ECE-656: Fall 2009

Lecture 28: Balance Equation Approach

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outline

1) **Introduction**
2) General continuity equation
3) Carrier continuity equation
4) Current equation
5) Summary

review

So far in ECE-656, we have discussed three general topics:

1) Landauer approach to low field transport
2) Boltzmann Transport equation
3) Carrier scattering

Landauer approach (1D)

$$I_x = -\frac{2q}{h}\int_0^{\infty} T(E)M(E)\left(f_1 - f_2\right)dE$$

- describes ballistic (*T* = 1) or diffusive (*T* < 1) transport
- works best for small bias
- leads to quantized conductance
- readily extended for thermoelectric effects
- can be derived without assuming a bandstructure (Datta: https://nanohub.org/resources/5346/

BTE

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar} \frac{\partial f}{\partial k_x} = \hat{C} f$$

- describes semi-classical transport near or far from equilibrium - hard to solve in general

$$\hat{C} f = -\left(f - f_S \right) / \tau_f$$

- describes semi-classical transport near equilibrium for specific types of scattering
- gives results that are very similar to the Landauer approach, easier to include B-field and anisotropic transport.

scattering

$$\hat{C} f = \sum_{\vec{p}'} S\left(\vec{p}', \vec{p}\right)\left[1 - f\left(\vec{p}\right)\right] - \sum_{\vec{p}'} S\left(\vec{p}, \vec{p}'\right)\left[1 - f\left(\vec{p}'\right)\right]$$

- Fermi's Golden Rule gives $S(p', p)$ or τ_f for BTE
- Also gives $\lambda(E)$ for Landauer approach

question

- physical quantities are moments of $f\left(\vec{r}, \vec{p}, t\right)$

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

e.g. $$\vec{J}_n\left(\vec{r}, t\right) = \sum_{\vec{p}} \left(-q\right) \vec{\upsilon}\, f\left(\vec{r}, \vec{p}, t\right)$$

Can we bypass solving the BTE and solve directly for the physical quantities of interest?

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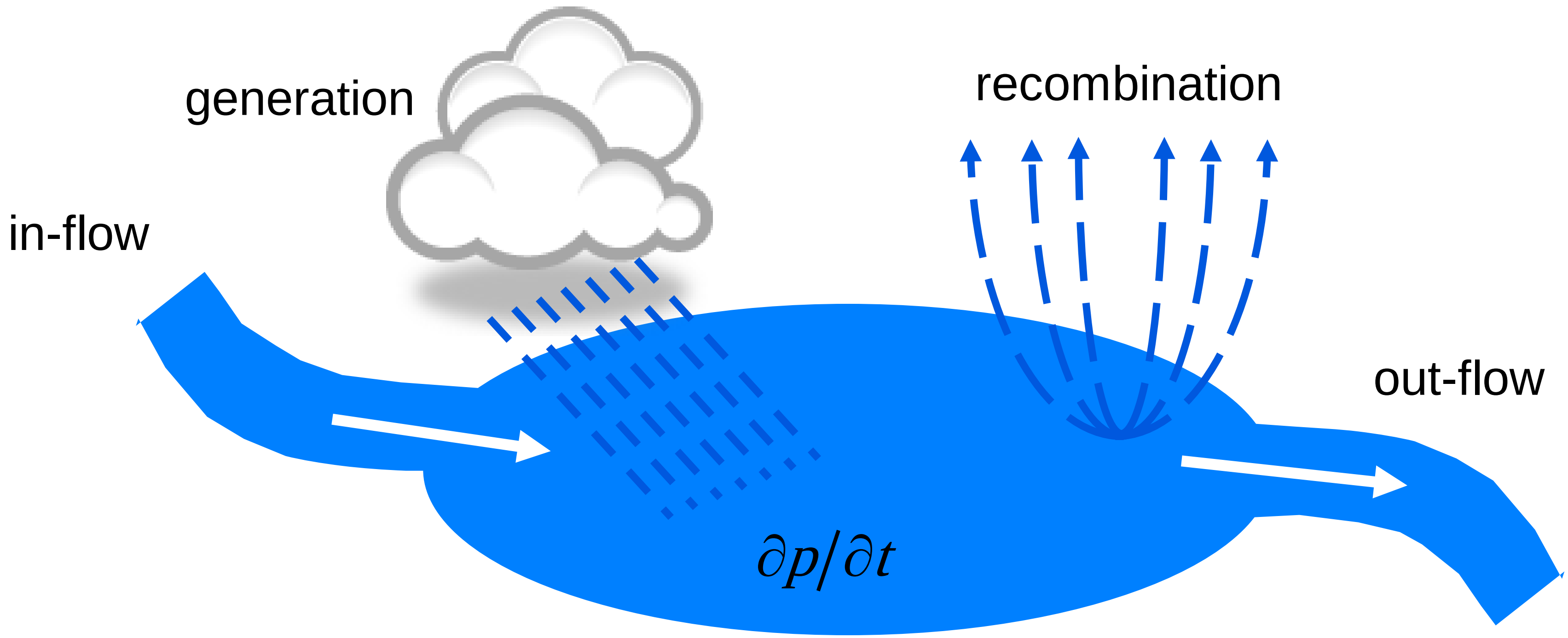
Reference: Chapter 5 of *Fundamentals of Carrier Transport* by Mark Lundstorm, Cambridge Univ. Press, 2000.

the continuity equation for holes

A familiar balance equation: $$\frac{\partial p}{\partial t} = -\nabla \bullet \frac{\vec{J}_p}{q} + G_p - R_p$$



in-flow -out-flow = - divergence of flux

balance equations for physical quantities

$$n_L = \frac{1}{L}\sum_p f(x,p,t) \qquad I_x = \frac{1}{L}\sum_p (-q)\upsilon_x f(x,p,t)$$

$$W = \frac{1}{L}\sum_p (E-\varepsilon_1) f(x,p,t) \qquad n_\phi(x,t) = \frac{1}{L}\sum_p \phi(p) f(x,p,t)$$

$$\frac{\partial p}{\partial t} = -\nabla \bullet \frac{\vec{J}_p}{q} + G_p - R_p \quad \rightarrow \quad \frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

balance equations examples

$\phi(\vec{p}) = 1: \quad n_\phi(\vec{r},t) = n(\vec{r},t)$ electron continuity equation

$\phi(\vec{p}) = (-q)\vec{\upsilon}(\vec{p}): \quad n_\phi(\vec{r},t) = \vec{J}_n(\vec{r},t)$ current balance equation

$\phi(\vec{p}) = E(\vec{p}): \quad n_\phi(\vec{r},t) = W(\vec{r},t)$ kinetic energy balance equation

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

What are the flux, generation rate, and recombination rate associated with the quantity n_ϕ?

moments of the BTE (1D)

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar}\frac{\partial f}{\partial k_x} = \hat{C} f$$

no explicit generation-recombination terms, but…

$$\phi(p_x)\frac{\partial f}{\partial t} + \phi(p_x)\upsilon_x \frac{\partial f}{\partial x} - q\mathcal{E}_x \phi(p_x)\frac{\partial f}{\partial p_x} = \phi(p_x)\hat{C} f$$

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t} + \frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x \frac{\partial f}{\partial x} + \frac{1}{L}\sum_{p_x} - q\mathcal{E}_x \phi(p_x)\frac{\partial f}{\partial p_x} = \frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C} f$$

moments of the BTE (1D)

$$\boxed{\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t}}+\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x\frac{\partial f}{\partial x}+\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}=\frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C}f$$

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t}=\frac{\partial}{\partial t}\left\{\frac{1}{L}\sum_{p_x}\phi(p_x)\,f(x,p_x,t)\right\}=\boxed{\frac{\partial n_\phi(x,t)}{\partial t}}$$

$$\boxed{n_\phi\equiv\frac{1}{L}\sum_{p_x}\phi(p_x)\,f(x,p_x,t)}$$

moments of the BTE (1D)

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t}+\boxed{\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x\frac{\partial f}{\partial x}}+\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}=\frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C}f$$

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x\frac{\partial f}{\partial x}=\frac{\partial}{\partial x}\left\{\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x f(x,p_x,t)\right\}\equiv\boxed{\frac{\partial F_\phi}{\partial x}}$$

$$\boxed{F_\phi\equiv\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x f(x,p_x,t)}$$

moments of the BTE (1D)

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t}+\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x\frac{\partial f}{\partial x}+\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}=\frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C}f$$

$$\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}=-q\mathcal{E}_x\left\{\frac{1}{L}\sum_{p_x}\frac{\partial}{\partial p_x}\big(\phi(p_x)f\big)-\frac{1}{L}\sum_{p_x}\frac{\partial\phi}{\partial p_x}f\right\}$$

$$\frac{1}{L}\int_{-\infty}^{+\infty}d\left[\phi(p_x)f\right]=\phi(p_x)f\Big|_{-\infty}^{+\infty}=0$$

$$\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}=-q\mathcal{E}_x\left\{-\frac{1}{L}\sum_{p_x}\frac{\partial\phi}{\partial p_x}f\right\}\equiv -G_\phi$$

“generation” of n_ϕ

$$G_\phi \equiv -q\mathcal{E}_x \left\{ \frac{1}{L} \sum_{p_x} \frac{\partial \phi}{\partial p_x} f \right\}$$ why?

$$G_\phi \equiv \left\{ \frac{1}{L} \sum_{p_x} \frac{\partial \phi}{\partial t} f \right\} = \left\{ \frac{1}{L} \sum_{p_x} \frac{\partial \phi}{\partial p_x} \frac{dp_x}{dt} f \right\}$$

$$\frac{dp_x}{dt} = -q\mathcal{E}_x$$ equation of motion in momentum (k) space

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

moments of the BTE (recap)

$$\underbrace{\frac{1}{L}\sum_{p_x}\phi(p_x)\frac{\partial f}{\partial t}}_{\frac{\partial n_\phi}{\partial x}}+\underbrace{\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x\frac{\partial f}{\partial x}}_{\frac{\partial F_\phi}{\partial x}}+\underbrace{\frac{1}{L}\sum_{p_x}-q\mathcal{E}_x\phi(p_x)\frac{\partial f}{\partial p_x}}_{-G_\phi}=\underbrace{\frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C}f}_{?}$$

$$n_\phi(x,t)=\frac{1}{L}\sum_{p}\phi(p)\,f(x,p,t)$$

$$F_\phi\equiv\frac{1}{L}\sum_{p_x}\phi(p_x)\upsilon_x f(x,p_x,t)$$

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

"recombination"

$$\frac{1}{L}\sum_{p_x}\phi\left(p_x\right)\hat{C}\,f = ?$$

$$\hat{C}\,f(p_x) = \sum_{p'_x}\left\{S\left(p'_x, p_x\right) f\left(p'_x\right)\left[1- f\left(p_x\right)\right] - S\left(p_x, p'_x\right) f\left(p_x\right)\left[1- f\left(p'_x\right)\right]\right\}$$

$$\frac{1}{L}\sum_{p_x}\phi\left(p_x\right)\hat{C}\,f = \frac{1}{L}\sum_{p_x}\phi\left(p_x\right)\sum_{p'_x}\left\{\begin{array}{l} S\left(p'_x, p_x\right) f\left(p'_x\right)\left[1- f\left(p_x\right)\right] \\ \qquad - S\left(p_x, p'_x\right) f\left(p_x\right)\left[1- f\left(p'_x\right)\right]\end{array}\right\}$$

To see how to evaluate this expression, for non-degenerate conditions ([1-f(p)] = 0),see the text, pp. 215-216.

phenomenological approach

$$\frac{\partial f}{\partial t}+\upsilon_x\frac{\partial f}{\partial x}-\frac{q\mathcal{E}_x}{\hbar}\frac{\partial f}{\partial k_x}=\hat{C}f \qquad \text{RTA:} \qquad \hat{C}f\approx-\frac{f-f_0}{\tau_f}$$

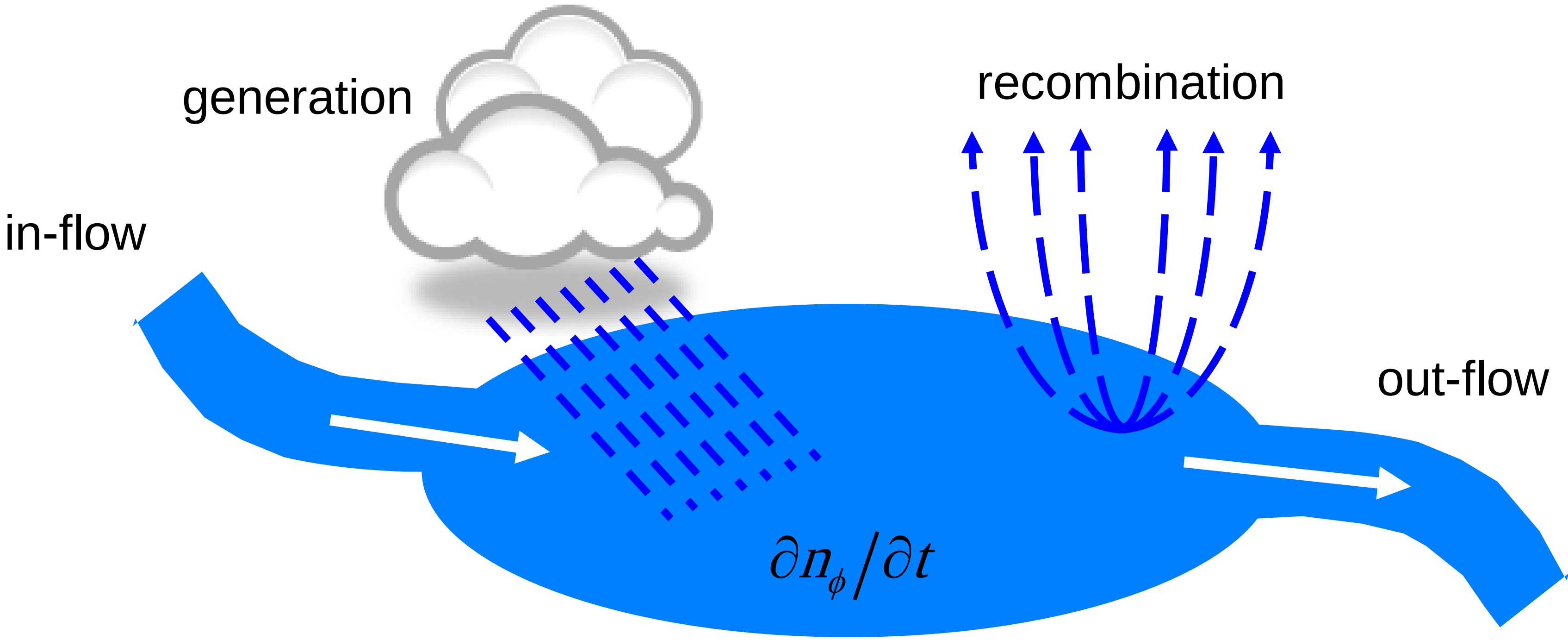
$/_f(p)$ is a “microscopic” relaxation time

$$\frac{1}{L}\sum_{p_x}\phi(p_x)\hat{C}f\equiv-\frac{n_\phi-n_\phi^0}{\langle\tau_\phi\rangle} \qquad \boxed{R_\phi\equiv\frac{n_\phi-n_\phi^0}{\langle\tau_\phi\rangle}}$$

$\langle\tau_\phi\rangle$ is a “macroscopic” relaxation time

the continuity equation for n_ϕ

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



in-flow -out-flow = - divergence of flux

putting it all together

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar} \frac{\partial f}{\partial k_x} = \hat{C} f$$

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

$$n_\phi(x,t) = \frac{1}{L}\sum_p \phi(p)\, f(x,p,t)$$

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

$$F_\phi \equiv \frac{1}{L}\sum_{p_x} \phi(p_x)\upsilon_x f(x, p_x, t)$$

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

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We will work this out in 1D. See Lundstrom, for 3D.

0th moment of the BTE (1D)

$$n_\phi(x,t) = \frac{1}{L}\sum_p \phi(p)\, f\left(x,p,t\right) \qquad \phi(p) = 1$$

$$n_\phi(x,t) = n_L(x,t)$$

$$F_\phi \equiv \frac{1}{L}\sum_{p_x} \phi\left(p_x\right)\upsilon_x f = \frac{I_x}{(-q)}$$

$$G_\phi = -q\mathcal{E}_x\left\{\frac{1}{L}\sum_{p_x}\frac{\partial \phi}{\partial p_x} f\right\} = 0$$

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

0th moment of the BTE

$$\phi(p) = 1$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \rightarrow \frac{\partial n_L(x,t)}{\partial t} = -\frac{d\left[I_{nx}/(-q)\right]}{dx}$$

$$\boxed{\frac{\partial n_L(x,t)}{\partial t} = \frac{1}{q}\frac{dI_{nx}}{dx}}$$

In steady-state, the current is constant because we have assumed that there is no generation-recomination of electrons.

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We will work this out in 1D. See Lundstrom, FCT, for 3D.

1st moment of the BTE

$$n_\phi(x,t) = \frac{1}{L}\sum_p \phi(p)\, f\left(x,p,t\right) \qquad \phi(p) = p_x$$

$$n_\phi(x,t) = P_x(x,t) = n_L \left\langle p_x \right\rangle$$

$$F_\phi \equiv \frac{1}{L}\sum_{p_x} \phi\left(p_x\right)\upsilon_x\, f\left(x,p_x,t\right) = \frac{1}{L}\sum_{p_x} p_x \upsilon_x\, f\left(x,p_x,t\right) \equiv 2W$$

$$F_\phi = 2W = n_L \left\langle p_x \upsilon_x \right\rangle$$

$$\left(W = n_L \left\langle \frac{1}{2} m^* \upsilon_x^2 \right\rangle \right)$$

1st moment of the BTE

$$\phi(p) = p_x \qquad n_\phi(x,t) = P_x \qquad F_\phi = 2W = n_L \left\langle p_x \upsilon_x \right\rangle$$

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

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{L} \sum_{p_x} \frac{\partial \phi}{\partial p_x} f \right\} = (-q) n_L \mathcal{E}_x$$

1st moment of the BTE

$$\phi(p) = 1$$

$$n_\phi(x,t) = P_x \qquad F_\phi = 2W = n_L \langle p_x \upsilon_x \rangle \qquad R_\phi = \frac{P_x}{\langle \tau_m \rangle} \qquad G_\phi = (-q) n_L \mathcal{E}_x$$

momentum balance equation

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \rightarrow \boxed{\frac{\partial P_x(x,t)}{\partial t} = -\frac{d(2W)}{dx} - n_L q \mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}}$$

current equation

$$\frac{\partial P_x(x,t)}{\partial t} = -\frac{d(2W)}{dx} - n_L q \mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

$$P_x = n_L \langle p_x \rangle = n_L m^* \langle \upsilon_x \rangle \qquad I_x = (-q) n_L \langle \upsilon_x \rangle \qquad I_x = \frac{(-q)}{m^*} P_x$$

$$\frac{\partial I_x(x,t)}{\partial t} = \frac{2q}{m^*}\frac{dW}{dx} + \frac{n_L q^2}{m^*}\mathcal{E}_x - \frac{I_x}{\langle \tau_m \rangle}$$

$$I_x + \langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} = \frac{n_L q^2 \langle \tau_m \rangle}{m^*}\mathcal{E}_x + \frac{2q\langle \tau_m \rangle}{m^*}\frac{dW}{dx} \qquad \mu_n \equiv \frac{q\langle \tau_m \rangle}{m^*}$$

drift-diffusion equation

$$I_x + \langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} = n_L q \mu_n \mathcal{E}_x + 2\mu_n \frac{dW}{dx}$$

assume:

$$\langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} << I_x$$

$$\frac{q\langle \tau_m \rangle}{m^*} = \mu_n \quad \mu_n \approx 1000 \text{ cm}^2/\text{V-s}, \quad \text{m}^* = m_0 \rightarrow \langle \tau_m \rangle = 0.5\,\text{ps}$$

$$f << \frac{1}{\langle \tau_m \rangle} = 2 \text{ THz}$$

drift-diffusion equation

$$I_x + \langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} = n_L q \mu_n \mathcal{E}_x + 2\mu_n \frac{dW}{dx}$$

assume:

$$\langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} << I_x \qquad W = n_L \frac{1}{2} m^* \langle \upsilon_x^2 \rangle \approx n_L \frac{k_B T}{2} \qquad T = \text{constant}$$

$$I_x = n_L q \mu_n \mathcal{E}_x + \mu_n \frac{d(n_L k_B T)}{dx} = n_L q \mu_n \mathcal{E}_x + k_B T \mu_n \frac{dn_L}{dx}$$

$$I_x = n_L q \mu_n \mathcal{E}_x + q D_n \frac{dn_L}{dx} \qquad D_n = \frac{k_B T}{q} \mu_n$$

DD equation with temperature gradients

assume:

$$\langle \tau_m \rangle \frac{\partial I_x(x,t)}{\partial t} << I_x \qquad W = n_L \frac{1}{2} m^* \langle \upsilon_x^2 \rangle \approx n_L \frac{k_B T}{2}$$

$T \neq \text{constant}$

$$I_x = n_L q \mu_n \mathcal{E}_x + 2\mu_n \frac{dW}{dx}$$

$$2\mu_n \frac{dW}{dx} = 2\mu_n \frac{d}{dx}\left(n_L \frac{k_B T}{2} \right) = \mu_n \frac{d}{dx}\left(n_L k_B T \right)$$

$$n_L = N_{1D} e^{(F_n - \varepsilon)/k_B T} = \frac{\sqrt{2m^* k_B T / \pi}}{\hbar} e^{(F_n - \varepsilon)/k_B T} = n_L(x, T)$$

DD equation with temperature gradients (ii)

$$I_x = n_L q \mu_n \mathcal{E}_x + 2\mu_n \frac{dW}{dx}$$

$$2\mu_n \frac{dW}{dx} = \mu_n \frac{d}{dx}\left(n_L k_B T\right) = \mu_n \left[k_B T \frac{\partial n_L}{\partial x} + n_L k_B \frac{dT}{dx} + k_B T \frac{\partial n_L}{\partial T} \frac{dT}{dx} \right]$$

$$n_L\left(x,T\right) = \frac{\sqrt{2m^* k_B T / \pi}}{\hbar} e^{\left(F_n - \varepsilon\right)/k_B T}$$

$$2\mu_n \frac{dW}{dx} = k_B T \mu_n \frac{\partial n_L}{\partial x} + n_L k_B T \mu_n \left[2 - \frac{\left(F_n - \varepsilon\right)}{k_B T} \right] \frac{dT}{dx}$$

final current equation

$$I_x = n_L q \mu_n \mathcal{E}_x + qD_n \frac{dn_L}{dx} - S_T \frac{dT}{dx}$$

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

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

$$S_T = n_L q \mu_n \frac{k_B}{(-q)} \left[2 - \frac{(E_F - \varepsilon)}{k_B T} \right]$$

(Soret coefficient)

Note error in eqn. (5.101), p. 236 of Lundstrom)

Seebeck coefficient

assume $dn_L/dx = 0$, and solve for $\mathcal{E}_x$:

$$I_x = n_L q \mu_n \mathcal{E}_x + qD_n \frac{dn_L}{dx} - S_T \frac{dT}{dx}$$

$$\mathcal{E}_x = \frac{I_x}{n_L q \mu_n} + \frac{S_T}{n_L q \mu_n} \frac{dT}{dx}$$

$$\mathcal{E}_x = \rho_0 I_x + S \frac{dT}{dx}$$

$$S = \frac{k_B}{(-q)}\left[2 - \eta_F\right]$$

recall: Lecture 8

$$S_{1D} = -\frac{k_B}{q}\left[(r+1) - \eta_F\right]$$

$$\lambda(E) = \lambda_0 \left(E/k_B T\right)^r$$

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moments of the BTE

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar}\frac{\partial f}{\partial k_x} = \hat{C} f \Rightarrow \frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

$$\frac{\partial n_L(x,t)}{\partial t} = \frac{dI_{nx}}{dx} \qquad \phi(p_x) = 1 = p_x^0$$

0th moment

$$I_x + \tau_m \frac{\partial I_x(x,t)}{\partial t} = n_L q \mu_n \mathcal{E}_x + 2\mu_n \frac{dW}{dx} \qquad \phi(p_x) = (-q)\frac{p_x^1}{m^*}$$

1st moment

Now we need an equation for *W* ….

terminating the hierarchy

Zeroth moment brings in the first moment

First moment brings in the second moment

$$W = \frac{1}{L}\sum_{p_x}\frac{p_x \upsilon_x}{2} f(x, p_x, t) = n_L u_{xx} \quad u_{xx} \approx \frac{k_B T}{2}$$

But what is *T*? Answer: Near equilibrium: $T \approx T_L$

questions

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