Week7 – Relaxation Time Approximation

ECE 695-O Semiconductor Transport Theory

Fall 2018

Instructor: Byoung-Don Kong

POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Contents

- Relaxation Time Approximation- continues.

Simple Example – Electric Field Only

- In the previous class, we arrived at the following expression,

$$\mathbf{G} = -e\tau\left\{\frac{\boldsymbol{\mathcal{F}} + \frac{e\tau}{m^*}\boldsymbol{\mathcal{F}} \times \mathbf{B} + \left(\frac{e\tau}{m^*}\right)^2 (\boldsymbol{\mathcal{F}} \cdot \mathbf{B})\mathbf{B}}{1 + \left(\frac{e\tau}{m^*}\right)^2 \mathbf{B} \cdot \mathbf{B}}\right\}$$

for the case of spherical energy band.

- Let's assume an electric field applied along x-axis: $\mathbf{E} = E_x \hat{\boldsymbol{x}}$.
- Then, there is no component related to $\mathbf{B}$ and $\mathbf{G}$ becomes

$$\mathbf{G} = -e\tau\mathbf{E}$$

(We defined electro thermal field in the previous class like $\boldsymbol{\mathcal{F}} = \mathbf{E} + \frac{T}{e} \nabla_{\mathbf{r}} \left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)$.)

- Then,

$$\phi = -\mathbf{v} \cdot \mathbf{G} = e\tau E_x v_x$$

Simple Example – Electric Field Only(2)

- The steady state distribution f becomes

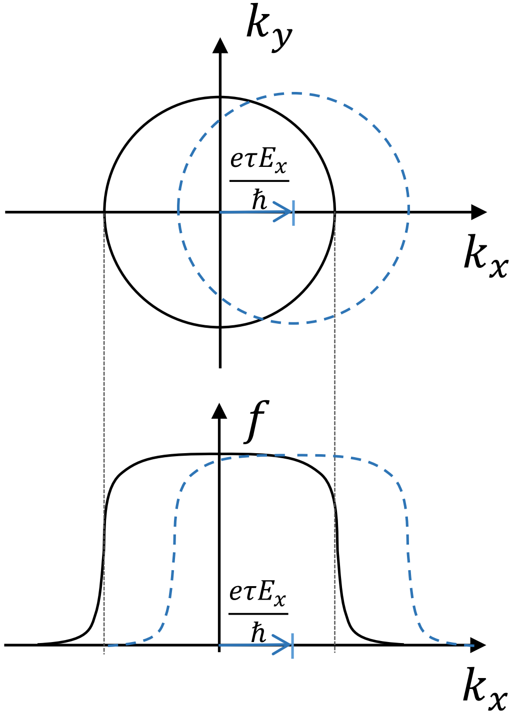
$$
\begin{aligned}
f &= f_0 + \mathbf{v} \cdot \mathbf{G} \frac{\partial f_0}{\partial \mathcal{E}} \\
&= f_0 - e\tau E_x v_x \frac{\partial f_0}{\partial \mathcal{E}} \\
&= f_0 - e\tau E_x \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial k_x} \frac{\partial f_0}{\partial \mathcal{E}} \\
&= f_0 - \frac{e\tau E_x}{\hbar} \frac{\partial f_0}{\partial k_x}
\end{aligned}
$$

- This looks like a Taylor expansion with respect to k_x.
- Thus, it can be written as

$$
f \cong f_0\left(k_x - \frac{e\tau E_x}{\hbar}, k_y, k_z\right)
$$

Simple Example – Electric Field Only(2)

$$f \cong f_0\left(k_x - \frac{e\tau E_x}{\hbar}, k_y, k_z\right)$$



- So the application of an electric field only results in displacement of the Fermi sphere in k-space.
- All points on these surface undergo the same displacement.
- No change in shape.
- One of the criteria to justify the relaxation time approximation was that $\left[\frac{\phi(\mathbf{k}')}{\phi(\mathbf{k})}\right]$ must be independent of the type of perturbation.

$$\frac{\phi(\mathbf{k}')}{\phi(\mathbf{k})} = \frac{e\tau(\mathbf{k}')E_x v_x(\mathbf{k}')}{e\tau(\mathbf{k}')E_x v_x(\mathbf{k}')} = \frac{\tau(\mathbf{k}')v_x(\mathbf{k}')}{\tau(\mathbf{k}')v_x(\mathbf{k}')}$$

→This justifies the adoption of the relaxation time approximation (external perturbation Ex cancels out)

Quiz-break (for fun)

- Let's assume a 1 m long copper wire and its diameter is 2mm. Try to guess how long does it take an electron travel from one end of wire to the other end when there is 1 A of current flow.

- Answer:

electron density in copper: 8.49 x 10^{28} m^{-3}

drift velocity $v_d = \frac{J}{qn} = \frac{I}{qnA} = \frac{1}{8.49\times10^{28}\times1.6\times10^{-19}\times\pi(1\times10^{-3})^2}$

$$\approx 2.34 \times 10^{-5}\, m/s$$

$$v = \frac{dx}{dt}$$

So, $\Delta t = \frac{\Delta x}{v_d} = \frac{1}{2.34\times10^{-5}} \approx 42735$ sec. = 11.87 Hours

Simple Example – Thermal Gradient Only

- Let's assume there is only thermal gradient along x direction.
- Then, $B = 0$ and $E = 0$.

$$\mathbf{G}(\mathcal{E}, \mathbf{r}) = -e\tau\mathbf{E} - \tau T\, \nabla_{\mathbf{r}}\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right) - \frac{e\tau}{\hbar^2}\mathbf{B} \times (\mathbf{G}\cdot\nabla_{\mathbf{k}})\nabla_{\mathbf{k}}\mathcal{E}$$

$$= -\tau T\, \nabla_{\mathbf{r}}\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)$$

: $\mathcal{E}_F$ has temperature dependence since density function is not uniform.

$$\phi = -\mathbf{v}\cdot\mathbf{G} = \tau T\mathbf{v}\cdot\nabla_{\mathbf{r}}\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)$$

$$= \tau T\mathbf{v}\cdot\left\{\frac{1}{T}\nabla_{\mathbf{r}}(\mathcal{E}-\mathcal{E}_F) - \frac{\mathcal{E}-\mathcal{E}_F}{T^2}\nabla_{\mathbf{r}}T\right\} = \tau\mathbf{v}\cdot\left\{\underbrace{\nabla_{\mathbf{r}}(\mathcal{E}-\mathcal{E}_F)} - \frac{\mathcal{E}-\mathcal{E}_F}{T}\underbrace{\nabla_{\mathbf{r}}T}_{\frac{\partial T}{\partial x}}\right\}$$

$$\nabla_{\mathbf{r}}(\mathcal{E}-\mathcal{E}_F) = \frac{\partial T}{\partial x}\frac{\partial(\mathcal{E}-\mathcal{E}_F)}{\partial T} = -\frac{\partial T}{\partial x}\frac{\partial \mathcal{E}_F}{\partial T}$$

Simple Example – Thermal Gradient Only(2)

$$\phi = \tau v_x \left\{ -\frac{\partial T}{\partial x}\frac{\partial \mathcal{E}_F}{\partial T} - \frac{\mathcal{E} - \mathcal{E}_F}{T}\frac{\partial T}{\partial x} \right\}$$

$$= \tau v_x \frac{\partial T}{\partial x}\left\{ -\frac{\partial \mathcal{E}_F}{\partial T} - \frac{\mathcal{E} - \mathcal{E}_F}{T} \right\}$$

- Then, this gives

They cancels to each other so long as we are dealing with elastic scattering.

$$\frac{\phi(\mathbf{k}')}{\phi(\mathbf{k})} = \frac{\tau(\mathbf{k}')v_x(\mathbf{k}')\cancel{\frac{\partial T}{\partial x}\left\{ -\frac{\partial \mathcal{E}_F}{\partial T} - \frac{\mathcal{E} - \mathcal{E}_F}{T} \right\}}}{\tau(\mathbf{k}')v_x(\mathbf{k}')\cancel{\frac{\partial T}{\partial x}\left\{ -\frac{\partial \mathcal{E}_F}{\partial T} - \frac{\mathcal{E} - \mathcal{E}_F}{T} \right\}}} = \frac{\tau(\mathbf{k}')v_x(\mathbf{k}')}{\tau(\mathbf{k}')v_x(\mathbf{k}')}$$

and the application of relaxation time approximation can be justified.

- $\frac{\partial \mathcal{E}_F}{\partial T}$ is small quantity so let's ignore for a while. Then,

$$\phi \cong \tau v_x \frac{\partial T}{\partial x}\left\{ -\frac{\mathcal{E} - \mathcal{E}_F}{T} \right\}$$

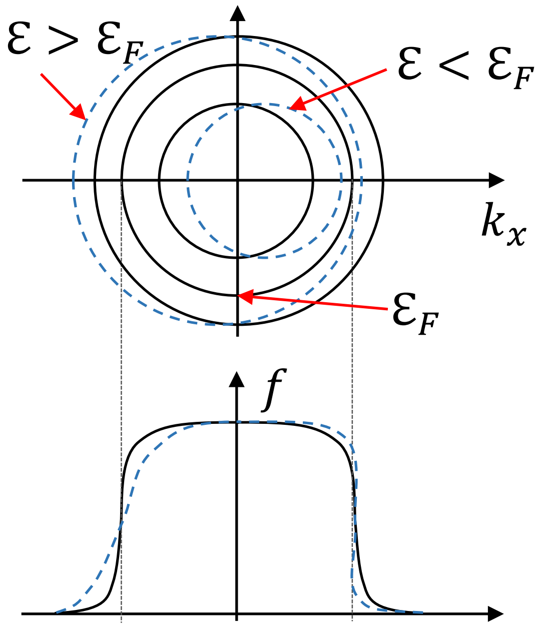
Simple Example – Thermal Gradient Only(3)

- The steady state distribution is

$$f = f_0 + \frac{\partial f_0}{\partial \mathcal{E}} \tau v_x \frac{\partial T}{\partial x}\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right) = f_0 + \frac{\partial f_0}{\partial \mathcal{E}} \frac{\partial \mathcal{E}}{\partial k_x} \tau \frac{\partial T}{\partial x}\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)$$

$$= f_0 + \tau \left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right) \frac{\partial T}{\partial x} \frac{\partial f_0}{\partial k_x}$$

$$\cong f_0\left(k_x + \tau \boxed{\left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)} \frac{\partial T}{\partial x}, k_y, k_z\right)$$



This is a similar shift of the distribution in E-field only but depending on the sign of $(\mathcal{E}-\mathcal{E}_F)$, the direction of shift changes.

Electrical Conductivity in the Relaxation Time Approximation

- The macroscopic response to an external perturbation can appear as current or heat flow.
- Let's consider first when there is only E-field along x.

$$\phi = -\mathbf{v} \cdot \mathbf{G} = e\tau E_x v_x$$

$$f = f_0 - \frac{e\tau E_x}{\hbar} \frac{\partial f_0}{\partial k_x}$$

- The electric current density is given by the product of electron charge and electron velocity, summed over all the electrons contributing (in the FBZ).

$$\mathbf{J} = \int e\mathbf{v}f \frac{d^3k}{4\pi^3}$$

Electrical Conductivity in the Relaxation Time Approximation-E-field only

- Since we are dealing with E-field along x, let's simplify the expression.

$$J_x = \int e v_x f \frac{d^3k}{4\pi^3} \qquad f = f_0 - e\tau E_x v_x \frac{\partial f_0}{\partial \mathcal{E}}$$

$$= \frac{e}{4\pi^3}\left\{\boxed{\int f_0(\mathbf{k}) v_x(\mathbf{k}) d^3k} - \int \phi(\mathbf{k}) \frac{\partial f_0}{\partial \mathcal{E}} v_x(\mathbf{k}) d^3k\right\}$$

This should be zero since equilibrium distribution times v_x (which is antisymmetric function) is an odd function.

$$= -\frac{e^2 E_x}{4\pi^3}\int v_x^2(\mathbf{k}) \frac{\partial f_0}{\partial \mathcal{E}} \tau(\mathbf{k}) d^3k$$

- Here, we will treat one type of carrier in one energy band.
- However, in general, $\mathbf{J} = \sum \int e \mathbf{v}_n f_n \frac{d^3k}{4\pi^3}$

n_{th} band

Electrical Conductivity in the Relaxation Time Approximation-E-field only (2)

$$J_x = -\frac{e^2 E_x}{4\pi^3}\int v_x^2(\mathbf{k})\frac{\partial f_0}{\partial \mathcal{E}}\tau(\mathbf{k})d^3k = e^2 E_x K_1$$

- We can define so-called transport integral (for later use) as

$$K_n = -\frac{1}{4\pi^3}\int d^3k\tau(\mathbf{k})v_x^2(\mathbf{k})[\mathcal{E}(\mathbf{k})]^{\boldsymbol{n-1}}\frac{\partial f_0}{\partial \mathcal{E}}$$

This is kinetic energy part.

- Note that external perturbation only shift the distribution function but does not change the total number carriers. In other words, $n = \frac{1}{4\pi^3}\int f_0 d^3k$ does not change even though there is a perturbation.

Electrical Conductivity in the Relaxation Time Approximation-E-field only (3)

- Thus, we can express the current density like

$$\frac{\partial f_0}{\partial \mathcal{E}} = -\frac{1}{k_B T} f_0(1 - f_0)$$

$$J_x = -e^2 E_x n \frac{\frac{1}{4\pi^3}\int v_x^2 \frac{\partial f_0}{\partial \mathcal{E}} \tau \, d^3k}{\frac{1}{4\pi^3}\int f_0 d^3k}$$
$$= \frac{e^2 E_x n}{k_B T} \frac{\int \tau v_x^2 f_0(1 - f_0) d^3k}{\int f_0 d^3k}$$

- Now, we assume a parabolic energy band $\mathcal{E} = \frac{\hbar^2 k^2}{2m^*} = \frac{1}{2} m^* v^2$ as usual.
- Another assumption we are going to make is the equipartition assumption: $v_x^2 = v_y^2 = v_z^2$.
- This means that the distribution is slightly shifted by E_x but still the energy is evenly distributed.
- In other words, the shape(Maxwellian shape) itself is not changed even though the center is slightly shifted.
- If E_x is small, this assumption is valid.

Electrical Conductivity in the Relaxation Time Approximation-E-field only (4)

- Then,

$$v_x^2 = v_y^2 = v_z^2 = \frac{1}{3}v^2$$

$$\Rightarrow v_x^2 \cong \frac{2\mathcal{E}}{3m^*}$$

- If we plug this into the current density expression,

$$J_x = \frac{2e^2E_xn}{3m^*k_BT}\frac{\int \tau\mathcal{E}f_0(1-f_0)d^3k}{\int f_0d^3k}$$

- Now, we change integral variable into energy by multiplying density of states $\sqrt{\mathcal{E}}$ for a 3D case.

$$J_x = \frac{2e^2E_xn}{3m^*k_BT}\frac{\int_0^{\mathcal{E}_m} \tau\mathcal{E}^{\frac{3}{2}}f_0(1-f_0)d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}}f_0d\mathcal{E}}$$

where $\mathcal{E}_m$ is conduction band maximum.

Electrical Conductivity in the Relaxation Time Approximation-E-field only (5)

- By the way, remember that τ is also a function of energy $\mathcal{E}$, although it is not the function on $\mathbf{k}$.
- Scattering usually have no directional preference.
- Let's consider this integral:

$$\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E} = -k_BT\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}} \frac{\partial f_0}{\partial \mathcal{E}} d\mathcal{E}$$

$$= -k_BT\left(f_0\mathcal{E}^{\frac{3}{2}}\Big|_0^{\mathcal{E}_m} - \frac{3}{2}\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}} f_0 d\mathcal{E}\right)$$

$$= -k_BT\left(\left[\cancel{f_0(\mathcal{E}_m)\mathcal{E}_m^{\frac{3}{2}}} - \underbrace{\cancel{f_0(0)0^{\frac{3}{2}}}}_{=0}\right] - \frac{3}{2}\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}} f_0 d\mathcal{E}\right)$$

Distribution at the conduction band maximum is almost zero

$$= \frac{3k_BT}{2}\boxed{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}} f_0 d\mathcal{E}}$$

This is denominator of the previous equation.

Electrical Conductivity in the Relaxation Time Approximation-E-field only (6)

$$\frac{2}{3k_BT}\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E} = \int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}} f_0 d\mathcal{E}$$

- Thus,

$$J_x = \frac{2e^2E_xn}{3m^*k_BT}\frac{\int_0^{\mathcal{E}_m} \tau\mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{1}{2}} f_0 d\mathcal{E}}$$

$$= \frac{2e^2E_xn}{3m^*k_BT}\frac{\int_0^{\mathcal{E}_m} \tau\mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E}}{\frac{2}{3k_BT}\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E}}$$

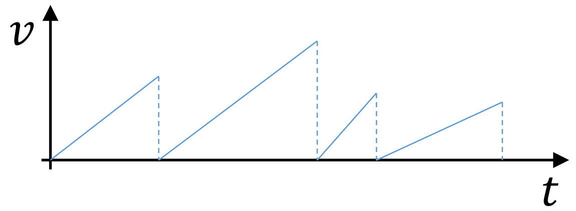
$$= \frac{e^2E_xn}{m^*}\boxed{\frac{\int_0^{\mathcal{E}_m} \tau\mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}} f_0(1-f_0)d\mathcal{E}}}$$

If we define this as $\langle\tau\rangle$

- We arrive at $J_x = \frac{e^2E_xn}{m^*}\langle\tau\rangle$ which is a very familiar expression: $J_x = nqE_x\mu$ where $\mu = \frac{q}{m^*}\langle\tau\rangle$.
- First, $\langle\tau\rangle$, we define here, is a certain average of τ but it is not an ensemble average. The ensemble average of $\langle\tau\rangle$ is : $\langle\tau\rangle_{ensemble} = \frac{\int \tau f d^3k}{\int f d^3k}$

Electrical Conductivity in the Relaxation Time Approximation-E-field only (7)

- Let's recall Drude model.



$$F = eE_x = m^* \frac{dv_x}{dt}$$

$$v_x(t) = \frac{eE_x}{m^*} t$$

$$v_d = \frac{eE_x}{m^*}\tau \quad \longrightarrow \quad J_x = nev_d = \frac{e^2 E_x n}{m^*}\tau$$

- Thus, $\langle J_x \rangle_{ensemble} = \dfrac{e^2 E_x n}{m^*} \langle \tau \rangle_{ensemble}$.
- And more generally, $\mathbf{J} = \sigma \mathbf{E} = nq\mu \mathbf{E}$ and $\mu = \dfrac{q}{m^*}\langle \tau \rangle_{ensemble}$ is the definition of mobility in Drude model.
- Although it looks like that BTE gives the same answer but there is a difference in evaluating in $\langle \tau \rangle$.