
Lecture12: BTE solver

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Homework#5

- Due: October 31st
- Calculate the phonon-limited mobility of a MOS structure.

BTE simulator (1)

- Equations

- For example, dispersion relation of graphene ($\mathbf{p} = \hbar\mathbf{k}$)

$$\epsilon(\mathbf{k}) = \hbar k v_F = \epsilon(k) = v \frac{\mathbf{k}}{k}$$

- Another example is the 2DEG in the MOS channel
- Isotropic band structure is understood.
- Boltzmann equation

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

- Electric force

$$\mathbf{F} = q \nabla \phi$$

BTE simulator (2)

- Derivation

- Boltzmann equation

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

- Explicitly,

$$\begin{aligned} \frac{\partial f(x, k, \phi)}{\partial t} + v \mathbf{a}_k \cdot \mathbf{a}_x \frac{\partial f(x, k, \phi)}{\partial x} + \frac{1}{\hbar} F \mathbf{a}_x \\ \cdot \left(\mathbf{a}_k \frac{\partial f(x, k, \phi)}{\partial k} + \mathbf{a}_\phi \frac{1}{k} \frac{\partial f(x, k, \phi)}{\partial \phi} \right) = \hat{S} \end{aligned}$$

- Dot products are written as

$$\begin{aligned} \mathbf{a}_x \cdot \mathbf{a}_k &= \cos \phi \\ \mathbf{a}_x \cdot \mathbf{a}_\phi &= -\sin \phi \end{aligned}$$

BTE simulator (3)

- Derivation

- Using the previous relations,

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

- Note that the above relation holds for arbitrary isotropic band structure. (Here, v is a function of k .)
 - In the energy space,

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

BTE simulator (4)

- Derivation

- We have the following relation:

$$kdkd\phi = \frac{\epsilon}{(\hbar v_F)^2} d\epsilon d\phi = \frac{k}{\hbar v} d\epsilon d\phi = (2\pi)^2 Z d\epsilon d\phi$$

- For graphene, $Z = \frac{1}{(2\pi)^2} \frac{\epsilon}{(\hbar v_F)^2}$

- For a parabolic band, $Z = \frac{1}{(2\pi)^2} \frac{m}{\hbar^2}$

- Transformed Boltzmann equation reads:

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

BTE simulator (5)

- 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 it,

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

BTE simulator (6)

- Derivation
 - Note that

$$\cos \phi Y_m = \frac{1}{c_1} Y_1 Y_m$$

$$\sin \phi Y_m = \frac{1}{c_{-1}} Y_{-1} Y_m$$

- By integration,

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

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

BTE simulator (7)

- 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 (8)

- 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 (9)

- 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,

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