Week8 – Relaxation Time Approximation

ECE 695-O Semiconductor Transport Theory

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Contents

- Relaxation Time Approximation- continues.

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

- We considered relaxation time approximation of BTE when there is only e-filed and arrived at

$$J_x = \frac{e^2 n}{m^*} \langle \tau \rangle E_x \quad .$$

- We can generalize this expression such as

$$\mathbf{J} = \frac{e^2 n}{m^*} \langle \tau \rangle \mathbf{E}$$

where

$$\langle \tau \rangle = \frac{\int_0^{\mathcal{E}_m} \tau\, \mathcal{E}^{\frac{3}{2}}\, f_0(1 - f_0) d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}}\, f_0(1 - f_0) d\mathcal{E}}$$

- Mobility $\mu = \frac{q}{m^*} \langle \tau \rangle$

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

- For non-degenerate semiconductors,

$$f_0(1-f_0) \cong f_0 \cong e^{-(\mathcal{E}-\mathcal{E}_F)/k_BT}$$

- This gives

$$J_x \cong \frac{e^2 n E_x}{m^*} \frac{\int_0^{\mathcal{E}_m} \tau\ \mathcal{E}^{\frac{3}{2}}\ e^{-(\mathcal{E}-\mathcal{E}_F)/k_BT}\ d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}}\ e^{-(\mathcal{E}-\mathcal{E}_F)/k_BT}\ d\mathcal{E}}$$

$$= \frac{e^2 n E_x}{m^*} \frac{\int_0^{\mathcal{E}_m} \tau\, \mathcal{E}^{\frac{3}{2}}\, e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}}\ e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}.$$

- Let's assume $\tau = A\mathcal{E}^{-s}$ where $s = \frac{1}{2}$ for acoustic phonon scattering and $s = -\frac{3}{2}$ for charge impurity scattering.
- This will be discussed in the scattering section later but we just use the results here.

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

- Let's assume $\tau = A\mathcal{E}^{-s}$ where $s = \frac{1}{2}$ for acoustic phonon scattering and $s = -\frac{3}{2}$ for charge impurity scattering.
- This will be discussed in the scattering section later but we just use the results here.
- However, you can understand this intuitively like followings.
- At high temperature, $\tau_{ac\,ph} = A\mathcal{E}^{-\frac{1}{2}}$ is dominant term, and as $\mathcal{E}$ increases, the scattering rate increases.
- At lower temperature, $\tau_{ii} = A\mathcal{E}^{\frac{3}{2}}$ is dominant term, and as $\mathcal{E}$ increases, the scattering rate decreases.
- τ_{ii} has Columbic origin. If incoming speed is fast, only electron trajectory is slightly affected.

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

- Thus, with $\tau = A\mathcal{E}^{-s}$,

$$\langle\tau\rangle = \frac{\int_0^{\mathcal{E}_m} A\mathcal{E}^{-s}\, \mathcal{E}^{\frac{3}{2}}\, e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}}\ e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}$$

→ $\mathcal{E}_m$ to ∞ since the integrand will become zero before $\mathcal{E}_m$.

$$= A\frac{\int_0^{\infty} \mathcal{E}^{\frac{3}{2}-s}\ e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}{\int_0^{\infty} \mathcal{E}^{\frac{3}{2}}\ e^{-\mathcal{E}/k_BT}\ d\mathcal{E}}$$

→ You can recognize gamma function forms in the numerator and the denominator.

- Let's put $\dfrac{\mathcal{E}}{k_BT} = x,$

$$\Rightarrow \langle\tau\rangle = \frac{A}{(k_BT)^s}\frac{\int_0^{\infty} x^{\frac{3}{2}-s}\ e^{-x}\ dx}{\boxed{\int_0^{\infty} x^{\frac{3}{2}}\, e^{-x} dx} = \Gamma\left(\frac{5}{2}\right)}$$

$$\Rightarrow \langle\tau\rangle = \frac{A}{(k_BT)^s}\frac{\Gamma\left(\frac{5}{2}-s\right)}{\Gamma\left(\frac{5}{2}\right)}$$

FYI

$$\Gamma(z) = \int_0^{\infty} x^{z-1}e^{-x}dx$$

$$\Gamma(z+1) = z\Gamma(z)$$

$$\Gamma(1) = 1$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

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

- For acoustic phonon scattering, $\tau = A\mathcal{E}^{-\frac{1}{2}}$ and $s = \frac{1}{2}$,

$$\Rightarrow \langle\tau\rangle_{ac\,ph} = \frac{A}{(k_BT)^s}\frac{\Gamma\left(\frac{5}{2}-s\right)}{\Gamma\left(\frac{5}{2}\right)}$$

$$= \frac{A}{(k_BT)^{\frac{1}{2}}}\frac{\Gamma\left(\frac{5}{2}-\frac{1}{2}\right)}{\Gamma\left(\frac{5}{2}\right)}$$

$$= \frac{A}{(k_BT)^{\frac{1}{2}}}\frac{\Gamma\left(\frac{4}{2}\right)}{\Gamma\left(\frac{5}{2}\right)} = \frac{A}{(k_BT)^{\frac{1}{2}}}\frac{\Gamma(2)}{\Gamma\left(\frac{5}{2}\right)}$$

$$= \frac{A}{(k_BT)^{\frac{1}{2}}}\frac{1\times\Gamma(1)}{\frac{3}{2}\times\Gamma\left(\frac{3}{2}\right)} = \frac{A}{(k_BT)^{\frac{1}{2}}}\frac{1}{\frac{3}{2}\times\frac{1}{2}\times\Gamma\left(\frac{1}{2}\right)}$$

$$= \frac{4}{3}\frac{A}{(\pi k_BT)^{\frac{1}{2}}}$$

FYI

$$\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx$$

$$\Gamma(z+1) = z\Gamma(z)$$

$$\Gamma(1) = 1$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

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

$$\Rightarrow \langle\tau\rangle_{ac\,ph} = \frac{4}{3}\frac{A}{(\pi k_B T)^{\frac{1}{2}}} \propto T^{-\frac{1}{2}}$$

- Thus, as T goes up, $\langle\tau\rangle_{ac\,ph}$ goes down. Shorter relaxation time means more scattering; <u>scattering or relaxation rate goes up</u>.

- For ionized impurity scattering, $\tau = A\mathcal{E}^{\frac{3}{2}}$ and $s = -\frac{3}{2}$,
- We repeat the same stuff here;

$$\Rightarrow \langle\tau\rangle_{ii} = \frac{A'}{(k_B T)^s}\frac{\Gamma\left(\frac{5}{2}-s\right)}{\Gamma\left(\frac{5}{2}\right)} = \frac{8A'}{\sqrt{\pi}}(k_B T)^{3/2} \propto T^{\frac{3}{2}}$$

- And, as temperature goes up, scattering rate goes down.

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

- Usually there are multiple scattering mechanisms.
- If we recall the way we calculated relaxation time,

$$\frac{1}{\tau} \propto \int P_{\mathbf{kk}'}\{\cdots\}d^3k'$$

and $P_{\mathbf{kk}'}$ is transition probability from $\mathbf{k}$ to $\mathbf{k}'$.

- If there are many scattering mechanism, let's say $P^1_{\mathbf{kk}'}$, $P^2_{\mathbf{kk}'}$, $P^3_{\mathbf{kk}'}$, etc., these can be added. Thus, the total scattering rate can be

$$\frac{1}{\tau_{total}} \propto \int \left(P^1_{\mathbf{kk}'} + P^2_{\mathbf{kk}'} + P^3_{\mathbf{kk}'} + \cdots\right)\{\cdots\}d^3k'$$

$$= \int P^1_{\mathbf{kk}'}\{\cdots\}d^3k' + \int P^1_{\mathbf{kk}'}\{\cdots\}d^3k' + \int P^1_{\mathbf{kk}'}\{\cdots\}d^3k' + \cdots$$

$$= \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3} + \cdots$$

Electrical Conductivity in the Relaxation Time Approximation-E-field only(8)

- Ideally, we can plug this,

$$\frac{1}{\tau_{total}} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3} + \cdots$$

into

$$\langle \tau \rangle = \frac{\int_0^{\mathcal{E}_m} \tau\, \mathcal{E}^{\frac{3}{2}}\, f_0(1 - f_0) d\mathcal{E}}{\int_0^{\mathcal{E}_m} \mathcal{E}^{\frac{3}{2}}\, f_0(1 - f_0) d\mathcal{E}}$$

and calculate $\langle \tau \rangle$, but that is not easy.

- As an approximation, we will use

$$\frac{1}{\langle \tau \rangle_{total}} \cong \frac{1}{\langle \tau \rangle_1} + \frac{1}{\langle \tau \rangle_2} + \frac{1}{\langle \tau \rangle_3} + \cdots$$

and this is so-called 'Matthiessen's rule'.

Electrical Conductivity in the Relaxation Time Approximation-E-field only(9)

- Thus,

$$\frac{1}{\langle\tau\rangle} = \frac{1}{\langle\tau\rangle_{ac\,ph}} + \frac{1}{\langle\tau\rangle_{ii}}$$

and

$$\frac{1}{\mu} = \frac{m^*}{q}\left(\frac{1}{\langle\tau\rangle_{ac\,ph}} + \frac{1}{\langle\tau\rangle_{ii}}\right) .$$

If there are more scattering mechanism, you can keep adding here.

Single ellipsoidal energy minima – an example

- In this case, the energy is given as

$$\mathcal{E} = \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} + \frac{\hbar^2 k_z^2}{2m_z^*}$$

and we assume electric field along x direction such as

$$\mathbf{E} = E_x\hat{\mathbf{x}}.$$

$$J_x = \frac{e^2 n}{m^*}\langle\tau\rangle E_x$$

- Generally, this should be

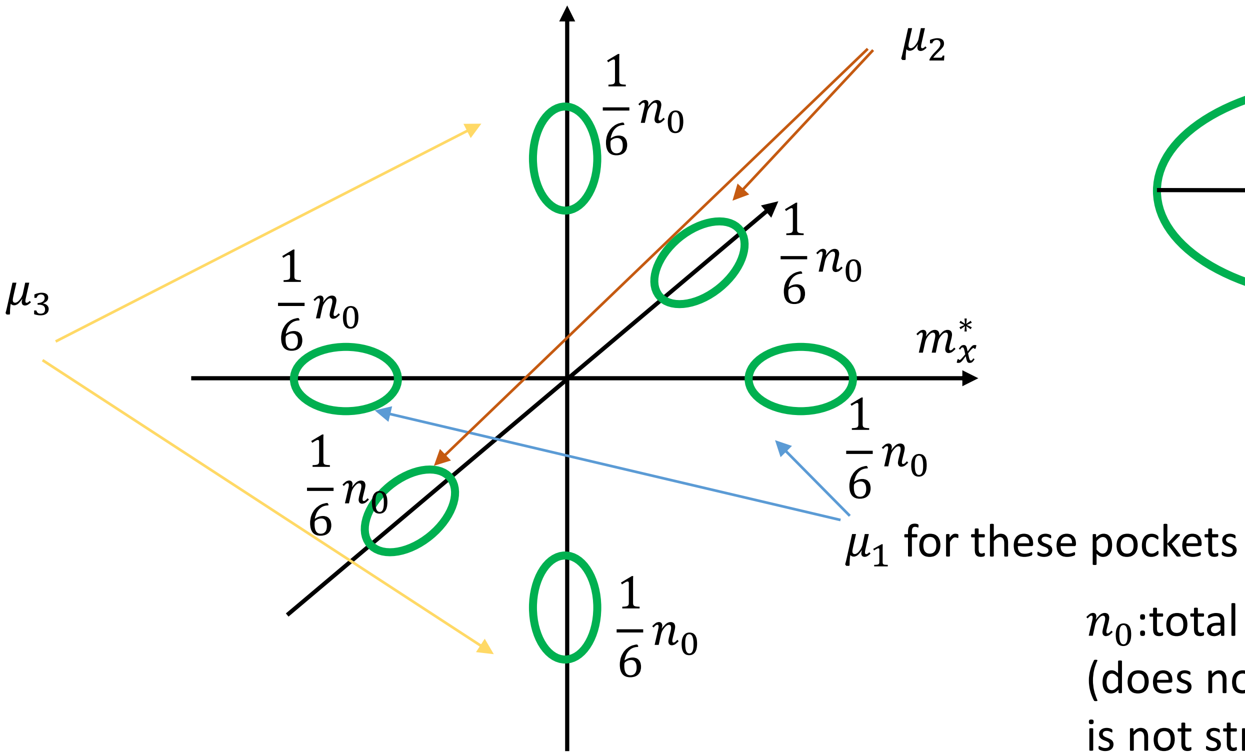
$$\mathbf{J} = \boldsymbol{\sigma}\mathbf{E}$$

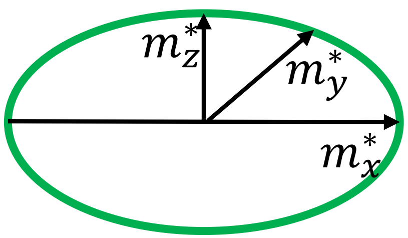
where $\boldsymbol{\sigma} = \begin{pmatrix} en\mu_1 & 0 & 0 \\ 0 & en\mu_2 & 0 \\ 0 & 0 & en\mu_3 \end{pmatrix}$ and $\mu_i = \dfrac{q\langle\tau\rangle}{m_i^*}$.

- If E-field direction is parallel to the principal axis (x, y, z) then the current is parallel to the E-field. However, if the E-field is applied along other directions, current is not parallel to E-field.

Multiple ellipsoidal energy minima

- However, normally there are multiple minima exist so they will compensate the effect.
- In the case of Si, there are 6 minima near X.





n_0:total electron population (does not change if the field is not strong)

Multiple ellipsoidal energy minima(2)

- When $\mathbf{E} = E_x\hat{\mathbf{x}}$,

$$J_x = \frac{1}{6}(n_0e\mu_1E_x + n_0e\mu_1E_x + n_0e\mu_2E_x + n_0e\mu_2E_x + n_0e\mu_3E_x + n_0e\mu_3E_x)$$
$$= \frac{n_0e}{3}(\mu_1 + \mu_2 + \mu_3)E_x$$

- If we change the field direction to along y-axis, we will get the same results since we will have the same μ_1 , μ_2 , and μ_3 .
- Thus,

$$\mathbf{J} = \sigma\mathbf{E}$$

where $\sigma = \frac{ne}{3}(\mu_1 + \mu_2 + \mu_3) \equiv ne\mu$.

- Since $\mu \equiv \frac{1}{3}(\mu_1 + \mu_2 + \mu_3)$,

$$\frac{q\langle\tau\rangle}{m^*} = q\langle\tau\rangle\boxed{\frac{1}{3}\left(\frac{1}{m_x^*} + \frac{1}{m_y^*} + \frac{1}{m_z^*}\right)}$$

$= \frac{1}{m_{cond}^*}$: conductivity effective mass

Multiple ellipsoidal energy minima(3)

- When $\mathbf{E} = E_x \hat{\mathbf{x}}$,

$$J_x = \frac{1}{6}(n_0 e\mu_1 E_x + n_0 e\mu_1 E_x + n_0 e\mu_2 E_x + n_0 e\mu_2 E_x + n_0 e\mu_3 E_x + n_0 e\mu_3 E_x)$$
$$= \frac{n_0 e}{3}(\mu_1 + \mu_2 + \mu_3)E_x$$

- If we change the field direction to along y-axis, we will get the same results since we will have the same μ_1 , μ_2 , and μ_3 .
- Thus,

$$\mathbf{J} = \sigma \mathbf{E}$$

where $\sigma = \dfrac{ne}{3}(\mu_1 + \mu_2 + \mu_3) \equiv ne\mu$.

- Since $\mu \equiv \frac{1}{3}(\mu_1 + \mu_2 + \mu_3)$,

$$\frac{q\langle\tau\rangle}{m^*} = q\langle\tau\rangle \boxed{\frac{1}{3}\left(\frac{1}{m_x^*} + \frac{1}{m_y^*} + \frac{1}{m_z^*}\right)} = \frac{1}{m_{cond}^*}$$

$= \frac{1}{m_{cond}^*}$: conductivity effective mass

Multiple ellipsoidal energy minima(4)

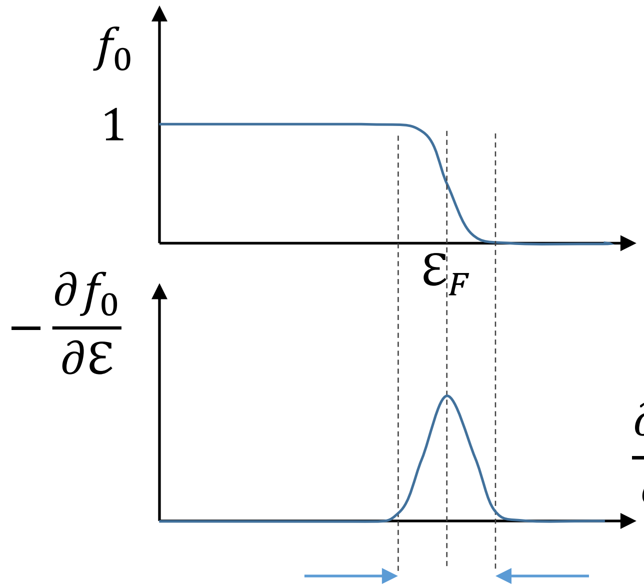
- Usually for silicon,

$$\frac{1}{m^*_{cond}} = \frac{1}{3}\left(\frac{1}{m^*_l} + \frac{2}{m^*_t}\right)$$

- FYI, $m^*_{DOS} = \left(m^*_x m^*_y m^*_z\right)^{1/3}$

Conductivity in metals

- In metals, we cannot use the approximation, $f_0(1-f_0) \approx$ Maxwell-Boltzmann distribution, since it is degenerate case.
- We will use $f_0(1-f_0) = -k_B T \frac{\partial f_0}{\partial \mathcal{E}}$.



Thermal broadening of order of $k_B T$

$$\frac{\partial f_0}{\partial \mathcal{E}} = -\delta(\mathcal{E} - \mathcal{E}_F)$$

So this is good approximation

$$\int_{-\infty}^{\infty} \frac{\partial f_0}{\partial \mathcal{E}} d\mathcal{E} = f_0\Big|_{-\infty}^{\infty} = -1$$

Conductivity in metals(2)

- Thus, for metals,

$$\langle \tau \rangle = \frac{\int \tau \ \mathcal{E}^{\frac{3}{2}} \frac{df_0}{d\mathcal{E}} d\mathcal{E}}{\int \mathcal{E}^{\frac{3}{2}} \ \frac{df_0}{d\mathcal{E}} \ d\mathcal{E}} = \frac{\int \tau \ \mathcal{E}^{\frac{3}{2}} \delta(\mathcal{E} - \mathcal{E}_F) d\mathcal{E}}{\int \mathcal{E}^{\frac{3}{2}} \delta(\mathcal{E} - \mathcal{E}_F) d\mathcal{E}}$$

$$\cong \frac{\tau(\mathcal{E}_F) \mathcal{E}_F^{3/2}}{\mathcal{E}_F^{3/2}} \cong \tau(\mathcal{E}_F) \quad .$$

- So, in metals, $\langle \tau \rangle$ near $\mathcal{E}_F$ is the dominant factor.
- In metal everything happens near Fermi level, and the states some energy under Fermi level do not have any empty spot to scatter in.
- So

$$\mu = \frac{q}{m^*} \tau(\mathcal{E}_F)$$