Lecture15

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Motivation

- Dimensionality of the Boltzmann equation
  - For the 2DEG, we must consider 2D (real space) + 2D (momentum space).
  - By assuming a certain channel direction, the problem can be regarded as 1D (real space) + 2D (momentum space).
  - Even further reduction is possible, when we employ the Fourier harmonics expansion for the momentum space.

BTE simulator (1)

- 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,

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

  - Dot products are written as $\mathbf{a}_x\cdot\mathbf{a}_k = \cos\phi$ and $\mathbf{a}_x\cdot\mathbf{a}_\phi = -\sin\phi$.

BTE simulator (2)

- 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 bnad 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 (3)

- 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:

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

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 it,

$$Zd\epsilon \frac{\partial f}{\partial t} Y_m d\phi + vZd\epsilon \frac{\partial f}{\partial x} \cos\phi \, Y_m d\phi + vFZd\epsilon \frac{\partial f}{\partial \epsilon} \cos\phi \, Y_m d\phi - F\frac{1}{\hbar k} Zd\epsilon \frac{\partial f}{\partial \phi} \sin\phi \, Y_m d\phi = Zd\epsilon \hat{S} Y_m d\phi$$

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,

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

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

BTE simulator (6)

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

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

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

BTE simulator (7)

- Derivation
  - When $m = 0$,

$$Zd\epsilon \frac{\partial}{\partial t} f_0(x,\epsilon,t) + \frac{\partial}{\partial x}\frac{1}{c_1} vZdH f_1(x,H,t)\Upsilon_{1,0,1} = ZdH\hat{S}_0$$

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

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

BTE simulator (8)

- Derivation
  - When $m = 1$,

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

  - For a general odd number,

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

BTE simulator (9)

- Derivation
  - The lowest expansion reads

$$Zd\epsilon \frac{\partial}{\partial t} f_0(x,\epsilon,t) + \frac{\partial}{\partial x}\frac{1}{c_1} vZdH f_1(x,H,t)\Upsilon_{1,0,1} = ZdH\hat{S}_0$$

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