
Lecture16

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

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

Review

- Our goal
 - Reduction of the dimensionality
- Our achievement
 - An explicit equation in the energy space

$$\frac{\partial f(x, \epsilon, \phi)}{\partial t} + v \cos \phi \frac{\partial f(x, \epsilon, \phi)}{\partial x} + F \left(v \cos \phi \frac{\partial f(x, \epsilon, \phi)}{\partial \epsilon} - \sin \phi \frac{1}{\hbar k} \frac{\partial f(x, \epsilon, \phi)}{\partial \phi} \right) = \hat{S}$$

- Next step
 - Fourier harmonics expansion



BTE simulator (4)

- Derivation

- Pham's Fourier harmonic, $Y_m(\phi)$, is defined as

$$Y_m(\phi) = c_m \cos(m\phi + \varphi_m)$$

$$c_m = \sqrt{\frac{1}{(1 + \delta_{m,0})\pi}}$$

- The phase, φ_m , is $\frac{\pi}{2}$ for negative m . Otherwise, it is zero.
 - Multiplying Y_m ,

$$\begin{aligned} Z d\epsilon \frac{\partial f}{\partial t} Y_m d\phi + v Z d\epsilon \frac{\partial f}{\partial x} \cos \phi Y_m d\phi + v F Z d\epsilon \frac{\partial f}{\partial \epsilon} \cos \phi Y_m d\phi \\ - F \frac{1}{\hbar k} Z d\epsilon \frac{\partial f}{\partial \phi} \sin \phi Y_m d\phi = Z d\epsilon \hat{S} Y_m d\phi \end{aligned}$$

BTE simulator (5)

- Derivation

- Note that $\cos \phi Y_m = \frac{1}{c_1} Y_1 Y_m$ and $\sin \phi Y_m = \frac{1}{c_{-1}} Y_{-1} Y_m$

- By integration over the angle,

$$\begin{aligned} & Zd\epsilon \frac{\partial}{\partial t} f_m(x, \epsilon, t) + vZd\epsilon \frac{\partial}{\partial x} \sum_{m'} \frac{1}{c_1} f_{m'}(x, \epsilon, t) Y_{m',m,1} \\ & + vFZd\epsilon \frac{\partial}{\partial \epsilon} \sum_{m'} \frac{1}{c_1} f_{m'}(x, \epsilon, t) Y_{m',m,1} \\ & - F \frac{1}{\hbar k} Zd\epsilon \sum_{m'} \frac{-m'}{c_{-1}} f_{m'}(x, \epsilon, t) Y_{-m',m,-1} = Zd\epsilon \hat{S}_m \end{aligned}$$

- Here, $Y_{m,m',m''}$ is the integral of the triple product.

BTE simulator (6)

- Derivation

- The H-transformation is introduced. $H = \epsilon - qV$

$$Zd\epsilon \frac{\partial}{\partial t} f_m(x, \epsilon, t) + vZdH \frac{\partial}{\partial x} \sum_{m'} \frac{1}{c_1} f_{m'}(x, H, t) Y_{m', m, 1} - \left(q \frac{\partial V}{\partial x} \right) \frac{1}{\hbar k} ZdH \sum_{m'} \frac{-m'}{c_{-1}} f_{m'}(x, H, t) Y_{-m', m, -1} = ZdH \hat{S}_m$$

- Let us explicitly write the above equation for a given m .

BTE simulator (7)

- Derivation

- When $m = 0$,

$$Zd\epsilon \frac{\partial}{\partial t} f_0(x, \epsilon, t) + \frac{\partial}{\partial x} \frac{1}{c_1} v Z dH f_1(x, H, t) Y_{1,0,1} = Z dH \hat{S}_0$$

- Where is the last term?
- Stabilization scheme is employed.
- For a general even number,

$$Zd\epsilon \frac{\partial}{\partial t} f_m(x, \epsilon, t) + \frac{\partial}{\partial x} v Z dH \sum_{m'} \frac{1}{c_1} f_{m'}(x, H, t) Y_{m',m,1} + \left(q \frac{\partial V}{\partial x} \right) \frac{1}{\hbar k} Z dH \sum_{m'} \frac{-m}{c_{-1}} f_{m'}(x, H, t) Y_{-m,m',-1} = Z dH \hat{S}_m$$

BTE simulator (8)

- Derivation

- When $m = 1$,

$$Zd\epsilon \frac{\partial}{\partial t} f_1(x, \epsilon, t) + vZdH \frac{\partial}{\partial x} \frac{1}{c_1} f_0(x, H, t) Y_{0,1,1} = ZdH \hat{S}_1$$

- For a general odd number,

$$Zd\epsilon \frac{\partial}{\partial t} f_m(x, \epsilon, t) + vZdH \frac{\partial}{\partial x} \sum_{m'} \frac{1}{c_1} f_{m'}(x, H, t) Y_{m',m,1} \\ - \left(q \frac{\partial V}{\partial x} \right) \frac{1}{\hbar k} ZdH \sum_{m'} \frac{-m'}{c_{-1}} f_{m'}(x, H, t) Y_{-m',m,-1} = ZdH \hat{S}_m$$

BTE simulator (9)

- Derivation
 - The lowest expansion reads

$$Zd\epsilon \frac{\partial}{\partial t} f_0(x, \epsilon, t) + \frac{\partial}{\partial x} \frac{1}{c_1} v Z dH f_1(x, H, t) Y_{1,0,1} = Z dH \hat{S}_0$$

$$Zd\epsilon \frac{\partial}{\partial t} f_1(x, \epsilon, t) + v Z dH \frac{\partial}{\partial x} \frac{1}{c_1} f_0(x, H, t) Y_{0,1,1} = Z dH \hat{S}_1$$

Homework#10

- Due: AM08:00, November 12
 - Do NOT upload your HW in this time. E-mail submission only.

- Problem#1

- Solve the following equations under a fixed H .

$$\frac{\partial}{\partial x} \frac{1}{c_1} v Z f_1(x, H) Y_{1,0,1} = 0$$
$$v Z \frac{\partial}{\partial x} \frac{1}{c_1} f_0(x, H) Y_{0,1,1} = -Z \frac{f_1(x, H)}{\tau}$$

- Consider both of the graphene ($\epsilon = \hbar v_F k$) and a parabolic band ($\epsilon = \frac{\hbar^2}{2m} k^2$).