ECE 656: Electronic Transport in Semiconductors Fall 2017

The Moment Equation Approach

Mark Lundstrom

Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA

11/7/17

ECE 656: Transport physics

Near-equilibrium:

✓ ballistic to diffusive
✓ electrons and phonons
✓ coupled flows
✓ magnetic fields
✓ electrical characterization

Far from equilibrium:

- diffusive high-field (hot carrier) transport in the bulk
- non-local transport in devices
- ballistic transport in devices under high bias

ECE 656: Analytical and numerical techniques

✓ 1) Landauer approach

✓ 2) Boltzmann Transport Equation

➔ 3) **Moments of the BTE**

4) Monte Carlo simulation

5) (Quantum transport)

Boltzmann Transport Equation (BTE)

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f$$

in general, **very** difficult to solve

Moments of the BTE

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.

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

$$\vec{J}_n\left(\vec{r},t\right)=\frac{1}{\Omega}\sum_{\vec{p}}\left(-q\right)\vec{\upsilon}\,f\left(\vec{r},\vec{p},t\right)$$

More moments

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

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

$\phi(\vec{p}) = E(\vec{p}):$ $\quad n_\phi(\vec{r},t) = W(\vec{r},t)$ K.E. density

$\phi(\vec{p}) = \vec{\upsilon}(\vec{p})\left(E(\vec{p}) - E_C\right)$ $\quad n_\phi(\vec{r},t) = \vec{F}_E(\vec{r},t)$ energy flux

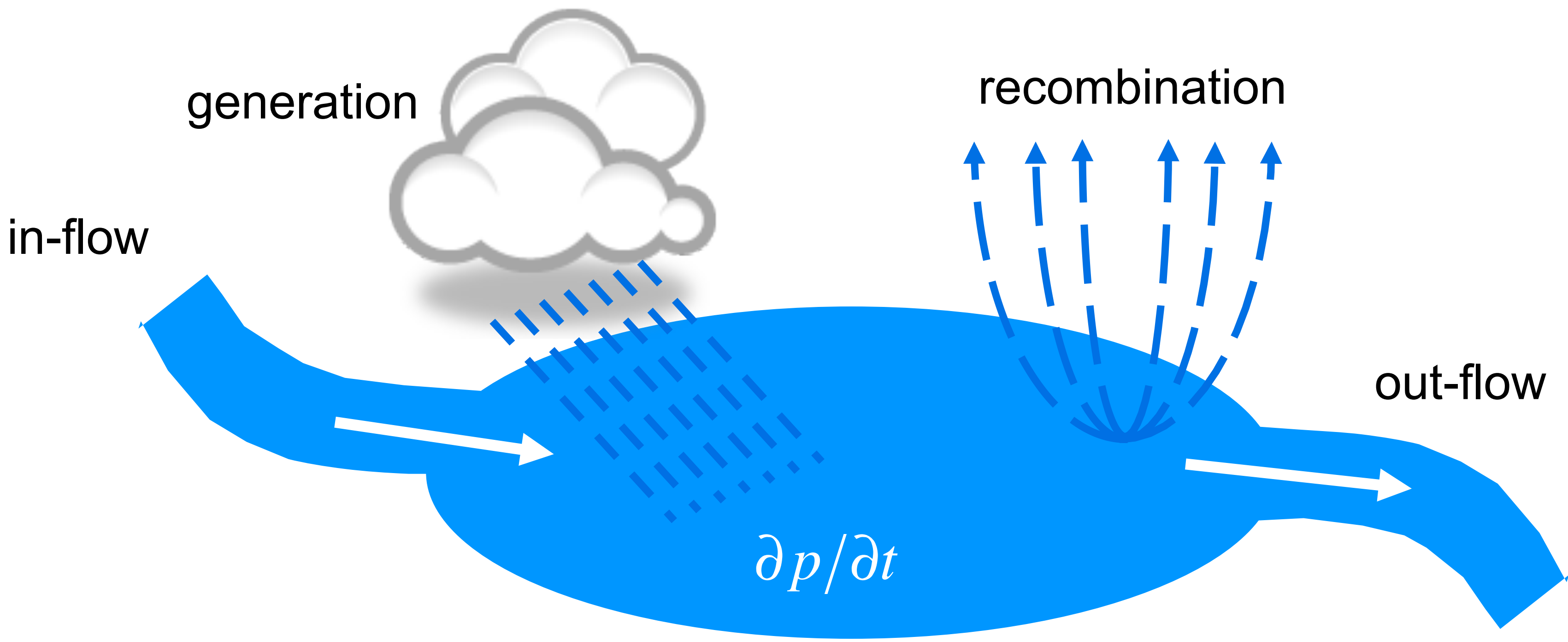
Can we bypass solving the BTE and solve directly for the physical quantities of interest?

Outline

1) Introduction
2) The prescription
3) Summary

The continuity equation for holes

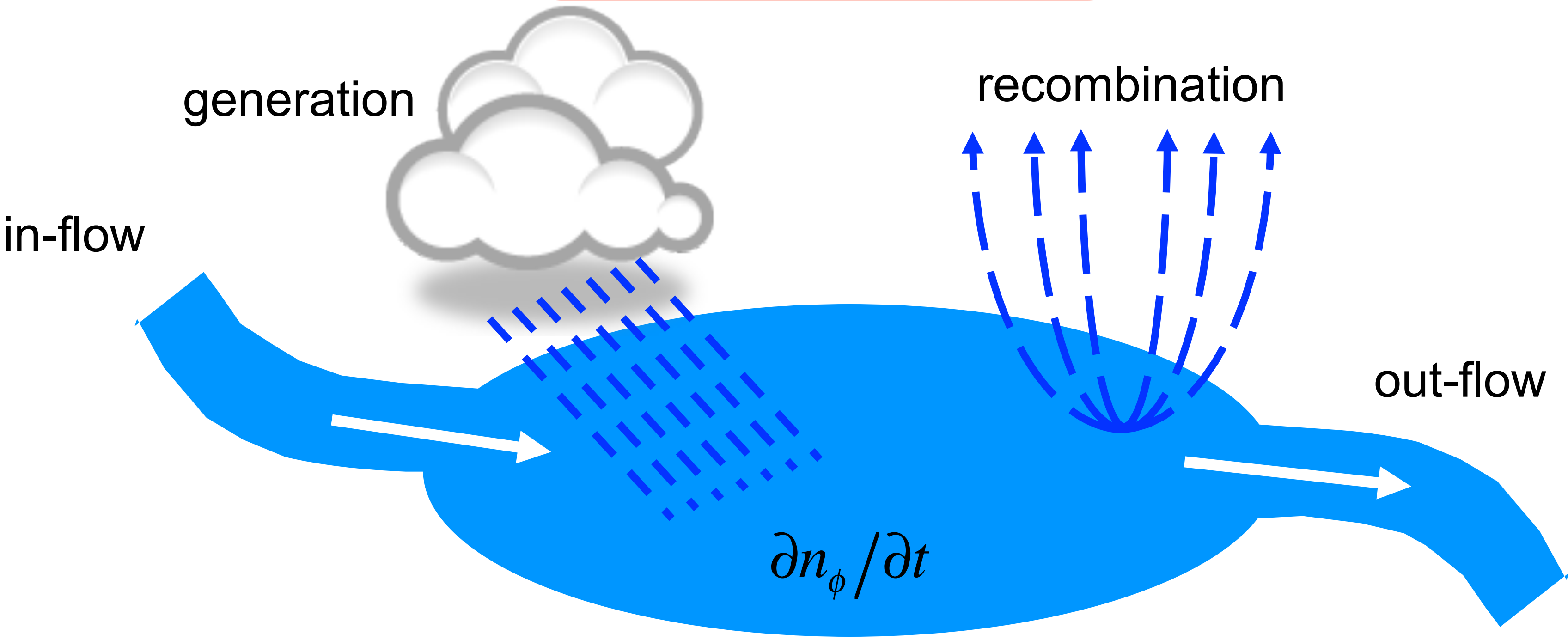
A familiar balance equation: $$\frac{\partial p}{\partial t} = -\nabla \bullet \frac{\vec{J}_p}{q} + G_p - R_p$$



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

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

Derivation

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

no explicit generation-recombination terms, but…

We will find "generation" and "recombination" terms in the moment equations.

Derivation (II)

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

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

Multiply by a function of momentum:

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

Derivation (iiI)

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

Sum (integrate) over momentum

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

(1) **(2)** **(3)** **(4)**

Recap

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \vec{\nabla}_r f - q\vec{\mathcal{E}} \bullet \vec{\nabla}_p f = \hat{C} f$$

$$\times \phi(\vec{p}) \qquad \sum_{\vec{p}} (\ )$$

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

(1) **(2)** **(3)** **(4)**

Term 1

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

(1) **(2)** **(3)** **(4)**

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

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

Term 2

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

(1) **(2)** **(3)** **(4)**

$$\sum_{\vec{p}} \frac{\partial\left(\phi(\vec{p}) \upsilon_x f\right)}{\partial x} = \frac{\partial}{\partial x} \sum_{\vec{p}} \phi(\vec{p}) \upsilon_x f = \frac{\partial F_{\phi x}}{\partial x}$$

$$\sum_{\vec{p}} \frac{\partial\left(\phi(\vec{p}) \upsilon_x f\right)}{\partial x} = \frac{\partial F_{\phi x}}{\partial x}$$

Term 3

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

(1) **(2)** **(3)** **(4)**

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

$$q\mathcal{E}_x \sum_{\vec{p}} \phi(\vec{p}) \frac{\partial f}{\partial p_x} = 0 - q\mathcal{E}_x \sum_{\vec{p}} \frac{\partial \phi(\vec{p})}{\partial p_x} f$$

$$q\mathcal{E}_x \sum_{\vec{p}} \phi(\vec{p}) \frac{\partial f}{\partial p_x} = -q\mathcal{E}_x \sum_{\vec{p}} \frac{\partial \phi(\vec{p})}{\partial p_x} f \equiv G_\phi$$

"Generation" of n_ϕ

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

Example:

Spatially uniform, no scattering

$$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - 0 \rightarrow$$

$$\frac{\partial n_\phi}{\partial t} = G_\phi$$

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

$$\frac{\partial W}{\partial t} = G_W$$

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

$$\frac{\partial W}{\partial t} = J_{nx}\mathcal{E}_x$$ ✓

Term 4

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

(1) **(2)** **(3)** **(4)**

$$\hat{C}f \equiv \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}$$

$$\sum_{\vec{p}} \phi(\vec{p}) \hat{C} f = ?$$

Term 4

$$\sum_{\vec{p}} \phi(\vec{p}) \hat{C} f = ?$$

(4)

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

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

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

Term 4: Simpler approach

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

(1) **(2)** **(3)** **(4)**

$$\hat{C} f \equiv \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}$$

$$\sum_{\vec{p}} \phi(\vec{p}) \hat{C} f \equiv -R_\phi$$

"Recombination" of n_ϕ

$$R_\phi = \sum_{\vec{p}} \phi(\vec{p}) \hat{C} f = -\frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle}$$ why?

$$\hat{C} f = -\frac{f - f_0}{\tau_m}$$ RTA

$$\sum_{\vec{p}} \phi(\vec{p}) \hat{C} f = -\sum_{\vec{p}} \phi(\vec{p}) \frac{f - f_0}{\tau_m} = -\frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle}$$

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

"recombination" due to scattering

About the Relaxation Time Approximation

"Microscopic RTA"

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

$$\hat{C} f(\vec{p}) = -\frac{f(\vec{p}) - f_S(\vec{p})}{\tau_m(\vec{p})}$$

"Macroscopic RTA"

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

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

Summary: Balance equation prescription

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

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

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

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

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

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

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

Questions

1) Introduction
2) The prescription
3) Summary