Lecture18: Drift-Diffusion

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How to derive the DD eqs.

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

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

Continuity equation (1)

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

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

  - In terms of the electron density,

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

  - It is now written as

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

Why?

Continuity equation (2)

- Moreover, for a position-independent band structure,
  - It is now written as

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

  - With the electron flux,

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

  - The continuity equation is obtained:

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

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.

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

  - 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 (2)

- 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

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

  - Using the effective mass,

$$-F_i\frac{1}{m^*}n \longleftarrow \text{Which approximation?}$$

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

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

Current density equation (3)

- 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

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

  - With the momentum relaxation time,

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

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