Lecture14:
BTE solver

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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,

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

  - Dot products are written as

$$\mathbf{a}_x\cdot\mathbf{a}_k = \cos\phi$$
$$\mathbf{a}_x\cdot\mathbf{a}_\phi = -\sin\phi$$

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 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 (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:

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

BTE simulator (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,

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

BTE simulator (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,

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

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

BTE simulator (7)

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

$$Zd\epsilon \frac{\partial}{\partial t} f_m(x,\epsilon,t) + vZdH \frac{\partial}{\partial x} \sum_{m\prime} \frac{1}{c_1} f_{m\prime}(x,H,t) \Upsilon_{m\prime,m,1}$$

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

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

BTE simulator (8)

- 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 (9)

- Derivation
  - When $m = 1$,

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

  - 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 (10)

- Derivation
  - The lowest expansion reads

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

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

  - For a scattering whose enery transfer is ΔE,

$$\hat{S} = -\frac{1}{(2\pi)^2}\iint S\delta\big(\epsilon(k,\phi) + \Delta E - \epsilon(k',\phi')\big)\big(1 - f(x,k',\phi')\big) f(x,k,\phi)\, k'dk'd\phi' + \frac{1}{(2\pi)^2}\iint S\delta(\epsilon(k,\phi) - \epsilon(k',\phi') - \Delta E)\big(1 - f(x,k,\phi\,)\big) f(x,k',\phi')\, k'dk'd\phi'$$

BTE simulator (11)

- Derivation
  - Integration over the energy yields,

$$\hat{S} = -SZ(\epsilon+\Delta E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x,\epsilon+\Delta E)\right) f(x,\epsilon,\phi)$$
$$+ SZ(\epsilon-\Delta E)\frac{1}{c_0} f_0(x,\epsilon-\Delta E)(1 - f(x,\epsilon,\phi))$$

  - For the zeroth order,

$ZdH\hat{S}_0$

$$= -dHSZ(\epsilon)Z(\epsilon+\mathit{\Delta}E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x,\epsilon+\mathit{\Delta}E)\right) f_0(x,\epsilon)$$
$$+ dHSZ(\epsilon)Z(\epsilon-\mathit{\Delta}E)\frac{1}{c_0} f_0(x,\epsilon-\mathit{\Delta}E)(\frac{1}{c_0} - f_0(x,\epsilon))$$

BTE simulator (12)

- Derivation
  - For the first order,

$$ZdH\hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon+\Delta E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x,\epsilon+\Delta E)\right)f_1(x,\epsilon) - dHSZ(\epsilon)Z(\epsilon-\Delta E)\frac{1}{c_0}f_0(x,\epsilon-\Delta E)f_1(x,\epsilon)$$

  - Without the Pauli principle

$$ZdH\hat{S}_0 = -dHSZ(\epsilon)Z(\epsilon+\Delta E)\frac{1}{c_0^2}f_0(x,\epsilon) + dHSZ(\epsilon)Z(\epsilon-\Delta E)\frac{1}{c_0^2}f_0(x,\epsilon-\Delta E)$$

$$ZdH\hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon+\Delta E)\frac{1}{c_0^2}f_1(x,\epsilon)$$

  - Do not neglect the Pauli principle for 2DEG!

BTE simulator (13)

- Derivation
  - For arbitrary order,

$$Z dH \hat{S}_m$$

$$= -dHSZ(\epsilon)Z(\epsilon + \Delta E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x, \epsilon + \Delta E)\right)f_m(x, \epsilon)$$

$$+ dHSZ(\epsilon)Z(\epsilon - \Delta E)\frac{1}{c_0}f_0(x, \epsilon - \Delta E)(\frac{1}{c_0}\delta_{m,0} - f_m(x, \epsilon))$$

BTE simulator (14)

- Derivation
  - Additionally, the electron density and the current density are given by

$$n = 4\frac{1}{c_0}\int f_0 Z d\epsilon$$

$$J_x = (-q)4\frac{1}{c_1}\int f_1 v_F Z d\epsilon$$

  - The leading coefficient, 4, was obtained by considering the spin degeneracy and two equivalent bands. (Of course, when we have further degeneracy, this number can be changed.)

Homework#6

- Due: November 14^{th}

- For a given energy level, solve the ballistic BTE with lmax=1.