ECE 656: Electronic Transport in Semiconductors Fall 2017

The Coupled Current Equations (Again)

Mark Lundstrom

Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA

ncn nanoHUB.org

11/16/17

PURDUE UNIVERSITY

The balance equation prescription

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

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

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

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

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

The balance equations

$$\frac{\partial n}{\partial t} = -\nabla \bullet \frac{\vec{J}_n}{(-q)}$$

$$\frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{m^*}\nabla W_{xx} + \frac{nq^2}{m^*}\vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

← Terminate here
(find a way to estimate *W* in terms of known quantities).

$$\frac{\partial W}{\partial t} = -\nabla \vec{F}_W - \vec{J}_n \vec{\mathcal{E}} - \frac{W - W_0}{\langle \tau_E \rangle}$$

$$\frac{\partial \vec{F}_W}{\partial t} = \ldots$$

The DD equation

$$\frac{\partial n}{\partial t} = -\nabla \bullet \frac{\vec{J}_n}{(-q)}$$

$$\frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{m^*}\nabla W_{xx} + \frac{nq^2}{m^*}\vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

← Terminate here.

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{\partial W_{xx}}{\partial x}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + \frac{2}{3}\mu_n \frac{\partial W}{\partial x}$$

$$W = \frac{3}{2} n k_B T_e$$

$$T_e = T_L = T$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{\partial n}{\partial x}$$

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

Coupled current equations

Recall that we derived the coupled current equations for the flow of charge and heat by solving the BTE in the Relaxation Time Approximation.

Coupled current equations

$$J = \sigma \mathcal{E} - \sigma S \, dT/dx$$

$$J_Q = T\sigma S \mathcal{E} - \kappa_0 \, dT/dx$$

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

$$J_Q = \pi J - \kappa_e \frac{dT}{dx}$$

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

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

$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T} \right) \sigma'(E) dE \bigg/ \int \sigma'(E) dE$$

$$\pi = TS$$

$$\kappa_0 = T \left(\frac{k_B}{q} \right)^2 \int \left(\frac{E - E_F}{k_B T} \right)^2 \sigma'(E) dE$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

Balance equation prescription

$$\frac{1}{\Omega}\sum_{\vec{p}}\phi(\vec{p})\left\{\frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_r f-q\vec{\mathcal{E}}\bullet\nabla_p f=\hat{C}f\right\}$$

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

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

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

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

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

Current equations

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

Charge current:

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

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

Heat current:

$$\phi(\vec{p}) = \left(E(\vec{p}) + E_C - F_n\right)\upsilon_x$$

$$n_\phi(\vec{r},t) = J_{Qx}(\vec{r},t) = \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r},\vec{p},t)$$

Charge current

$$J_{nx} = nq\mu_n \mathcal{E}_x + \frac{2}{3}\mu_n \frac{\partial W}{\partial x}$$

(assumes $W_{xx} = W/3$)

Now assume: $W = \frac{3}{2} n k_B T$

$$J_{nx} = nq\mu_n \mathcal{E}_x + \frac{2}{3}\mu_n \frac{\partial\left(\frac{3}{2} n k_B T\right)}{\partial x}$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + \mu_n \frac{\partial\left(n k_B T\right)}{\partial x}$$

Seebeck coefficient

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

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

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

Seebeck coefficient

$$\mu_n \frac{d}{dx}\left(n k_B T\right) = k_B T \mu_n \frac{\partial n}{\partial x} + n q \mu_n \left(\frac{k_B}{q}\right)\left\{1 + T \frac{1}{n}\frac{\partial n}{\partial T}\right\}\frac{dT}{dx}$$

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

$$\mu_n \frac{d}{dx}\left(n k_B T\right) = k_B T \mu_n \frac{\partial n}{\partial x} + n q \mu_n \left(\frac{k_B}{q}\right)\left\{\frac{3}{2} - \frac{F_n - E_C}{k_B T}\right\}\frac{dT}{dx}$$

Seebeck coefficient

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

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx} + nq\mu_n \left(\frac{k_B}{q} \right) \left\{ \frac{E_C - F_n}{k_B T} + \frac{3}{2} \right\} \frac{dT}{dx}$$

Seebeck coefficient

$$J_{nx} = nq\mu_n \mathcal{E}_x - \sigma_n S_n \frac{dT}{dx}$$

$$S_n = \left(-\frac{k_B}{q} \right) \left\{ \frac{E_C - F_n}{k_B T} + \frac{3}{2} \right\}$$

Comparison

Landauer or BTE

$$J_{nx} = \sigma_n \mathcal{E}_x - \sigma_n S_n \frac{dT_L}{dx}$$

$$\sigma_n = nq\mu_n$$

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

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

Moment of BTE

$$J_{nx} = \sigma_n \mathcal{E}_x - \sigma_n S_n \frac{dT}{dx}$$

$$\sigma_n = nq\mu_n$$

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

$$S_n = -\left(\frac{k_B}{q}\right)\left\{\frac{E_C - F_n}{k_B T} + \frac{3}{2}\right\}$$

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.

Charge and heat flow balance equations

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

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

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

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

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

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

Heat current

Repeat the process for the heat current.

Is the Kelvin Relation satisfied?

What is the Wiedemann-Franz Law in this approach?

Questions