(E) CALCULATION OF THE ELECTRICAL CONDUCTIVITY

The goal of this section is, by using the RTA, to calculate the electrical conductivity. Within the RTA, the distribution function is given by:

$$f(k) = f_0(k) + e\mathcal{E} v \cos\theta \, \tau_m(k)\left(\frac{\partial f_0}{\partial E}\right) \quad , \quad \theta = \measuredangle(\vec{\mathcal{E}}, \vec{v})$$

The current density is then given by:

$$\vec{J} = -\frac{e}{V}\sum_{\vec{k}} \vec{v}\, f(k) = -\frac{e}{V}\sum_{\vec{k}} \vec{v}\left[\cancel{f_0(k)} + e\mathcal{E} v\cos\theta\, \tau_m(k)\left(\frac{\partial f_0}{\partial E}\right)\right]$$

This term averages to zero because $f_0(k)$ is symmetric in k.

$$\vec{J} = -\frac{e}{V}\sum_{\vec{k}} \vec{v} e\mathcal{E}\, v\cos\theta\, \tau_m(k)\left(\frac{\partial f_0}{\partial E}\right)$$

If the electric field is along z-axis, and if we are interested in the current along z-direction, then $v_z = v\cos\theta$ and we get:

$$J_z = -\frac{e}{V}\sum_{\vec{k}} e\mathcal{E}\, v^2\cos^2\theta\, \tau_m(k)\left(\frac{\partial f_0}{\partial E}\right)$$

$$= -\frac{e^2\mathcal{E}\, 2\cancel{V}}{\cancel{V}\, 8\pi^3}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\int_0^{\infty} k^2 dk\; v^2\cos^2\theta\, \tau_m(k)\left(\frac{\partial f_0}{\partial E}\right)$$

$$= -e^2\mathcal{E}\,\frac{1}{\cancel{4\pi^3}_{\,2\pi^2}}\,\cancel{2\pi}\int_{-1}^{1} d(\cos\theta)\cos^2\theta\int_0^{\infty}\underbrace{k^2 dk}\,\frac{2E}{m^*}\,\tau_m(E)\left(\frac{\partial f_0}{\partial E}\right)$$

$$k\cdot k\,dk = \sqrt{\frac{2m^*}{\hbar^2}E}\;\frac{m^*}{\hbar^2}\,dE = a\sqrt{E}\,dE$$

$$= -\frac{1}{2\pi^2}\,e^2\mathcal{E}\,a\left(\cos^3\theta\Big|_{-1}^{1}\right)\frac{\cancel{2}}{m^*}\int_0^{\infty} E^{3/2}\tau_m(E)\left(\frac{\partial f_0}{\partial E}\right)dE$$

$$= -\frac{e^2\mathcal{E}a}{m^*\pi^2}\,\frac{2}{3}\int_0^{\infty} E^{3/2}\,\tau_m(E)\left(\frac{\partial f_0}{\partial E}\right)dE$$

The electron density is, on the other hand, given by:

$$n = 2\frac{1}{(2\pi)^3}\cdot 4\pi \int_0^\infty k^2 dk\, f_0(E) = \frac{1}{\pi^2}\int_0^\infty f_0(E)\, a\sqrt{E}\, dE = \frac{a}{\pi^2}\int_0^\infty f_0(E)\sqrt{E}\, dE$$

Hence: $a/\pi^2 = n \Big/ \int_0^\infty \sqrt{E} f_0(E) dE$, or:

$$J_z = -\frac{e^2\mathcal{E}}{m^*} n \frac{2}{3} \frac{\int_0^\infty E^{3/2}\tau_m(E)(\partial f_0/\partial E)\, dE}{\int_0^\infty f_0(E) E^{1/2} dE}$$

We now manipulate the denominator of this expression to bring it into a more convenient form:

$$\int_0^\infty E^{1/2} f_0(E)\, dE = \int_0^\infty f_0(E)\, d(E^{3/2})\,\frac{2}{3} =$$

$$= \frac{2}{3}\Big[\underbrace{E^{3/2} f_0(E)\Big|_0^\infty}_{0} - \int_0^\infty E^{3/2}\frac{\partial f_0}{\partial E} dE\Big] = -\frac{2}{3}\int_0^\infty E^{3/2}\left(\frac{\partial f_0}{\partial E}\right) dE$$

Substituting this result back into our expression for the conductivity gives:

$$J_z = \cancel{-}\frac{e^2\mathcal{E} n}{m^*}\cancel{\frac{2}{3}} \frac{\int_0^\infty E^{3/2}\left(\frac{\partial f_0}{\partial E}\right)\tau_m(E)\, dE}{\cancel{-\frac{2}{3}}\int_0^\infty E^{3/2}\left(\frac{\partial f_0}{\partial E}\right) dE} = \frac{ne^2}{m^*}\mathcal{E}\frac{\int_0^\infty E^{3/2}\tau_m(E)\left(\frac{\partial f_0}{\partial E}\right) dE}{\int_0^\infty E^{3/2}\left(\frac{\partial f_0}{\partial E}\right) dE}$$

Since: $\vec{J} = -en\langle\vec{v_d}\rangle$, we have $\vec{v_d} = -\mu_n\vec{\mathcal{E}}$, which gives:

$$\vec{J} = +en\mu_n\vec{\mathcal{E}} \quad \Rightarrow \quad J_z = en\mu_n\mathcal{E}_z = en\mu_n\mathcal{E}$$

Comparing this result with our expression for J_z suggests that:

$$\mu_n = \frac{e}{m^*}\langle\langle\tau_f\rangle\rangle = \frac{e}{m^*}\frac{\int_0^\infty E^{3/2}\tau_m(E)\left(\frac{\partial f_0}{\partial E}\right) dE}{\int_0^\infty E^{3/2}\left(\frac{\partial f_0}{\partial E}\right) dE} = \frac{e}{m^*}\frac{\langle E\tau_m(E)\rangle}{\langle E\rangle}$$

and: $\sigma = en\mu_n = \frac{ne^2}{m^*}\langle\langle\tau_f\rangle\rangle$

To summarize, the drift velocity (average) is given by:

$$\langle \vec{v}_d \rangle = -\mu_n \vec{\mathcal{E}} = -\frac{e}{m^*} \frac{\int_0^\infty E^{3/2} \tau_m(E) \frac{\partial f_0}{\partial E} dE}{\int_0^\infty E^{3/2} \frac{\partial f_0}{\partial E} dE} \vec{\mathcal{E}}$$

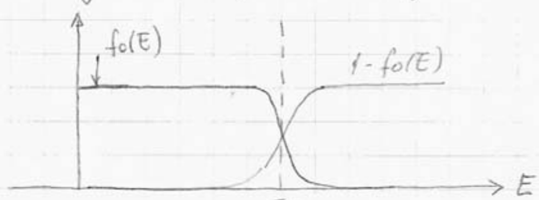
- for general Fermi-dirac statistics, we have:

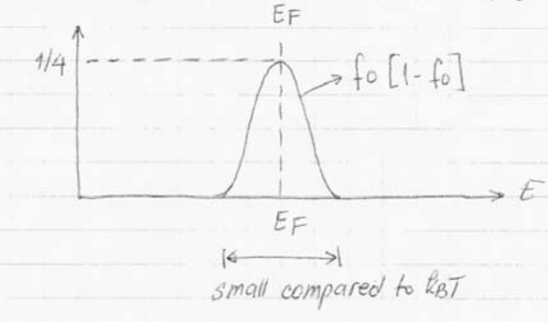
$$f_0(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}$$

$$\frac{\partial f_0}{\partial E} = -\frac{1}{k_BT} \frac{\exp[(E-E_F)/k_BT]}{\left[1+\exp\left(\frac{E-E_F}{k_BT}\right)\right]^2} = -\frac{1}{k_BT} \underbrace{\frac{\exp\left[\frac{E-E_F}{k_BT}\right]}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}}_{1-f_0(E)} \underbrace{\frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}}_{f_0(E)}$$

$$\frac{\partial f_0}{\partial E} = -\frac{1}{k_BT} f_0(E)\,(1-f_0(E)]$$

For $T \ll T_F$ ($k_BT \ll E_F$), the Fermi function $f_0(E)$ is small for E significantly in excess of E_F, and $1-f(E)$ is very small for E smaller than E_F. The product function $f_0(1-f_0)$ is, therefore, very small except in the neighborhood of E_F. As a result of this, there will be negligible contribution in the expression for $\langle\langle \tau_f \rangle\rangle$ except when E takes on values within a few k_BT units of E_F.





If we now assume that $E^{3/2}\tau_m(E)$ does not change significantly in this region, we can replace $f_0(1-f_0)$ with a Dirac δ-function:

$$f_0[1-f_0] = A\delta(E-E_F)$$

where the normalization constant A takes care of the area.

Using these observations into the expression for $\langle\langle \tau_f \rangle\rangle$, we have:

$$\langle\langle \tau_f \rangle\rangle \cong \frac{\int_0^\infty E^{3/2} \tau_m(E) \cancel{\left(-\frac{1}{k_B T}\right)} A\delta(E-E_F)\, dE}{\int_0^\infty E^{3/2} \cancel{\left(-\frac{1}{k_B T}\right)} A\delta(E-E_F)\, dE}$$

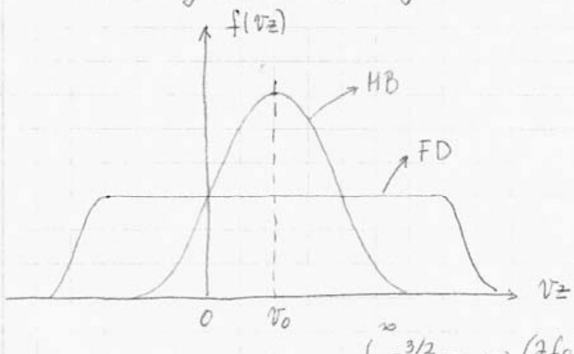
$$\langle\langle \tau_f \rangle\rangle \approx \frac{E_F^{3/2} \tau_m(E_F)}{E_F^{3/2}} \approx \tau_m(E_F)$$

Therefore, the conductivity at low temperatures equals to:

$$\sigma \approx \frac{n e^2 \tau_m(E_F)}{m^*} \Rightarrow J_z = \frac{n e^2 \tau_m(E_F)}{m^*} \mathcal{E}_z$$

i.e. carriers with energies very close to the Fermi energy contribute to the current.

- The above discussion also suggests that the statistics only will make difference in the details of the averaging procedure and will not affect the conductivity even at higher temperatures by orders of magnitude.



$$\langle\langle \tau_f \rangle\rangle = \frac{\int_0^\infty E^{3/2} \tau_m(E) \left(\frac{\partial f_0}{\partial E}\right) dE}{\int_0^\infty E^{3/2} \left(\frac{\partial f_0}{\partial E}\right) dE}$$

The double brackets in the expression for $\langle\langle \tau_f \rangle\rangle$ indicate that this is not a simple average of $\tau_f(E)$ over the symmetric part of the distribution function. It represents specially-defined average that arises in transport calculations.

- Let us assume that: $\tau_f(E) = \tau_0 (E/k_BT)^s$, where τ_0 is energy independent and s is characteristic exponent. Then; using $\partial f_0/\partial E = -f_0(E)/k_BT$, we get:

$$\langle\langle \tau_f \rangle\rangle = \frac{\int_0^\infty E^{3/2} \tau_0 \left(\frac{E}{k_BT}\right)^s \left(-\frac{1}{k_BT}\right) e^{-E/k_BT} dE}{\int_0^\infty E^{3/2} \left(-\frac{1}{k_BT}\right) e^{-E/k_BT} dE} = \frac{\tau_0 \int_0^\infty x^{s+3/2} e^{-x} dx}{\int_0^\infty x^{3/2} e^{-x} dx}$$

where we have used $x = E/k_BT$. The Γ-function is defined as:

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

and has the following properties: $\Gamma(p+1) = p\Gamma(p)$
$\Gamma(1/2) = \sqrt{\pi}$
$\Gamma(n) = (n-1)!$ when n is integer

Using the Γ-function definition, we have:

$$\langle\langle \tau_f \rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

Example:

For acoustic phonon scattering $s = -1/2$. Then:

$\Gamma(5/2) = 3/2\, \Gamma(3/2) = \frac{3}{2} \cdot \frac{1}{2} \sqrt{\pi} = \frac{3\sqrt{\pi}}{4}$. Also $\Gamma(5/2 - 1/2) = 1! = 1$.

Then:

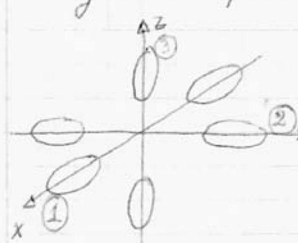
$$\langle\langle \tau_f \rangle\rangle = \tau_0 \frac{4}{3\sqrt{\pi}}$$

Characteristic exponents for common power law scattering mechanisms:

Scattering mechanism	exponent
1. acoustic phonon	$s = -1/2$
2. ionized impurity (weekly screened)	$s = 3/2$
3. ionized impurity (strongly screened)	$s = -1/2$
4. neutral impurity	$s = 0$
5. piezoelectric scattering	$s = 1/2$

Semiconductors with anisotropic mass

Consider now an anisotropic material such as Si, for which in near equilibrium conditions the electrons are almost equally distributed along the six equivalent valleys.



1,2,3 are valley pairs

$$\vec{J}_1 = \overleftrightarrow{\sigma}_1 \vec{E} = 2\frac{ne^2 \langle\langle\tau\rangle\rangle}{6} \begin{bmatrix} \frac{1}{m_l} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$\vec{J}_2 = \overleftrightarrow{\sigma}_2 \vec{E} = 2\frac{ne^2}{6} \langle\langle\tau\rangle\rangle \begin{bmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_l} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$\vec{J}_3 = \overleftrightarrow{\sigma}_3 \vec{E} = 2\frac{ne^2}{6} \langle\langle\tau\rangle\rangle \begin{bmatrix} 1/m_t & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_l \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

Total conductivity is thus:

$$\vec{J} = \overleftrightarrow{\sigma}\vec{E} = \frac{ne^2}{3} \langle\langle\tau\rangle\rangle \begin{bmatrix} \frac{1}{m_l} + \frac{2}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_l} + \frac{2}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} + \frac{2}{m_t} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \frac{ne^2 \langle\langle\tau\rangle\rangle}{3} \left(\frac{1}{m_l} + \frac{2}{m_t}\right) I \vec{E}$$

i.e. $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \dfrac{ne^2 \langle\langle\tau\rangle\rangle}{m_c}$, where $\dfrac{1}{m_c} = \dfrac{1}{3}\left(\dfrac{1}{m_l} + \dfrac{2}{m_t}\right)$

conductivity mass: $m_c = \dfrac{3}{1/m_l + 2/m_t} \cong 0.26\, m_0$

- Consider next the case when several scattering mechanisms are important. Then:

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -\frac{f_A}{\tau_1} - \frac{f_A}{\tau_2} \qquad \text{(for two mechanisms)}$$

where: $\frac{1}{\tau_{eff}} = \frac{1}{\tau_1} + \frac{1}{\tau_2}$ i.e. $\tau_{eff} = \frac{\tau_1 \tau_2}{\tau_1 + \tau_2}$. Let suppose

now that the characteristic exponents for these two mechanisms are s_1 and s_2. Then:

$$\tau_{eff} = \frac{\tau_{01}(E/k_BT)^{s_1} \; \tau_{02}(E/k_BT)^{s_2}}{\tau_{01}(E/k_BT)^{s_1} + \tau_{02}(E/k_BT)^{s_2}} \rightarrow \text{rather complicated expression}$$

If it happens that $s_1 = s_2 = s$, we get:

$$\tau_{eff} = \frac{\tau_{01}\tau_{02}}{\tau_{01}+\tau_{02}} \left(\frac{E}{k_BT}\right)^s$$

and: $$\mu_{eff} = \frac{e}{m^*} \langle\langle \tau_{eff} \rangle\rangle = \frac{e}{m^*} \frac{\tau_{01}\tau_{02}}{\tau_{01}+\tau_{02}} \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

or: $$\frac{1}{\mu_{eff}} = \frac{m^*}{e\tau_{01}} \frac{\Gamma(5/2)}{\Gamma(s+5/2)} + \frac{m^*}{e\tau_{02}} \frac{\Gamma(5/2)}{\Gamma(s+5/2)} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$$

This last result is known as MATHIESSEN'S RULE. It is usually used in calculating mobility when multiple scattering mechanisms occur.

Note: Mathiessen's rule is only valid when the scattering mechanisms considered have the same energy dependence.