2 k_B T / q}$$

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non-degenerate: Seebeck

$$S = -\left(\frac{k_B}{q}\right)\left(\frac{E_J - E_F}{k_B T}\right) = -\left(\frac{k_B}{q}\right)\left((r+2) - \eta_F\right) \quad \pi = TS$$

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3} = N_C e^{\eta_F} \quad \eta_F = \ln\left(\frac{n_0}{N_C}\right) \quad N_C = \frac{1}{4} \left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{3/2}$$

$$S = -\left(\frac{k_B}{q}\right)\left((r+2) + \ln\left(\frac{N_C}{n}\right)\right)$$

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6

non-degenerate: thermal conductivity

$$\sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle = \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right) \Gamma(r+2) e^{\eta_F}$$

$$e^{\eta_F} = \frac{\sigma}{\frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right) \Gamma(r+2)}$$

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non-degenerate

$$e^{\eta_F} = \frac{\sigma}{\frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right) \Gamma(r+2)}$$

$$\begin{aligned}\kappa_e &= T \left(\frac{k_B}{q} \right)^2 \frac{2q^2}{h} \lambda_0 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right) \times \Gamma(r+3) e^{\eta_F} \\ &= T \left(\frac{k_B}{q} \right)^2 \frac{\Gamma(r+3)}{\Gamma(r+2)} \sigma\end{aligned}$$

$$\kappa_e = T \left(\frac{k_B}{q} \right)^2 \mathcal{L} \sigma$$

$$\mathcal{L} = \frac{\Gamma(r+3)}{\Gamma(r+2)}$$

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electrical current:

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heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$\sigma = n_0 q \mu_n \quad \mu_n = \frac{v_T \lambda_0 \Gamma(r+2)}{2 k_B T / q}$$

$$S = -\left(\frac{k_B}{q}\right) \left((r+2) + \ln\left(\frac{N_C}{n}\right) \right)$$

$$\pi = TS$$

$$\kappa_e = T \left(\frac{k_B}{q}\right)^2 \mathcal{L} \sigma \quad \mathcal{L} = \frac{\Gamma(r+3)}{\Gamma(r+2)}$$

9

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balance equation prescription

$$\sum_{\vec{p}} \phi(\vec{p}) \left\{ \frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} - \frac{q \mathcal{E}_x}{\hbar} \frac{\partial f}{\partial k_x} = \hat{C} f \right\}$$

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

$$n_\phi(\vec{r}, t) = \frac{1}{\Omega} \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r}, \vec{p}, t) \quad G_\phi = -q \vec{E} \cdot \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \vec{\nabla}_{\vec{p}} \phi f \right\}$$

$$\vec{F}_\phi \equiv \frac{1}{\Omega} \sum_{\vec{p}} \phi(\vec{p}) \vec{v} f(\vec{r}, \vec{p}, t) \quad R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle}$$

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10

balance equation prescription

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

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$J_x = \sigma \mathcal{E}_x - S \sigma \frac{dT}{dx}$$

$$\phi(\vec{p}) = (-q) \vec{v}(\vec{p})$$

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$\phi(\vec{p}) = (E - F_n) \vec{v}$$

current

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

$$n_\phi(\vec{r}, t) = \frac{1}{\Omega} \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r}, \vec{p}, t)$$

$$\phi(\vec{p}) = (-q)v_x(\vec{p})$$

$$n_\phi(\vec{r}, t) = J_{nx}(\vec{r}, t)$$

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12

associated flux

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

$$\vec{F}_\phi \equiv \frac{1}{\Omega} \sum_{\vec{p}} \phi(\vec{p}) \vec{v} f(\vec{r}, \vec{p}, t)$$

$$\phi(\vec{p}) = (-q) v_x(\vec{p})$$

$$\vec{F}_\phi = F_{\phi_x} = \frac{1}{\Omega} \sum_{\vec{p}} (-q) v_x^2 f(\vec{r}, \vec{p}, t)$$

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13

current “generation”

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

$$G_\phi = -q \vec{\mathcal{E}} \cdot \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \vec{\nabla}_p \phi f \right\}$$

$$\phi(\vec{p}) = (-q) v_x(\vec{p})$$

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

$$\begin{aligned} \frac{\partial \phi(\vec{p})}{\partial p_x} &= (-q) \frac{\partial v_x}{\partial p_x} = (-q) \frac{\partial}{\partial p_x} \frac{\partial E(p)}{\partial p_x} \\ &= (-q) \frac{\partial^2 E(p)}{\partial p_x^2} = (-q) \frac{1}{m^*(E)} \end{aligned}$$

$$G_\phi = q^2 \mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \frac{1}{m^*(E)} f \right\}$$

$$G_\phi = n q^2 \mathcal{E}_x \left\langle \frac{1}{m^*(E)} \right\rangle$$

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14

current “recombination”

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

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle}$$

$$\phi(\vec{p}) = (-q)v_x(\vec{p})$$

$$R_\phi \equiv \frac{J_{nx}}{\langle \tau_J \rangle}$$

$$R_\phi \equiv \frac{J_{nx}}{\langle \tau_J \rangle}$$

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15

balance equation prescription

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

$$\phi(\vec{p}) = (-q)\vec{v}(\vec{p})$$

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$\phi(\vec{p}) = E - F_n$$

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

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16

result

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

$$\frac{\partial J_{nx}}{\partial t} = -\frac{d}{dx} n \langle v_x^2 \rangle + n q^2 \mathcal{E}_x \left\langle \frac{1}{m^*(E)} \right\rangle - \frac{J_{nx}}{\langle \tau_J \rangle}$$

$$\langle \tau_J \rangle \frac{\partial J_{nx}}{\partial t} + J_{nx} = n q \left\{ q \langle \tau_J \rangle \left\langle \frac{1}{m^*(E)} \right\rangle \right\} \mathcal{E}_x + q \langle \tau_J \rangle \frac{d}{dx} n \langle v_x^2 \rangle$$

simplify

$$\langle \tau_J \rangle \frac{\partial J_{nx}}{\partial t} + J_{nx} = nq \left\{ q \langle \tau_J \rangle \left\langle \frac{1}{m^*(E)} \right\rangle \right\} \mathcal{E}_x + q \langle \tau_J \rangle \frac{d}{dx} n \langle v_x^2 \rangle$$

$$\mu_n \equiv q \langle \tau_J \rangle \left\langle \frac{1}{m^*(E)} \right\rangle$$

$$\langle \tau_J \rangle \frac{\partial J_{nx}}{\partial t} + J_{nx} = nq \mu_n \mathcal{E}_x + q \langle \tau_J \rangle \frac{d}{dx} n \langle v_x^2 \rangle$$

Now assume that the current varies slowly on the scale of the relaxation time.

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18

simplify

$$J_{nx} = nq\mu_n \mathcal{E}_x + q\langle\tau_J\rangle \frac{d}{dx} n\langle v_x^2 \rangle$$

Now assume parabolic bands
and isotropic distribution

$$\frac{2}{m^*} \left\langle \frac{1}{2} m^* v_x^2 \right\rangle = \frac{2}{m^*} \frac{k_B T_e}{2}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + \frac{2q}{m^*} \langle\tau_J\rangle \frac{d}{dx} \left\{ n \frac{k_B T_e}{2} \right\}$$

result

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \{ nk_B T_e \}$$

Now assume near-equilibrium: $J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \{ nk_B T_L \}$

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \{ nk_B T_L \}$$

uniform temperature

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \{ n k_B T_L \}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + k_B T_L \mu_n \frac{dn}{dx}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx}$$

$$\frac{D_n}{\mu_n} = \frac{k_B T_L}{q}$$

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21

did we get something for free?

$$\mu_n = \frac{q\langle\tau_J\rangle}{m^*}$$

See equation (5.13) in *Fundamentals of Carrier Transport*

Seebeck coefficient

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \left\{ n k_B T_L \right\}$$

$$\mu_n \frac{d}{dx} \left(nk_B T_L \right) = \mu_n \left[k_B T_L \frac{\partial n}{\partial x} + nk_B \frac{dT_L}{dx} + k_B T_L \frac{\partial n}{\partial T_L} \frac{dT_L}{dx} \right]$$

$$\mu_n \frac{d}{dx} \left(nk_B T_L \right) = k_B T_L \mu_n \frac{\partial n}{\partial x} + nq\mu_n \left(\frac{k_B}{q} \right) \left\{ 1 + T_L \frac{1}{n} \frac{\partial n}{\partial T_L} \right\} \frac{dT_L}{dx}$$

Seebeck coefficient

$$\mu_n \frac{d}{dx} (nk_B T_L) = k_B T_L \mu_n \frac{\partial n}{\partial x} + nq \mu_n \left(\frac{k_B}{q} \right) \left\{ 1 + T_L \frac{1}{n} \frac{\partial n}{\partial T_L} \right\} \frac{dT_L}{dx}$$

$$n = N_C e^{(F_n - E_C)/k_B T} \quad N_C = \frac{1}{4} \left(\frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$\mu_n \frac{d}{dx} (nk_B T_L) = k_B T_L \mu_n \frac{\partial n}{\partial x} + nq \mu_n \left(\frac{k_B}{q} \right) \left\{ 2 + \frac{F_n - E_C}{k_B T_L} \right\} \frac{dT_L}{dx}$$

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24

Seebeck coefficient

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{d}{dx} \left\{ nk_B T_L \right\}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx} + nq\mu_n \left(\frac{k_B}{q} \right) \left\{ 2 - \frac{F_n - E_C}{k_B T_L} \right\} \frac{dT_L}{dx}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x - \sigma_n \left(-\frac{k_B}{q} \right) \left\{ 2 - \frac{F_n - E_C}{k_B T_L} \right\} \frac{dT_L}{dx}$$

(uniform carrier concentration)

Seebeck coefficient

$$J_{nx} = nq\mu_n E_x - \sigma_n S_n \frac{dT_L}{dx}$$

$$S_n = \left(-\frac{k_B}{q} \right) \left\{ 2 - \frac{F_n - E_C}{k_B T_L} \right\}$$

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

$$S_n = \left(-\frac{k_B}{q} \right) \left\{ 2 + \ln \left(\frac{N_C}{n} \right) \right\}$$

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26

comparison

Landauer or BTE

$$J_{nx} = \sigma_n E_x - \sigma_n S_n \frac{dT_L}{dx}$$

$$\sigma_n = nq\mu_n$$

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

$$S_n = -\left(\frac{k_B}{q}\right) \left((r+2) + \ln\left(\frac{n}{N_C}\right) \right)$$

Moment of BTE

$$J_{nx} = nq\mu_n E_x - \sigma_n S_n \frac{dT_L}{dx}$$

$$\sigma_n = nq\mu_n$$

$$\mu_n = \frac{q\langle\tau_J\rangle}{m^*}$$

$$S_n = -\left(\frac{k_B}{q}\right) \left\{ 2 + \ln\left(\frac{N_C}{n}\right) \right\}$$

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27

Landauer / BTE vs. moments

See *Fundamentals of Carrier Transport*, Sec. 5.5.2 for a discussion of how to make the moment equations consistent with the Landauer/BTE approach.

balance equation prescription

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

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$J_x = \sigma \mathcal{E}_x - S \sigma \frac{dT}{dx}$$

$$\phi(\vec{p}) = (-q) \vec{v}(\vec{p})$$

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$\phi(\vec{p}) = (E - F_n) v(\vec{p})$$

heat current

Repeat the process for the heat current.

Is the Kelvin Relation satisfied?

What is the Wiedemann-Franz Law in this approach?