# Lecture19: Drift-Diffusion

Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Lab.
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

GIST Lecture on November 21, 2016 (Internal use only)

# Final exam. (Presentation)

- Date: December 12$^{th}$, 2016 (Tentative)
  – Depending on the situation, December 14$^{th}$ can be also used.
- Present your own work:
  – Non-equilibrium Green's function simulator
  – Mobility calculator
  – Graphene simulator
  – Drift-diffusion simulator
  – And so on…
  – *Please discuss with me, before your final presentation.*
- Your grade
  – Homework
  – Final presentation

# Calendar

- Plan for remaining lectures
  - IEDM business trip
  - *<u>Four make-up sessions</u>* will be made.

| Mon | Tue | Wed | Thu | Fri | Sat | Sun |
|---|---|---|---|---|---|---|
| | | 16 (L18) | 17 | 18 | 19 | 20 |
| 21 (L19) | 22 | 23 (L20) | 24 | 25 (L21) | 26 | 27 |
| 28 (No lecture) | 29 | 30 (L22) | Dec.1 | 2 (L23) | 3 | 4 |
| 5 (No lecture) | 6 | 7 (No lecture) | 8 | 9 | 10 | 11 |
| 12 (L24) | 13 | 14 (L25) | 15 | 16 (Final) | 17 | 18 |

# How to derive the DD eqs.

- Starting from the Boltzmann equation,
  - Let's derive the first two equations!
  - Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \frac{1}{\hbar}\mathbf{F} \cdot \nabla_k f = \hat{S}$$

# Continuity equation (1)

- Integrating the Boltzmann equation,
  - We have (neglecting the spin degeneracy)

$$\frac{\partial}{\partial t}\frac{1}{(2\pi)^3}\int_{BZ} f\,d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ} \mathbf{v}\cdot\nabla_r f\,d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ}\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\,d\mathbf{k}$$
$$= \frac{1}{(2\pi)^3}\int_{BZ}\hat{S}\,d\mathbf{k}$$

  - In terms of the electron density,

$$n = \frac{1}{(2\pi)^3}\int_{BZ} f\,d\mathbf{k}$$

  - It is now written as

$$\frac{\partial}{\partial t}n + \frac{1}{(2\pi)^3}\int_{BZ} \mathbf{v}\cdot\nabla_r f\,d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ}\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\,d\mathbf{k} = 0$$

Why?

# Continuity equation (2)

- Moreover, for a position-independent band structure,
  - It is now written as

$$\frac{\partial}{\partial t}n + \nabla_r \cdot \frac{1}{(2\pi)^3}\int_{BZ} \mathbf{v} f d\mathbf{k} + \cancel{\frac{1}{\hbar}\mathbf{F} \cdot \frac{1}{(2\pi)^3}\int_{BZ} \nabla_k f d\mathbf{k}} = 0$$

  - With the electron flux,

$$\mathbf{F}_n = \frac{1}{(2\pi)^3}\int_{BZ} \mathbf{v} f d\mathbf{k}$$

  - The continuity equation is obtained:

$$\frac{\partial}{\partial t}n + \nabla_r \cdot \mathbf{F}_n = 0$$

# Current density equation (1)

- Now, instead of just integrating the Boltzmann equation,
  - The velocity is multiplied.

$$\mathbf{v}\,\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{v}\cdot\nabla_r f) + \mathbf{v}\left(\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\right) = \mathbf{v}\hat{S}$$

  - Then, it is integrated.

$$\frac{\partial}{\partial t}\frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}f\,d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}(\mathbf{v}\cdot\nabla_r f)d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}\left(\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\right)d\mathbf{k}$$
$$= \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}\hat{S}d\mathbf{k}$$

  - It is readily found that

$$\frac{\partial}{\partial t}\mathbf{F}_n + \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}(\mathbf{v}\cdot\nabla_r f)d\mathbf{k} + \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}\left(\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\right)d\mathbf{k}$$
$$= \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}\hat{S}d\mathbf{k}$$

# Current density equation (2)

- Consider the third term.
  - For a given direction, $x_i$,

$$\frac{1}{(2\pi)^3}\int_{BZ} v_i\left(\frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f\right)d\mathbf{k} = -\mathbf{F}\cdot\frac{1}{(2\pi)^3}\int_{BZ}\frac{1}{\hbar}(\nabla_k v_i)f\,d\mathbf{k}$$

  - From the definition of the inverse mass, it is now noted that

$$-\sum_j F_j\frac{1}{(2\pi)^3}\int_{BZ} m_{ij}^{-1} f\,d\mathbf{k}$$

  - Using the effective mass,

$$-F_i\frac{1}{m^*}n \longleftarrow$$

Which approximation?

  - Therefore, in a vector form, the third term becomes

$$-\boldsymbol{F}\frac{1}{m^*}n$$

# Current density equation (3)

- Consider the second term.
  - For a given direction, $x_i$, it is

$$\sum_j \frac{1}{(2\pi)^3} \int_{BZ} v_i v_j \frac{\partial f}{\partial x_j} d\mathbf{k} = \sum_j \frac{1}{(2\pi)^3} \frac{\partial}{\partial x_j} \int_{BZ} v_i v_j f \, d\mathbf{k}$$

- Collecting the above discussion,
  - The equation looks like

$$\frac{\partial}{\partial t} F_{n,i} + \sum_j \frac{1}{(2\pi)^3} \frac{\partial}{\partial x_j} \int_{BZ} v_i v_j f \, d\mathbf{k} - F_i \frac{1}{m^*} n = \frac{1}{(2\pi)^3} \int_{BZ} v_i \hat{S} \, d\mathbf{k}$$

  - With the momentum relaxation time,

$$\frac{\partial}{\partial t} F_{n,i} + \sum_j \frac{1}{(2\pi)^3} \frac{\partial}{\partial x_j} \int_{BZ} v_i v_j f \, d\mathbf{k} - F_i \frac{1}{m^*} n = -\frac{F_{n,i}}{\tau_j}$$

  - We have to calculate a complicated quantity, $v_i v_j$. How?