Lecture18

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GIST Lecture on November 14, 2018

Notice

- No lecture days due to my business trip
  - December 3 and December 5
- One makeup seesion will be made either December 10 or December 12.
  - Check your schedule.
- Term project
  - No presentation
  - Just submit your final report and code.

How to derive the DD eqs.

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

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

- The continuity equation is the first equation.
- The current density is obtained in the second equation.

Continuity equation (1)

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

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

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

  - The electron density (per spin) is given by

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

Continuity equation (2)

- The first term can be easily converted.
  - It is now written as

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

  - Moreover, for a position-independent band structure,

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

  - The last term vanishes!

Continuity equation (3)

- We have only two terms.
  - The electron flux is defined.

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

  - The continuity equation is obtained as

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

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.

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

$$= \frac{1}{(2\pi)^3}\int_{BZ}\mathbf{v}\hat{S}d\mathbf{k}$$

Current density equation (2)

- Remember the electron flux.
  - 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 (3)

- 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

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

Current density equation (4)

- Effective mass
  - We assume that

$$m_{ij}^{-1} = \frac{1}{m^*}\delta_{ij}$$

  - Then, along the given direction, we have

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

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

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

Current density equation (5)

- 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

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

Current density equation (6)

- Collecting the above discussion,
  - With the momentum relaxation time,

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

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

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

  - Then, the electron diffusion coefficient, D_n, is introduced.

Current density equation (7)

- In a vector form,
  - A simple equation is obtained.

$$q\tau\frac{\partial}{\partial t}\mathbf{F}_n + q\nabla(D_n n) - \mathbf{F}\frac{q\tau}{m^*}n = -q\mathbf{F}_n$$

  - When the steady-state is considered, the current density $\mathbf{J}_n = -q\mathbf{F}_n$ becomes

$$\mathbf{J}_n = +q\mu_n n\mathbf{E} + qD_n\nabla n$$

  - (We neglect the spatial variation of D_n. $\mathbf{F} = -q\mathbf{E}$)

Homework#11

- Due: AM08:00, November 19
- Problem#1
  - Consider the system in Lecture17.
  - Select a value for V_D. (It's your own choice.)
  - Then, draw a 3D graph of $f_0(x, H)$.
  - Also draw a 3D graph of $f_1(x, H)$.
  - Of course, you need some constants. Those constants (such as τ) should be set by yourself.