ECE 656: Electronic Transport in Semiconductors Fall 2017

Moment Equations:

0, 1, 2, and 3

Mark Lundstrom

Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA

11/9/17

The balance equation prescription

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

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

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

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

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

Balance equations hierarchy

$\phi(\vec{p}) = 1$ — electron continuity equation

$\phi(\vec{p}) = \vec{p}$ — momentum balance equation

$\phi(\vec{p}) = E(\vec{p})$ — energy balance equation

$\phi(\vec{p}) = \upsilon(\vec{p})E(\vec{p})$ — energy flux balance equation

Outline

1) **Zeroth moment (continuity eqn.)**
2) First moment (current eqn.)
3) Second moment (energy balance eqn.)
4) The third moment (energy flux eqn.)
5) Summary

Zeroth moment

$$\phi(\vec{p}) = p^0 = 1$$

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

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

$$G_\phi = -q\vec{\mathcal{E}} \bullet \left\{\frac{1}{\Omega}\sum_{\vec{p}} \vec{\nabla}_p (1) f\right\} = 0$$

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

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{n - n_0}{\tau_n} \, ?$$

Zeroth moment "recombination" term

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{n - n_0}{\tau_n} \ ?$$

Since we have included no recombination terms in our BTE, electrons much be conserved.

$$R_\phi = 0$$

How can we show this rigorously?

Zeroth moment "recombination" term

$$R_\phi \equiv \frac{1}{\Omega}\sum_{\vec{p}}\phi(\vec{p})\hat{C}f$$

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

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

$$-\frac{1}{\Omega}\sum_{\vec{p}}\phi(\vec{p})\sum_{\vec{p}'}S(\vec{p},\vec{p}')f(\vec{p})\left[1-f(\vec{p}')\right]$$

$$\phi(\vec{p}) = 1$$

Zeroth moment "recombination" term

$$\phi(\vec{p}) = 1$$

$$R_\phi = \frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p}',\vec{p}) f(\vec{p}')\left[1 - f(\vec{p})\right]$$
$$-\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p},\vec{p}') f(\vec{p})\left[1 - f(\vec{p}')\right]$$

Work on the first term on the RHS:

$$\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p}',\vec{p}) f(\vec{p}')\left[1 - f(\vec{p})\right]$$

Zeroth moment "recombination" term

We are integrating out p and p' – they are dummy variables. Let's change their names.

$$\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p}',\vec{p}) f(\vec{p}')\left[1-f(\vec{p})\right] \rightarrow \frac{1}{\Omega}\sum_{\vec{p}'}\sum_{\vec{p}} S(\vec{p},\vec{p}') f(\vec{p})\left[1-f(\vec{p}')\right]$$

Now let's interchange the order of summation (integration):

$$\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p},\vec{p}') f(\vec{p})\left[1-f(\vec{p}')\right]$$

Zeroth moment "recombination" term

New term 1 on RHS: $\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p},\vec{p}')f(\vec{p})\left[1-f(\vec{p}')\right]$

$$R_\phi = \frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p}',\vec{p})f(\vec{p}')\left[1-f(\vec{p})\right]$$
$$-\frac{1}{\Omega}\sum_{\vec{p}}\sum_{\vec{p}'} S(\vec{p},\vec{p}')f(\vec{p})\left[1-f(\vec{p}')\right]$$

$$R_\phi = 0$$

Scattering conserves electrons.

Zeroth moment

$$\phi(\vec{p}) = p^0 = 1$$

$$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi \qquad \rightarrow \quad \rightarrow \qquad \boxed{\frac{\partial n}{\partial t} = -\nabla \bullet \frac{\vec{J}_n}{(-q)}}$$

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

$$G_\phi = -q\vec{\mathcal{E}} \bullet \left\{ \frac{1}{\Omega}\sum_{\vec{p}} \vec{\nabla}_p (1) f \right\} = 0$$

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

$$R_\phi = 0$$

Zeroth moment summary

$$\phi(\vec{p}) = p^0 = 1$$

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

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

$$\vec{J}_n = ?$$

Write another moment equation!

Outline

1) Zeroth moment (continuity eqn.)
2) First moment (current eqn.)
3) Second moment (energy balance eqn.)
4) The third moment (energy flux eqn.)
5) Summary

First moment

$$\phi(\vec{p}) = p_x$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{\partial F_{\phi x}}{\partial x} + G_\phi - R_\phi \quad \rightarrow \quad \rightarrow \quad ?$$

$$n_\phi(\vec{r},t) = \frac{1}{\Omega}\sum_{\vec{p}}\left(p_x\right) f\left(\vec{r},\vec{p},t\right) = P_x(\vec{r},t) \qquad W \equiv \frac{1}{\Omega}\sum_{\vec{p}} E\left(\vec{p}\right) f = \frac{1}{\Omega}\sum_{\vec{p}}\frac{1}{2}m^*\upsilon^2 f$$

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}}\left(p_x\right)\upsilon_x f\left(\vec{r},\vec{p},t\right) \equiv 2W_{xx} \qquad W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}}\frac{1}{2}m^*\upsilon_x^2 f = \frac{1}{\Omega}\sum_{\vec{p}}\frac{1}{2}p_x\upsilon_x f$$

First moment

$$\phi(\vec{p}) = p_x$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{\partial F_{\phi x}}{\partial x} + G_\phi - R_\phi \quad \rightarrow \quad \rightarrow \quad \frac{\partial P_x}{\partial t} = -\frac{\partial (2W_{xx})}{\partial x} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

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

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

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}} (p_x) \upsilon_x f(\vec{r},\vec{p},t) \equiv 2W_{xx}$$

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{P_x - P_{x0}}{\langle \tau_m \rangle} = \frac{P_x}{\langle \tau_m \rangle}$$

Momentum balance equation

$$\phi(\vec{p}) = p_x \qquad \frac{\partial P_x}{\partial t} = -\frac{\partial(2W_{xx})}{\partial x} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

What is W_{xx}?

Answer: Write another balance equation to find out.

$$n_\phi(\vec{r},t) = \frac{1}{\Omega}\sum_{\vec{p}} \phi(\vec{p}) f(\vec{r},\vec{p},t) \qquad \phi(\vec{p}) = \frac{1}{2} p_x \upsilon_x \quad W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}} \left(\frac{1}{2} p_x \upsilon_x\right) f(\vec{r},\vec{p},t)$$

Momentum balance equation

$$\phi(\vec{p}) = p_x \qquad \frac{\partial P_x}{\partial t} = -\frac{\partial(2W_{xx})}{\partial x} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

$$W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}}\left(\frac{1}{2}p_x \upsilon_x\right) f(\vec{r},\vec{p},t)$$

$$W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}}\left(\frac{1}{2}m^* \upsilon_x^2\right) f(\vec{r},\vec{p},t) \qquad W = \frac{1}{\Omega}\sum_{\vec{p}}\left(\frac{1}{2}m^* \upsilon^2\right) f(\vec{r},\vec{p},t)$$

Assume an isotropic distribution of velocities: $W_{xx} = W/3$

Momentum balance equation

$$\phi(\vec{p}) = p_x \qquad \frac{\partial P_x}{\partial t} = -\frac{2}{3}\frac{\partial W}{\partial x} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

Next, we need to write a balance equation for the kinetic energy density, *W*.

But first, let's re-cap.

Re-cap

$$\phi(\vec{p}) = p^0 = 1 \qquad \frac{\partial n}{\partial t} = -\nabla \bullet \frac{\vec{J}_n}{(-q)}$$

$$\phi(\vec{p}) = \vec{p} \qquad \frac{\partial \vec{P}}{\partial t} = -\frac{2}{3}\nabla W - nq\vec{\mathcal{E}} - \frac{\vec{P}}{\langle \tau_m \rangle}$$

$$\vec{P} = nm^* \langle \vec{\upsilon} \rangle \qquad \vec{J}_n = n(-q)\langle \vec{\upsilon} \rangle \qquad (-q)\frac{\vec{P}}{m^*} = \vec{J}_n$$

$$\phi(\vec{p}) = \vec{p} \qquad \frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{3m^*}\nabla W + \frac{nq^2}{m^*}\vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

Outline

1) Zeroth moment (continuity eqn.)
2) First moment (current eqn.)
3) **Second moment (energy balance eqn.)**
4) The third moment (energy flux eqn.)
5) Summary

Second moment

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

$$\frac{\partial n_\phi}{\partial t} = -\frac{\partial F_{\phi x}}{\partial x} + G_\phi - R_\phi \quad \rightarrow \quad \rightarrow \quad \frac{\partial W}{\partial t} = -\frac{\partial F_{Wx}}{\partial x} - J_{nx}\mathcal{E}_x - \frac{W - W_0}{\langle \tau_E \rangle}$$

$$n_\phi(\vec{r},t) = \frac{1}{\Omega}\sum_{\vec{p}} \left(E(\vec{p})\right) f(\vec{r},\vec{p},t) = W(\vec{r},t) \qquad G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega}\sum_{\vec{p}} \frac{\partial\left(E(\vec{p})\right)}{\partial p_x} f \right\} = J_{nx}\mathcal{E}_x$$

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}} \left(E(\vec{p})\right)\upsilon_x f(\vec{r},\vec{p},t) \equiv F_{Wx} \qquad R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{W - W_0}{\langle \tau_E \rangle}$$

The balance equations

$$\phi(\vec{p}) = p^0 = 1$$

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

$$\phi(\vec{p}) = p_x$$

$$\frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{3m^*}\nabla W + \frac{nq^2}{m^*}\vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

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

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

Outline

1) Zeroth moment (continuity eqn.)
2) First moment (current eqn.)
3) Second moment (energy balance eqn.)
4) **Third moment (energy flux eqn.)**
5) Summary

Third moment

$$\phi(\vec{p}) = E(p)\upsilon_x$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{\partial F_{\phi x}}{\partial x} + G_\phi - R_\phi \quad \rightarrow \quad \rightarrow \quad \frac{\partial F_{Wx}}{\partial t} = ?$$

$$n_\phi(\vec{r},t) = \frac{1}{\Omega}\sum_{\vec{p}}\left(\upsilon_x E(\vec{p})\right) f(\vec{r},\vec{p},t) = F_{Wx}(\vec{r},t) \qquad G_\phi = -q\mathcal{E}_x\left\{\frac{1}{\Omega}\sum_{\vec{p}}\frac{\partial\left(\upsilon_x E(\vec{p})\right)}{\partial p_x} f\right\} = ?$$

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}}\left(\upsilon_x E(\vec{p})\right)\upsilon_x f(\vec{r},\vec{p},t) \equiv X_{xx} \qquad R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle} = \frac{F_{Wx}}{\langle \tau_{F_W} \rangle}$$

The balance equations

$$\frac{\partial n}{\partial t} = -\nabla \bullet \frac{J_{nx}}{(-q)}$$

$$\frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{3m^*}\nabla W + \frac{nq^2}{m^*}\vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

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

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

We need to terminate the hierarchy of moment equations.

The balance equations

$$\frac{\partial n}{\partial t} = -\nabla \bullet \left[\vec{J}_n / (-q) \right]$$

$$\frac{\partial \vec{J}_n}{\partial t} = \frac{2q}{3m^*} \nabla W + \frac{nq^2}{m^*} \vec{\mathcal{E}} - \frac{\vec{J}_n}{\langle \tau_m \rangle}$$

← Terminate here and get the DD equations.

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

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

← Terminate here and get the energy transport equations.

Questions

1) Zeroth moment (continuity eqn.)
2) First moment (current eqn.)
3) Second moment (energy balance eqn.)
4) The third moment (energy flux eqn.)
5) Summary