Low-Field Transport

Note Title 10/17/2010

Flow of charge : $\vec{J} = \sigma \vec{\mathcal{E}}$

Flow of charge & heat : $\begin{cases} \vec{J} = L_{11}\vec{\mathcal{E}} + L_{12}\nabla T_L \\ J_Q = L_{21}\vec{\mathcal{E}} + L_{22}\nabla T_L \end{cases}$

Electrons transfer both heat & charge - so the two equations are coupled.

$$\text{BTE} \Longrightarrow L_{ij} = ?$$

Assumptions: low field
RTA
spherical parabolic bands

Low field solution (B=0):

$$f = f_S + f_A \qquad f_S = \frac{1}{1+e^{\theta}} \qquad \theta = \frac{E_C(r,t) + \overbrace{E(p)}^{\frac{p^2}{2m}} - \overbrace{F_n(r,t)}^{\text{quasi fermi level}}}{k_B T_L}$$

f_S: symmetric part (equilibrium)

f_A: Anti-symmetric (Perturbed)

Steady-state BTE:

$$\cancelto{0}{\frac{\partial f}{\partial t}} + v \cdot \nabla_r (f_S + f_A) + F \cdot \nabla_p (f_S + f_A) = -\frac{f_A}{\tau}$$

We also assume: $f_S \gg f_A$

$$|\nabla_r f_S| \gg |\nabla_r f_A|$$

$$|\nabla_p f_S| \gg |\nabla_p f_A|$$

$$\Rightarrow \quad \vec{v}\cdot\vec{\nabla}_r f_s + \vec{F}\cdot\vec{\nabla}_p f_s = -\frac{f_A}{\tau}$$

$$v\cdot \frac{\partial f_s}{\partial \theta}\nabla_r\theta + \underset{\underset{\nabla_r E_c \ (\text{since } B=0)}{\downarrow}}{F}\cdot\frac{\partial f_s}{\partial\theta}\nabla_p\theta = -\frac{f_A}{\tau}$$

$$\theta = \frac{E_c(r,t) + E(p) - F_n(r,t)}{k_B T_L}$$

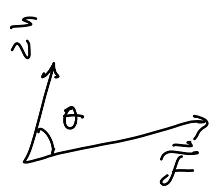
$$\begin{cases} \vec{\nabla}_r\theta = \dfrac{1}{k_B T_L}\left(\nabla_r E_c - \nabla_r F_n\right) + \left(E_c + E(p) - F_n\right)\nabla_r\left(\dfrac{1}{k_B T_L}\right) \\ \vec{\nabla}_p\theta = \dfrac{p}{m}\dfrac{1}{k_B T_L} = \vec{v}\,\dfrac{1}{k_B T_L} \end{cases}$$

insert in BTE $\rightarrow$ $$f_A = \frac{\tau}{k_B T_L}\left(-\frac{\partial f_s}{\partial\theta}\right)\vec{v}\cdot\underset{\underset{\text{generalized force}}{\downarrow}}{\vec{\mathcal{F}}}$$

$$\mathcal{F} = -\nabla_r F_n + T_L\left[E_c + E(p) - F_n\right]\nabla_r\left(\frac{1}{T_L}\right)$$

The generalized force has the influence of gradients of potential, carrier concentration, and Temperature.

$$f_A = \frac{\tau}{k_B T_L}\left(-\frac{\partial f_s}{\partial\theta}\right)\vec{v}\cdot\vec{\mathcal{F}} \equiv \underset{\underset{\substack{\text{function of magnitude of } p. \\ \text{doesn't depend on direction.}}}{\downarrow}}{g(p)}\cos\theta$$



$$\begin{cases} \text{Electric current:} \quad \vec{J} = \dfrac{-q}{\Omega}\sum_p \vec{v}\,(\overset{\overset{\text{even}}{\uparrow}}{f_s} + f_A) = \dfrac{-q}{\Omega}\sum_p \vec{v} f_A \quad \checkmark \\ \\ \text{Heat current:} \quad J_W = \dfrac{1}{\Omega}\sum_p \underset{\underset{\text{heat is associated with kinetic energy}}{\downarrow}}{E(\vec{p})}\,\vec{v} f_A \quad \times \end{cases}$$

But $E(p)$ includes also the drift kinetic energy due to the applied electric field. Heat is only associated by the random component of the kinetic energy. From Thermodynamics:

$$\underbrace{dU}_{\substack{\text{internal energy}\\ \text{(potential + kinetic)}\\ E_c+E(p)}} = \underbrace{dQ}_{\text{heat}} + \underbrace{F_n}_{\text{quasi fermi energy}} \underbrace{dN}_{\#\text{ of particles}}$$

$$dQ = dU - F_n dN \rightarrow \vec{J}_Q = \underbrace{\vec{J}_U}_{\frac{1}{\Omega}\sum_p (E_c+E(p))v f_A} - F_n \underbrace{\vec{J}_N}_{\frac{1}{\Omega}\sum_p v f_A}$$

$$\vec{J}_Q = \frac{1}{\Omega}\sum_p \left(E_c+E(p)-F_n\right)\vec{v} f_A$$

insert $f_A = \frac{\tau}{k_B T_L}\left(\frac{-\partial f}{\partial \theta}\right)\vec{v}\cdot\vec{\mathcal{F}}$ in J and J_Q =>

$$\vec{J} = \frac{-q}{\Omega}\sum_p \vec{v} f_A(p) \rightarrow \vec{J} = \frac{-q}{\Omega k_B T_L}\sum_{\vec{p}} \vec{v}\,(\vec{v}\cdot\vec{\mathcal{F}})\,\tau\left(\frac{-\partial f_s}{\partial \theta}\right)$$

for J_Q → $$\vec{J}_Q = \frac{1}{\Omega k_B T_L}\sum_p \vec{v}\,(\vec{v}\cdot\vec{\mathcal{F}})\,\tau\left(-\frac{\partial f_s}{\partial \theta}\right)\left[E_c+E(p)-F_n\right]$$

we may expand versus the vector components:

$$\vec{A}\cdot\vec{B} = \sum_{j=1}^{3} A_j B_j \equiv A_j B_j$$ repeated indices are summed over the three coordinates.

The i'th component of $\vec{J}$ is:

$$J_i = \frac{-q}{\Omega k_B T_L} \sum_p v_i v_j \mathcal{F}_j \tau \left(-\frac{\partial f_s}{\partial \theta}\right)$$

where: $\vec{\mathcal{F}} = -\nabla_r F_n(r) + T_L (E_c + E_p - F_n) \nabla_r \left(\frac{1}{T_L}\right)$

define $\partial_j(\cdot) \equiv \frac{\partial}{\partial x_j}(\cdot) \rightarrow$

$$\mathcal{F}_j = -\partial_j F_n + T_L (E_c + E_p - F_n) \partial_j \left(\frac{1}{T_L}\right) \Rightarrow$$

$$J_i = \underbrace{\frac{q \times q}{\Omega k_B T_L} \sum_p v_i v_j \tau \left(-\frac{\partial f_s}{\partial \theta}\right)}_{\sigma_{ij}} \left(\frac{\partial_j F_n}{q}\right) + \underbrace{\frac{q}{\Omega k_B T_L} \sum_p v_i v_j T_L (E_c + E_p - F_n) \tau \left(-\frac{\partial f_s}{\partial \theta}\right)}_{B_{ij}} \partial_j \left(\frac{1}{T_L}\right)$$

$$J_i = \sigma_{ij}\, \partial_j \left(\frac{F_n}{q}\right) + B_{ij}\, \partial_j \left(\frac{1}{T_L}\right)$$

$$\sigma_{ij} = \frac{q^2}{\Omega k_B T_L} \sum_p v_i v_j \tau \left(-\frac{\partial f_s}{\partial \theta}\right)$$

$$B_{ij} = \frac{-q}{\Omega k_B T_L} \sum_p v_i v_j \tau T_L (E_c + E_p - F_n) \left(-\frac{\partial f_s}{\partial \theta}\right)$$

In matrix form: recall $[A]X = \sum_{j=1}^{3} A_{ij} X_j = A_{ij} X_j$

$$\vec{J} = [\sigma] \nabla_r \left(\frac{F_n}{q}\right) + [B] \nabla_r \left(\frac{1}{T_L}\right)$$

If isotropic $\Rightarrow [\sigma] = \sigma_o [I]$ or $\sigma_{ij} = \sigma_o \delta_{ij}$

Similarly for $\vec{J}_Q$:

$$J_{Q_i} = P_{ij}\, \partial_j \left(\frac{F_n}{q}\right) + k_{ij}\, \partial_j \left(\frac{1}{T_L}\right)$$

$$P_{ij} = \frac{-q}{\Omega k_B T_L} \sum_p v_i v_j \tau [E_c + E_p - F_n] \left(-\frac{\partial f_s}{\partial \theta}\right)$$

$$k_{ij} = \frac{1}{\Omega k_B} \sum_p v_i v_j \tau [E_c + E_p - F_n]^2 \left(-\frac{\partial f_s}{\partial \theta}\right)$$

In matrix form: $$\vec{J}_Q = [P]\,\nabla_r\left(\frac{F_n}{q}\right) + [K]\,\nabla_r\left(\frac{1}{T_L}\right)$$

For anisotropic materials, $\vec{J}$ and $\vec{J}_Q$ may not be parallel to the deriving force.

For **cubic** semiconductors, the tensors are diagonal =>

For CB electrons

$$\begin{cases} \vec{J} = \overset{\oplus}{\sigma_0}\,\vec{\nabla}_r\left(\frac{F_n}{q}\right) + \overset{\ominus}{B_0}\,\vec{\nabla}_r\left(\frac{1}{T_L}\right) \\ \vec{J}_Q = \underset{\ominus}{P_0}\,\vec{\nabla}_r\left(\frac{F_n}{q}\right) + \overset{\oplus}{K_0}\,\vec{\nabla}_r\left(\frac{1}{T_L}\right) \end{cases}$$ For Cubic semiconductors

For CB electrons

The deriving forces are $\vec{\nabla}_r\left(\frac{F_n}{q}\right)$ and $\nabla_r\left(\frac{1}{T_L}\right)$.

In general $\nabla_r\left(\frac{F_n}{q}\right)$ has the effect of both drift & diffusion forces.
If the carrier concentration is uniform $n(r) = n \Rightarrow \vec{\nabla}_r F_n = q\vec{\mathcal{E}}$

Transport Coefficients

Four tensors that describe the low field transport at $B=0$ are:

$$\begin{bmatrix} \sigma_{ij} \\ B_{ij} \\ P_{ij} \\ K_{ij} \end{bmatrix} = \frac{1}{\Omega} \underbrace{\sum_{\vec{p}}}_{\text{vector } \vec{p}} \left(-\frac{\partial f_s}{\partial \theta}\right) \overbrace{\tau}^{\text{depends on } |P|} \frac{v_i v_j}{k_B T_L} \begin{bmatrix} q^2 \\ -q T_L (E_c + E_p - F_n) \\ -q\,(E_c + E_p - F_n) \\ T_L\,(E_c + E_p - F_n)^2 \end{bmatrix}$$

$$\begin{cases} \vec{J} = [\sigma]\,\vec{\nabla}_r\left(\frac{F_n}{q}\right) + [B]\,\vec{\nabla}_r\left(\frac{1}{T_L}\right) \\ \vec{J}_Q = [P]\,\vec{\nabla}_r\left(\frac{F_n}{q}\right) + [K]\,\vec{\nabla}_r\left(\frac{1}{T_L}\right) \end{cases}$$

σ, B, P, K are similar in form. Let's look at one, say σ:

Assume non-degenerate for simple math: $f_s = e^{-\theta} \rightarrow \frac{\partial f_s}{\partial \theta} = -f_s$

note: $J_i = \sum_j \sigma_{ij} \partial_j \left(\frac{F_n}{q}\right)$

For parabolic spherical band:

$$\rightarrow \sigma_{ij} = \frac{q^2}{k_B T_L} \frac{1}{\Omega} \sum_{\vec{p}} v_i v_j \overset{\text{magnitude of } \vec{p}}{\downarrow}\tau(p) f_s = \frac{q^2}{m^* k_B T_L/2} \frac{1}{\Omega} \sum_{\vec{p}} \frac{m^* \overbrace{v_i v_j}^{v_i^2 \delta_{ij} = \frac{1}{3} v^2 \delta_{ij}}}{2} \tau f_s$$

$$= \frac{q^2}{m^* \underbrace{\frac{3}{2} k_B T_L}_{\langle E \rangle}} \underbrace{\frac{1}{\Omega} \sum_p \left(\frac{m^* v^2}{2}\right) \tau f_s}_{n \langle E\tau \rangle} = nq \frac{q}{m^*} \frac{\langle E\tau \rangle}{\langle E \rangle} = nq \underbrace{\frac{q \langle\langle \tau \rangle\rangle}{m^*}}_{\mu_n} \delta_{ij}$$

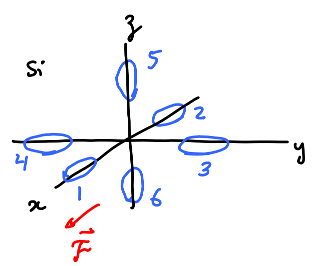
Similarly for B_{ij}, P_{ij}, and K_{ij}. If $\tau \propto E^s$, for non-degenerate case we have:

$$\begin{cases} \sigma_{ij} = q n \mu_n \delta_{ij} \qquad \mu_n = \dfrac{q \langle\langle \tau \rangle\rangle}{m^*} \\[2ex] B_{ij} = \dfrac{k_B}{-q} T_L^2 \left[\ln\left(\dfrac{N_c}{n}\right) + \left(s + \dfrac{5}{2}\right) \right] \sigma_{ij} \qquad N_c = 2\left(\dfrac{2\pi m^* k_B T}{h^2}\right)^{3/2} \\[2ex] P_{ij} = \dfrac{1}{T_L} B_{ij} \\[2ex] K_{ij} = \dfrac{k_B^2 T_L^3}{q^2} \left\{ \left[\ln \dfrac{N_c}{n} + \left(s + \dfrac{5}{2}\right) \right]^2 + \left(s + \dfrac{5}{2}\right) \right\} \sigma_{ij} \end{cases}$$

Ellipsoidal energy bands

For many semiconductors the energy bands are ellipsoidal & there are several CB minima:

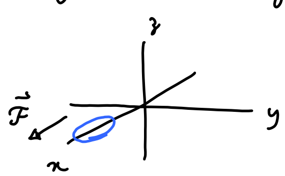
$$E_p = \frac{(P_x - P_{x_0})^2}{2m_{xx}} + \frac{(P_y - P_{y_0})^2}{2m_{yy}} + \frac{(P_z - P_{z_0})^2}{2m_{zz}}$$



This E_p goes into the transport coefficient for integration over P.

To find σ, we consider one ellipsoid at a time and add the contributions together as at equilibrium carriers are evenly distributed in the ellipsoids.

Consider ellipsoid 1 whose major axis is along $\hat{x}$-axis. Assume the generalized field is also along $\hat{x}$-axis.



$\Rightarrow$ so carriers respond with longitudinal effective mass m_ℓ^*.

$$\sigma_1 = \frac{n}{6} q \overbrace{\frac{q\langle\langle\tau\rangle\rangle}{m_l^*}}^{\mu} \qquad \text{also} \qquad \sigma_2 = \frac{n}{6} q \frac{q\langle\langle\tau\rangle\rangle}{m_l^*}$$

$$\text{but} \qquad \sigma_3 = \sigma_4 = \sigma_5 = \sigma_6 = \frac{n}{6} q \frac{q\langle\langle\tau\rangle\rangle}{m_t^*}$$

$$\sigma = \sum_{i=1}^{6} \sigma_i = nq \underbrace{\frac{1}{3}\left(\frac{1}{m_l} + \frac{2}{m_t}\right)}_{\frac{1}{m_c}} q\langle\langle\tau\rangle\rangle = nq \frac{q\langle\langle\tau\rangle\rangle}{m_c}$$

conductivity effective mass

Multiple Scatterings :

using RTA:

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -\frac{f_A}{\tau_1} - \frac{f_A}{\tau_2} \equiv -\frac{f_A}{\tau} \rightarrow \frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} \qquad \text{Mathiessen's rule.}$$

If $\tau_1 \propto E^{s_1}$ and $\tau_2 \propto E^{s_2}$ and $s_1 = s_2 \Rightarrow \frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$

Transport in weak magnetic field

we need to add the force by $\vec{B}$: $-q\vec{v}\times\vec{B}$ to BTE. The math is a bit tedeous so we only consider weak magnetic field and present the result.

$$\vec{v}\cdot\vec{\nabla}_r f + \left(-q\vec{\mathcal{E}} - q\vec{v}\times\vec{B}\right)\cdot\vec{\nabla}_p f = -\frac{f_A}{\tau}$$

For low field we can use superposition ① $B=0 \Rightarrow f_A'$ as before.

② $\mathcal{F}$ due to concentration, temperature gradients & electric field $=0 \Rightarrow$

$$-q(\vec{v}\times\vec{B})\cdot\vec{\nabla}_p f = -\frac{f_A''}{\tau} \rightarrow f_A'' = q\tau(\vec{v}\times\vec{B})\vec{\nabla}_p f$$

Can we approximate $\vec{\nabla}_p f = \vec{\nabla}_p f_0$?

$\theta = (E_C + E_p - F_n)/k_BT$

note that: $\nabla_p f_s = \frac{\partial f_s}{\partial\theta}\nabla_p\theta = \frac{\partial f_s}{\partial\theta}\frac{v}{k_BT}$

But $(\vec{v}\times\vec{B})\cdot\vec{v} = 0 \Rightarrow f_A'' = 0 \rightarrow$ so this is not a good approximation.

A better approx. is $\nabla_p f \simeq \nabla_p f' = \nabla_p\left[\frac{\tau}{k_BT}\left(-\frac{\partial f_0}{\partial\theta}\right)(\vec{v}\cdot\vec{\mathcal{F}})\right]$

Functions of energy like $h(E)$

$\nabla_p h(E) = \frac{\partial h}{\partial E}\nabla_p E = \frac{\partial h}{\partial E} v$ so the gradient of a function of energy is proportional to velocity.

$$\Rightarrow (\vec{v}\times\vec{B})\cdot\vec{\nabla}_p h(E) = 0 \rightarrow f_A'' = \tau q(\vec{v}\times\vec{B})\cdot\vec{\nabla}_p f' = \tau q(\vec{v}\times\vec{B})\cdot\underbrace{\vec{\nabla}_p\left[\frac{\tau}{k_BT}\left(-\frac{\partial f_0}{\partial\theta}\right)(\vec{v}\cdot\vec{\mathcal{F}})\right]}$$

$$\frac{1}{k_BT}(\vec{\nabla}_p\tau)\left(-\frac{\partial f}{\partial\theta}\right)(\vec{v}\cdot\vec{\mathcal{F}}) + \frac{\tau}{k_BT}\vec{\nabla}_p\left(-\frac{\partial f_0}{\partial\theta}\right)(\vec{v}\cdot\vec{\mathcal{F}}) + \frac{\tau}{k_BT}\left(-\frac{\partial f_0}{\partial\theta}\right)\underbrace{\vec{\nabla}_p(\vec{v}\cdot\vec{\mathcal{F}})}$$

$(v\times B)\cdot(\cdot) = 0$

0

$$(\vec{\mathcal{F}}\cdot\vec{\nabla}_p)\vec{v} + (\vec{v}\cdot\vec{\nabla}_p)\vec{\mathcal{F}} + \vec{\mathcal{F}}\times(\vec{\nabla}_p\times\vec{v}) + \vec{v}\times(\vec{\nabla}_p\times\vec{\mathcal{F}})$$

0 $\quad$ 0 $\quad$ parallel to $\vec{v}$

$$\boxed{f_A'' = \tau q\,(\vec{\nabla}_p\cdot\vec{v})\,(\vec{v}\times\vec{B})\cdot\vec{\mathcal{F}}}$$

$\frac{1}{m^*}$ for spherical band $\Rightarrow f_A'' = \frac{-q\tau^2}{m^*}\frac{1}{k_BT}\frac{\partial f_0}{\partial\theta}(\vec{v}\times\vec{B}\cdot\vec{\mathcal{F}})$

$A\cdot(B\times C) = B\cdot(C\times A) \Rightarrow$ $\boxed{f_A'' = -\frac{q\tau^2}{mk_BT}\frac{\partial f_0}{\partial\theta}\vec{v}\cdot(\vec{B}\times\vec{\mathcal{F}})}$

So we can calculate the current:

$$\vec{J} = \frac{-q}{\Omega} \sum_{p} \vec{v}\,(f_A' + f_A'') = \overbrace{\frac{-q}{\Omega}\sum_{p} \vec{v} f_A'}^{J' = [\sigma']\vec{\mathcal{E}}} + \overbrace{\frac{-q}{\Omega}\sum_{p} \vec{v} f_A''}^{J''}$$

replace f_A'' for spherical band:

$$\vec{J}'' = \frac{1}{\Omega} \sum_{\vec{p}} \frac{q^3 \tau^2}{m^* k_B T} \left(-\frac{\partial f_0}{\partial \theta}\right) v \left[\vec{v} \cdot (\vec{B} \times \vec{\mathcal{E}})\right]$$

$i \to j \to k \to i$

Recall: $\vec{A} \times \vec{B} = \varepsilon_{1jk} A_j B_k \hat{x}_1 + \varepsilon_{2jk} A_j B_k \hat{x}_2 + \varepsilon_{3jk} A_j B_k \hat{x}_3$; $\varepsilon_{ijk} = \begin{cases} 1 & i,j,k \text{ in cyclic order} \\ -1 & \text{" in anti-cyclic order} \\ 0 & \text{otherwise} \end{cases}$

The i^{th} component of the cross product is: $(\vec{A} \times \vec{B}) \cdot \hat{x}_i = \varepsilon_{ijk} A_j B_k$

e.g.: $(\vec{A} \times \vec{B}) \cdot \hat{x} = \overbrace{\varepsilon_{xyz}}^{1} A_y B_z + \overbrace{\varepsilon_{xzy}}^{-1} A_z B_y = A_y B_z - A_z B_y$

So we can write: $J_i'' = \underbrace{\frac{1}{\Omega} \sum_{\vec{p}} \frac{q^3 \tau^2}{m^* k_B T} \left(-\frac{\partial f_0}{\partial \theta}\right) v_i v_m \varepsilon_{mnj} B_n}_{\sigma_{ij}'' :\ \text{conductivity tensor}} \mathcal{E}_j$

$$\sigma_{ij}'' = \frac{1}{\Omega} \sum_{\vec{p}} \frac{q^3 \tau^2}{m^* k_B T} \left(-\frac{\partial f_0}{\partial \theta}\right) (v_i v_m \varepsilon_{mnj} B_n)$$

Consider the diagonal element σ_{11}'':

$$\sigma_{11}'' = (\,\cdots) (\underbrace{v_1 v_m}_{v_1^2 \delta_{1m}} \varepsilon_{mn1} B_n) = 0$$

$v_1^2 \delta_{1m}$ when integrated over θ & ϕ $\to m=1 \to \varepsilon_{1n1} = 0$

Similarly other diagonal terms are zero. So the presence of small magnetic field doesn't affect the diagonal terms of $[\sigma]$.

Consider now the off-diagonal terms:

similar to σ_{11} but has τ^2 instead of τ

$$\sigma''_{12} = \frac{1}{\Omega}\sum_{\vec{p}}\frac{q^3\tau^2}{m^* k_B T}\left(-\frac{\partial f_0}{\partial \theta}\right)\underbrace{v_1 v_m \varepsilon_{mn2} B_n}_{\text{only } v_1^2\varepsilon_{132}B_3 \text{ is not zero: } m=1,\ n=3} = \frac{-qB_3}{m^*}\overbrace{\left\{\frac{q^2}{k_B T\Omega}\sum_{\vec{p}}\underbrace{v_1^2}_{\frac{v^2}{3}}\tau^2\left(-\frac{\partial f_0}{\partial \theta}\right)\right\}}$$

$$= \frac{-qB_3}{m^*}\frac{q^2}{\underbrace{m^*\frac{3k_BT}{2}}_{\langle E\rangle}}\underbrace{\frac{1}{\Omega}\sum_{\vec{p}}\frac{m^*}{2}v^2\tau^2\left(-\frac{\partial f_0}{\partial \theta}\right)}_{n\langle E\tau^2\rangle} = \frac{-qB_3}{m^*}\frac{q^2}{m^*}n\frac{\langle E\tau^2\rangle}{\langle E\rangle}$$

$$= -\overbrace{qn\overbrace{\frac{q}{m^*}\frac{\langle E\tau\rangle}{\langle E\rangle}}^{\mu}}^{\sigma_0}\underbrace{\overbrace{\frac{\langle E\tau^2\rangle\langle E\rangle^2}{\langle E\rangle\langle E\tau\rangle^2}}^{\langle\langle\tau^2\rangle\rangle/\langle\langle\tau\rangle\rangle^2}\overbrace{\frac{q\langle E\tau\rangle}{m^*\langle E\rangle}}^{\mu}}_{\mu_H \text{ Hall mobility}}B_3 = -\sigma_0\mu_H B_3$$

$$\mu_H = \overbrace{\frac{\langle\langle\tau^2\rangle\rangle}{\langle\langle\tau\rangle\rangle^2}}^{r_H}\mu$$

$$\mu_H = \underbrace{r_H}_{\text{Hall factor}}\mu$$

$(\tau \propto E^s)$

Scattering	s	r_H
Acoustic Phonon	$-1/2$	1.18
Ionized Impurity	$3/2$	1.93

So weak magnetic field does not affect the diagonal elements of σ but introduces off-diagonal terms:

$$J_i = \sigma_{ij}\,\mathcal{E}_j$$

$$\sigma_{ij} = \sigma_0\delta_{ij} - \sigma_0\mu_H\varepsilon_{ijk}B_k \implies$$

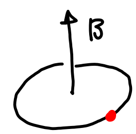
$$\sigma(B) = \begin{bmatrix} 1 & -\mu_H B_z & \mu_H B_y \\ \mu_H B_z & 1 & -\mu_H B_x \\ -\mu_H B_z & \mu_H B_x & 1 \end{bmatrix}$$

magneto conductivity tensor

$$\boxed{\vec{J} = \sigma_0\vec{\mathcal{E}} - \sigma_0\mu_H\vec{\mathcal{E}}\times\vec{B}}$$

We can improve the approximation by using the obtained $f_A' + f_A''$ for $\nabla_p f$. The resut will have terms proportional to B^2. We may iterate for better approximation and for any strength of magnetic field B.

strong B is defined by: $\omega_c \tau \gg 1$ where $\omega_c = \frac{qB}{m}$ cyclotron frequency



Weak B: Carriers scatter many times before completing an orbit.
Strong B: Carriers complete several orbits before being scattered.

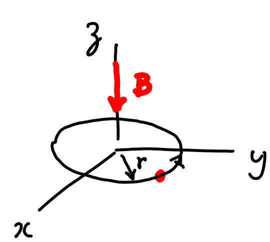
Strong B affects both the diagonal & off-diagonal terms of $[\sigma]$. Also $r_H \to 1$

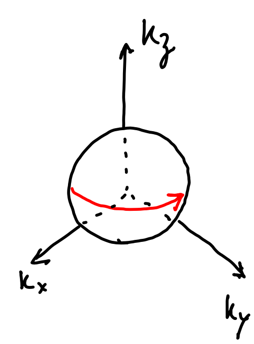
Strong B parallel to σ => Longitudinal magnetoresistance
Strong B perpendicular to σ => Transverse magnetoresistance + Quantized Landau levels separated by $\hbar\omega_c$

At low T: $k_B T \ll \hbar\omega_c$ => strong influence on carrier transport.

Measurement of Effective mass

$$\frac{mv^{\cancel{2}}}{r} = qv \times B_z = q\cancel{v}B_z$$

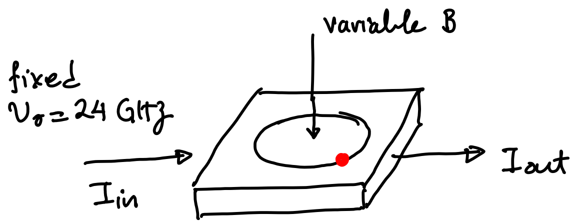


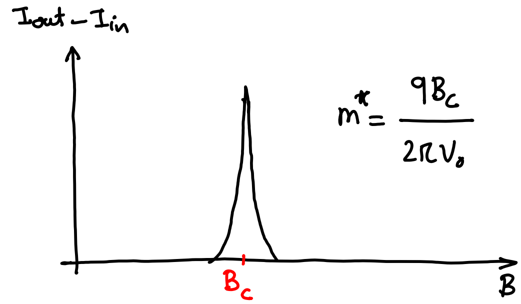


$$v = \frac{qBr}{m} \qquad \tau = \frac{2\pi r}{v} = \frac{2\pi \cancel{r} m}{qB\cancel{r}}$$

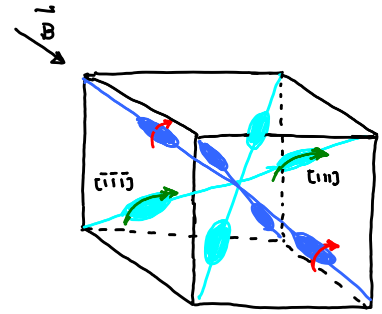
$$\nu_c = \frac{1}{\tau} = \frac{qB}{2\pi m^*} \quad \text{or} \quad \boxed{\omega_c = \frac{qB}{m^*}}$$

$B = 1T \quad m^* = m_0 \to \nu_c \cong 28$ GHz





$$m^* = \frac{qB_c}{2\pi\nu_0}$$



Example: Germanium

$$\omega_c = \frac{qB}{m^*}$$

* 8 Ellipsoids:

[111] [1̄11] [11̄1] [111̄]

[1̄1̄1] [1̄11̄] [11̄1̄] [1̄1̄1̄]

* 4 angles between B & the ellipsoids

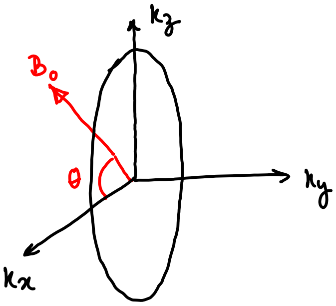
we want to show that: $\dfrac{1}{m_c^2} = \dfrac{\cos^2\theta}{m_t^2} + \dfrac{\sin^2\theta}{m_l m_t}$ we measure m_c & θ $\Rightarrow$ Calculate m_t & m_l

Start from: $\vec{F} = m\vec{a}$

$$q\vec{v}\times\vec{B} = [m]\frac{d\vec{v}}{dt} \longrightarrow F_x = q(v_yB_z - v_zB_y) = m_t^*\frac{dv_x}{dt}$$

$$F_y = q(v_zB_x - v_xB_z) = m_t^*\frac{dv_y}{dt}$$

$$F_z = q(v_xB_y - v_yB_x) = m_l^*\frac{dv_z}{dt}$$



$$\begin{cases} B_x = B_0\cos\theta \\ B_y = 0 \\ B_z = B_0\sin\theta \end{cases} \rightarrow \begin{cases} F_x = qv_yB_0\sin\theta = m_t^*\dfrac{dv_x}{dt} \\ F_y = q(v_zB_0\cos\theta - v_xB_0\sin\theta) = m_t^*\dfrac{dv_y}{dt} \\ F_z = -qv_yB_0\cos\theta = m_l^*\dfrac{dv_z}{dt} \end{cases}$$

$$\frac{dF_y}{dt} = qB_0\left(\frac{dv_z}{dt}\cos\theta - \frac{dv_x}{dt}\sin\theta\right) = m_t^* \frac{d^2 v_y}{dt}$$

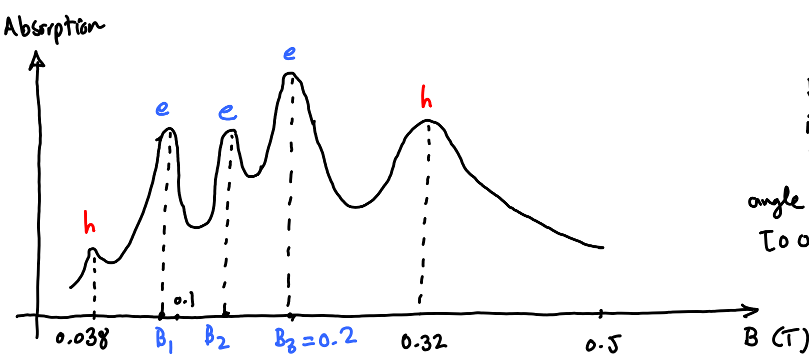
$$= qB_0\left(\frac{-qB_0\cos^2\theta}{m_l} v_y - \frac{qB_0\sin^2\theta}{m_t} v_y\right) = m_t^* \frac{d^2 v_y}{dt}$$

$$\rightarrow \frac{d^2 v_y}{dt^2} + \underbrace{\left(\underbrace{\frac{q^2}{B_0^2 m_l m_t}}_{\omega_l \omega_t}\cos^2\theta + \underbrace{\frac{q^2}{B_0^2 m_t^2}}_{\omega_t^2}\sin^2\theta\right)}_{\omega_c^2} v_y = 0 \quad \Rightarrow \quad \frac{d^2 v_y}{dt^2} + \omega_c^2 v_y = 0$$

$$\omega_c = \frac{q}{B_0 m_c}$$

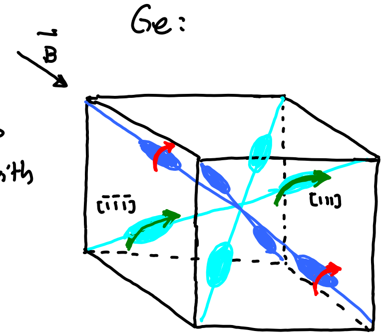
$$\omega_c^2 = \frac{\cancel{q^2}}{\cancel{B_0^2} m_c^2} = \frac{\cancel{q^2}}{\cancel{B_0^2} m_l m_t}\cos^2\theta + \frac{\cancel{q^2}}{\cancel{B_0^2} m_t^2}\sin^2\theta$$

$$\Rightarrow \quad \frac{1}{m_c^2} = \frac{\cos^2\theta}{m_l m_t} + \frac{\sin^2\theta}{m_t^2}$$



B in [110] plane => angle of 60° with [001] axis

Ge:



$B_1, B_2, B_3 \Rightarrow m_{c_1}, m_{c_2}, m_{c_3}$ each peak corresponds to a mass $m_{c_1} = \frac{q}{\omega_c B_1}$ $m_{c_2} = \frac{q}{\omega_c B_2}$ ...

we also know the three angles: 7, 65, 73 (two angles are equal; otherwise there are four angles)

$$\begin{cases} \dfrac{1}{m_{c_1}^2} = \dfrac{\cos^2\theta_1}{m_t^2} + \dfrac{\sin^2\theta_1}{m_l m_t} \\[2ex] \dfrac{1}{m_{c_2}^2} = \dfrac{\cos^2\theta_2}{m_t^2} + \dfrac{\sin^2\theta_2}{m_l m_t} \\[2ex] \dfrac{1}{m_{c_3}^2} = \dfrac{\cos^2\theta_3}{m_t^2} + \dfrac{\sin^2\theta_3}{m_l m_t} \end{cases} \rightarrow m_l, m_t, m_t$$

The Phenomenological current equations

$$\begin{cases} J_i = \sigma_{ij}(\vec{B})\,\mathcal{E}_j + B_{ij}(\vec{B})\,\partial_j(1/T_L) \\ J_{\varphi_i} = \underbrace{p_{ij}}_{}(\vec{B})\,\mathcal{E}_j + K_{ij}(\vec{B})\,\partial_j(1/T_L) \end{cases}$$

$$\downarrow$$

$$\partial_j F_{n/q} = \mathcal{E}_j \quad \text{when } n(r) \text{ is constant.}$$

These equations are valid regardless of RTA and simplifications. However, the matrices of coefficients depends on the approximations such as RTA, etc.

Inversion of the equations

We often like to send a current to the material/device and measure the voltage. So we prefer the following shape for the equations:

$$\begin{cases} \mathcal{E}_j = \overset{\text{resistivity}}{\rho_{jk}}\, J_k + \overset{\text{Seebeck coefficient (TE power)}}{\alpha_{jk}}\, \partial_k T_L \\ J_{\varphi_j} = \underset{\text{Peltier Coefficient}}{\pi_{jk}}\, J_k - \underset{\text{Thermal Conductivity}}{K_{jk}}\, \partial_k T_L \end{cases}$$

To find these coefficients:

$$\vec{J} = [\sigma]\vec{\mathcal{E}} + [B]\vec{\nabla}_r\left(\frac{1}{T}\right) = [\sigma]\vec{\mathcal{E}} - \frac{[B]}{T^2}\vec{\nabla}_r T$$

$$\Rightarrow \quad \vec{\mathcal{E}} = \underbrace{[\sigma]^{-1}}_{[\rho]}\vec{J} + \underbrace{\frac{[\sigma]^{-1}[B]}{T^2}}_{[\alpha]}\vec{\nabla}_r T$$

Similarly for $[\pi]$ and $[K]$:

$$\begin{cases} [\rho] = [\sigma]^{-1} \\ [\alpha] = \dfrac{[\sigma]^{-1}[B]}{T^2} \\ [\pi] = [p][\rho] \\ [K] = \dfrac{1}{T^2}\left\{[K] - [p][\rho][B]\right\} \end{cases}$$

Taylor series of transport tensors:

It is difficult to work with arbitrary $\vec{B}$. We may expand the equations to approximate for weak or moderate $\vec{B}$:

If $\nabla_r T = 0 \rightarrow \quad \mathcal{E}_i = \rho_{ij}(\vec{B}) J_j$ (B_k, B_l are like B_x, B_y)

Sum over k   Sum over k and l

$$\rho_{ij}(\vec{B}) = \underbrace{\rho_{ij}(0)}_{\rho_{ij}} + \underbrace{\left.\frac{\partial \rho_{ij}}{\partial B_k}\right|_{B=0}}_{\rho_{ijk}} B_k + \underbrace{\frac{1}{2}\left.\frac{\partial^2 \rho_{ij}}{\partial B_k \partial B_l}\right|_{B=0}}_{\rho_{ijkl}} B_k B_l + \cdots = \rho_{ij} + \rho_{ijk} B_k + \rho_{ijkl} B_k B_l + \cdots$$

$$\Rightarrow \quad \boxed{\mathcal{E}_i = \rho_{ij} J_j + \rho_{ijk} B_k J_j + \rho_{ijkl} B_k B_l J_j + \cdots}$$

electrical conduction   Hall effect   magnetoresistance

Other transport coefficient can be expanded similarly.

For Cubic Semiconductors like Si, GaAs:

From the crystal symmetry we can find which elements in the matrices are zero or are equal.

for $\vec{B} = 0$, $[\sigma]$ is diagonal: $\sigma_{ij} = \sigma_0 \delta_{ij}$ or $\rho_{ij} = \rho_0 \delta_{ij}$ $\quad \rho_0 = \frac{1}{\sigma_0}$

To find $\rho_{ijk} = \left.\frac{\partial \rho_{ij}}{\partial B_k}\right|_{B=0} B_k$ $\quad [\rho] = [\sigma]^{-1} = \begin{bmatrix} 1 & -\mu_H B_z & \mu_H B_y \\ \mu_H B_z & 1 & -\mu_H B_x \\ -\mu_H B_z & \mu_H B_x & 1 \end{bmatrix}^{-1} \Rightarrow \frac{\partial \rho_{ij}}{\partial B_k} \cdots$

alternating unit tensor   recall magnetoconductivity tensor

The result is: $\rho_{ijk} = \rho_0 \mu_H \underset{\sim}{\varepsilon_{ijk}}$

To find ρ_{ijkl}, we must work with the magnetoconductivity tensor valid to 2^{nd} order in $\vec{B}$.

For cubic semiconductor, only a few of the 81 terms of this tensor are non-zero:

ρ_{ijkl} tensor $\rightarrow$ $3\times3\times3\times3 = 81$ elements

non-zero terms: $\rho_{\alpha\alpha\alpha\alpha}$, $\rho_{\alpha\alpha\beta\beta}$, $\rho_{\alpha\beta\alpha\beta} = \rho_{\alpha\beta\beta\alpha}$ (no sum over Greek letters)

$\rightarrow$ For Cubic Semiconductor: $\boxed{\mathcal{E}_i = \rho_0 J_i + \rho_0 \mu_H \varepsilon_{ijk} J_j B_k + \rho_{ijkl} J_j B_k B_l + \cdots}$

other transport tensors are similar. for example: $\kappa_{ij} = \kappa_0 \delta_{ij}$ $\quad \kappa_{ijk} = \kappa_1 \varepsilon_{ijk}$

$\kappa_{ijkl} \neq 0$ when $\rho_{ijkl} \neq 0$

We can find for non-degenerate $n < N_c$ + spherical + parabolic band + RTA:

$$\begin{cases} \rho_0 = \dfrac{1}{\sigma_0} = \dfrac{1}{q n \mu_n} \\ \alpha_0 = \dfrac{\rho_0 B_0}{T^2} = \overbrace{\dfrac{k_B}{-q}}^{86\,\mu V/K} \left[\ln\left(\dfrac{N_c}{n}\right) + \left(s + \dfrac{5}{2}\right)\right] \\ \Pi_0 = \alpha_0 T \quad \text{Kelvin relation. Generally true.} \\ \kappa_0 = T \left(\dfrac{k_B}{q}\right)^2 \left(s + \dfrac{5}{2}\right) \sigma_0 \quad \text{electronic part of thermal conduction} \end{cases}$$

$$N_c = 2\left(\frac{2\pi m^* k_B T}{h^2}\right)^{3/2}$$

Applications:

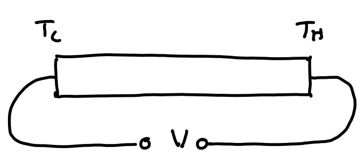
Thermoelectric: $\vec{\nabla} T + \vec{\mathcal{E}}$

Thermomagnetic: $\vec{\nabla} T + \vec{B}$

Galvanomagnetic: $\vec{\mathcal{E}} + \vec{B}$

Thermoelectric Effect:

① Seebeck effect:



$B = 0$

$j_x = 0$

$\Delta T \Rightarrow V$

$$\mathcal{E}_j = \rho_{jk} J_k + \alpha_{jk} \partial_k T \qquad \begin{cases} J_x = J_y = J_z = 0 \\ \partial_y T = \partial_z T = 0 \end{cases} \Rightarrow \qquad \mathcal{E}_x = \alpha_{xx} \partial_x T = \alpha_{xx} \frac{dT}{dx}$$

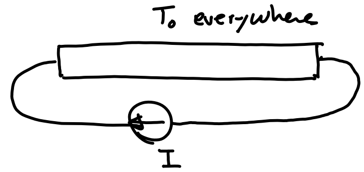
diagonal element of $[\alpha]$

$$\rightarrow \quad \mathcal{E}_x = \alpha_0 \frac{T_H - T_c}{L} \rightarrow \underbrace{\mathcal{E}_x L}_{-V} = \alpha_0 \underbrace{(T_H - T_c)}_{\Delta T} \Rightarrow V = -\alpha_0 \Delta T$$

$$\begin{cases} \text{n-Type} : \alpha < 0 \\ \text{p-Type} : \alpha > 0 \end{cases}$$

② Peltier Effect:

$$J_{\varphi j} = \pi_{jk} J_k - \kappa_{jk} \partial_k T$$

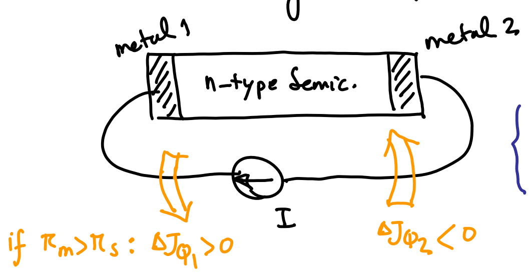


$$\Rightarrow \partial_k T = 0 \Rightarrow$$

$$J_{\varphi x} = \pi_{xx} J_x = \pi_0 J_x$$

diagonal element of $[\pi]$

Considering the effect of contacts: metal : π_m Semiconductor : π_s



$$\begin{cases} \Delta J_{\varphi_1} = J_{\varphi_{in}} - J_{\varphi_{out}} = \pi_m J_x - \pi_s J_x = (\pi_m - \pi_s) J_x \\ \Delta J_{\varphi_2} = J_{\varphi_{in}} - J_{\varphi_{out}} = (\pi_s - \pi_m) J_x \end{cases}$$

Transport Coefficient for Isotropic Material at small field & B=0 :

$$\vec{\mathcal{E}} = \rho \vec{J} + S \vec{\nabla} T \Rightarrow \vec{J} = \overbrace{\frac{1}{\rho}}^{\sigma} \vec{\mathcal{E}} - \frac{S}{\rho} \vec{\nabla} T = \sigma \vec{\mathcal{E}} - S\sigma \vec{\nabla} T$$

$$\begin{cases} \vec{J} = \sigma \vec{\mathcal{E}} - S \sigma \vec{\nabla} T \\ \vec{J}_\varphi = \pi \vec{J} - \kappa \vec{\nabla} T \end{cases}$$

$$\sigma = \frac{2e^2}{3m^*}\int_0^\infty E\tau\left(-\frac{\partial f}{\partial E}\right) g(E)\, dE$$

$$S = \frac{1}{eT}\,\frac{\int_0^\infty E\tau\,(E-E_f)\left(-\frac{\partial f}{\partial E}\right) g(E)\,dE}{\int_0^\infty E\tau\left(-\frac{\partial f}{\partial E}\right) g(E)\,dE}$$

$$K_e = \frac{2}{3m^*T}\left\{\frac{\left[\int_0^\infty E^2\tau\left(-\frac{\partial f}{\partial E}\right) g(E)\,dE\right]^2}{\int_0^\infty \tau\left(-\frac{\partial f}{\partial E}\right) g(E)\,dE} - \int_0^\infty E^3\tau\left(-\frac{\partial f}{\partial E}\right) g(E)\,dE\right\}$$

$$K = K_e + K_L + K_b$$

K_e: electronic part; K_L: lattice part; K_b: bipolar part

It is convenient to define:

$$K_s = -\frac{2T}{3m^*}\int_0^\infty E^{s+1}\tau\,\frac{\partial f}{\partial E}\, g(E)\,dE$$

$$\begin{cases} \sigma = \dfrac{e^2}{T} K_1 \\[2ex] S = \dfrac{1}{eT}\left(E_f - \dfrac{K_1}{K_0}\right) \\[2ex] K_e = \dfrac{1}{T^2}\left(K_2 - \dfrac{K_1^2}{K_0}\right) \end{cases}$$

Multiband equations:

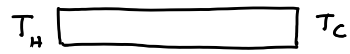
$$\sigma = \sum_i \sigma_i$$

$$S = \frac{\sum_i \sigma_i S_i}{\sum_i \sigma_i}$$

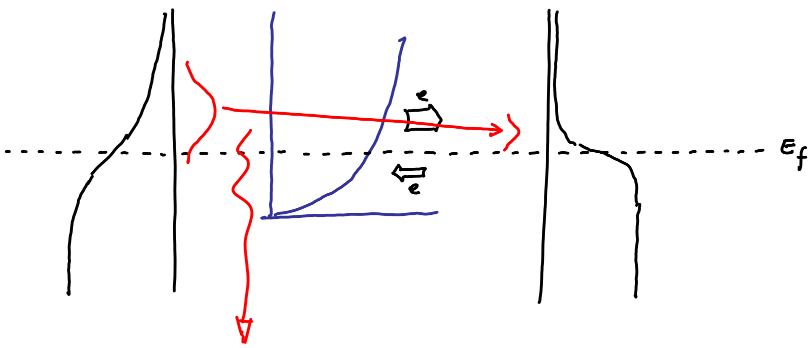
$$K_e = \sum K_{e_i}$$

Pictorial descriptions:

Power Generation: Seebeck coefficient



n-type

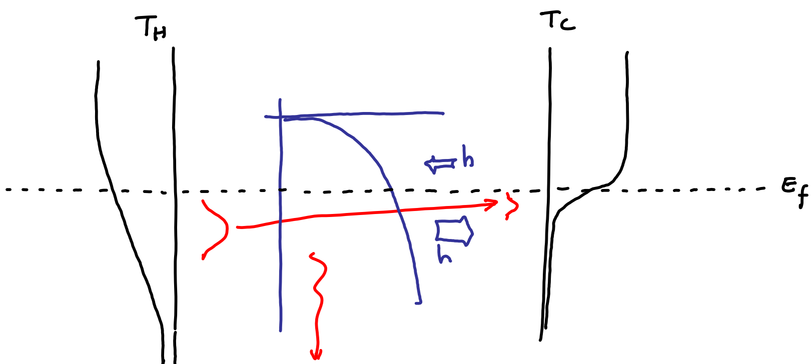


n-type:

ⓔ flow from T_H to T_C

Extra energy is given to the lattice heating it up → Thomson effect in power generation

P-type:



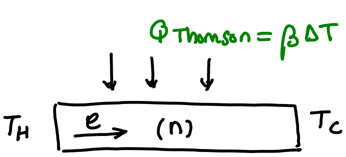
P-type:

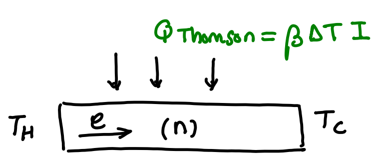
ⓗ from T_H to T_C

Extra energy is given to the lattice → Thomson effect

So in power generation, majority charge carriers always move from T_H to T_C.
In n-type this is ⓔ and in p-type ⓗ.

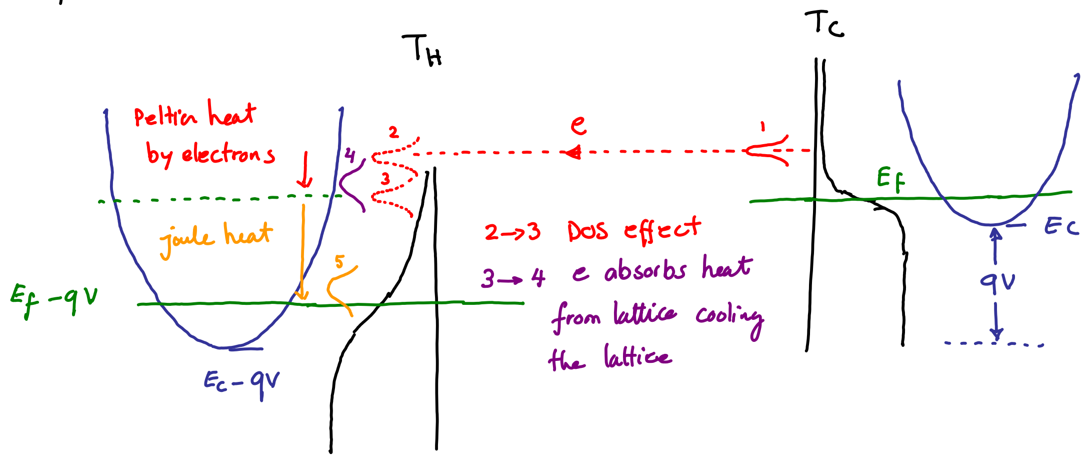
Thomson Coefficient: $\beta = T \frac{dS}{dT}$ (same unit as Seebeck $\frac{V}{K}$)

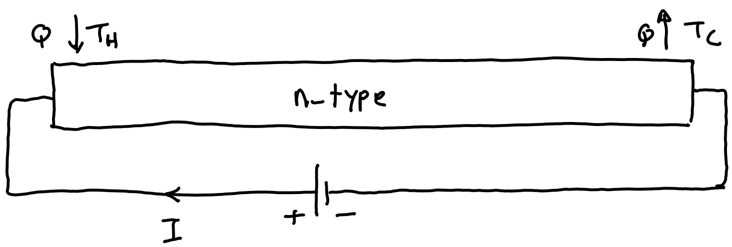




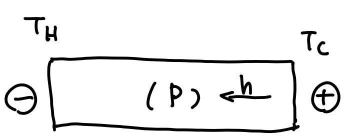
Cooling :

n-type:





P-type:

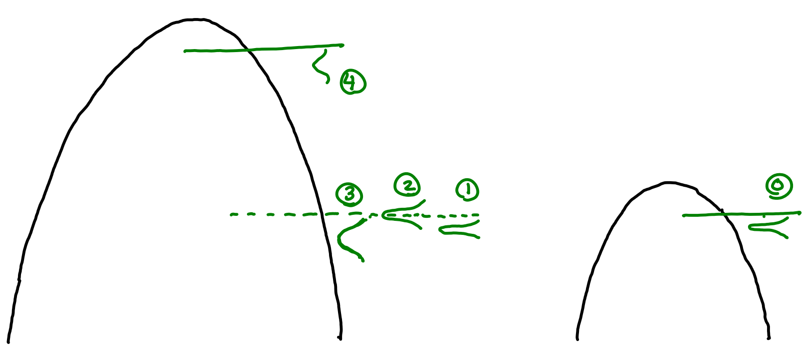


0→1: transport

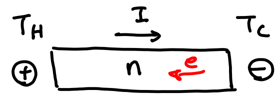
1→2: DOS effet => release heat

2→3: broaden the distribution due to T_H => shift the energy => absorb heat from lattice (Thomson effect)

3→4: joule heating

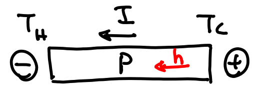


n type:



e from $T_c \to T_H$

p type:

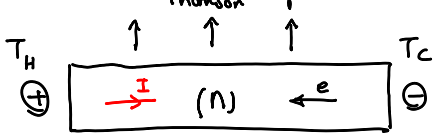


h from $T_c \to T_H$

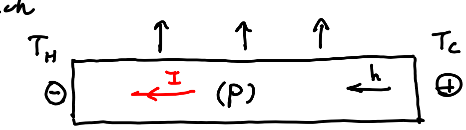
} for cooling, majority charge carriers flow from $T_c \to T_H$

Thomson effect in Peltier Cooling:

$\varphi_{Thomson} = \overset{\ominus}{\beta} \Delta T I < 0$ for majority carrier Seebeck

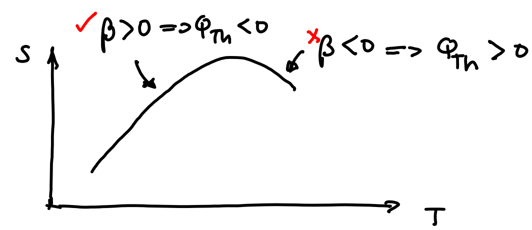


$\varphi_{Thomson} = -\overset{\oplus}{\beta} \Delta T I < 0$ for majority carrier Seebeck



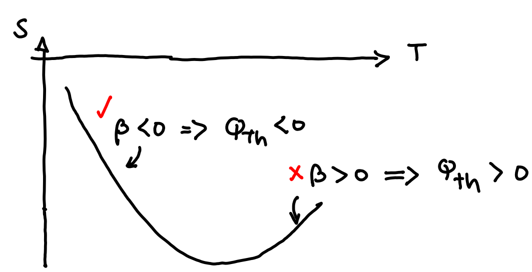
p-type

$$\beta = T \frac{dS}{dT}$$



n-type

$$\beta = T \frac{dS}{dT}$$



Thomson heat like joule heating dissipates in all of the device. But peltier heat is at interface.

ZT :

$$\eta = \underbrace{\left(1 - \frac{T_C}{T_H}\right)}^{\text{Carnot efficiency}} \frac{M-1}{M + \frac{T_C}{T_H}} \qquad M = \sqrt{1+\bar{T}} \qquad \bar{T} = \frac{T_C + T_H}{2}$$

$$ZT = \frac{S^2 \sigma}{\kappa} T$$

Thomson effect on ZT:

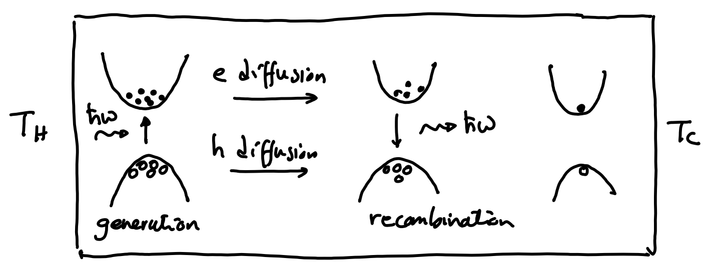
Cooling : $\frac{\left(S_H + \frac{1}{2}\beta \frac{\Delta T}{T_H}\right)^2 \sigma}{\kappa}$ As carriers move from $T_C \to T_H$, they carry heat & absorb heat

Generation : $\frac{\left(S_H - \frac{1}{2}\beta \frac{\Delta T}{T_H}\right)^2 \sigma}{\kappa}$ As carriers move from $T_H \to T_C$, they dissipate heat

$\beta \simeq 129\ \mu V/K$ for non-deg model.

For Bi_2Te_3 : $\beta \simeq 60-80\ \mu V/K$ usually small as TE's are highly doped.

Bipolar thermal Conduction (Ambipolar diffusion):



$$\boxed{\kappa_b = \frac{\sigma_1 \sigma_2}{\sigma_1 + \sigma_2} (S_1 - S_2)^2 T}$$

Thermomagnetic Effect

At presence of ΔT and B there are several different effects.

$$\mathcal{E}_i = \rho_{ik} J_k + \alpha_{ik} \partial_k T$$

At presence of B, expand to 2^{nd} order in $\vec{B}$:

Assume isotropic and $\vec{B} = B\hat{z}$:

$$\mathcal{E}_i = \rho_0 J_i + \rho_0 \mu_H \epsilon_{ijk} J_j B_k + \rho_{ijk} J_j B_k B_\ell + \alpha_0 \partial_i T + \overbrace{\alpha_{ijk}}^{=\alpha_1 \epsilon_{ijk}} \partial_j T_L B_k + \alpha_{ijk\ell} \partial_j T B_k B_\ell$$

If $J_i = 0$ and $\partial T/\partial y = 0 \Rightarrow$

$$\mathcal{E}_x = \alpha_0 \partial_x T + \alpha_1 \overbrace{\epsilon_{xxz}}^{=0} \partial_x T B_z + \alpha_{xxzz} \partial_x T B_z^2$$

$$\mathcal{E}_x = (\alpha_0 + \alpha_{xxzz} B_z^2) \frac{\partial T}{\partial x} \quad \rightarrow \quad \Delta\alpha = \alpha(B) - \alpha(0) = \alpha_{xxzz} B_z^2$$ magneto Seebeck effect

Other Thermomagnetic effects are: Nernst, Ettingshaussen, Righi-Leduc effects.

Nernst effect: no current flow $J = 0$

$\vec{B} = B\hat{z}$ & x-directed T gradient: $\mathcal{E}_i = \alpha_0 \partial_j T_L + \alpha_1 \epsilon_{ijz} \partial_j T B_z + \alpha_{ijzz} \partial_j T B_z^2$

For $i = x \Rightarrow$ magneto-Seebeck effect. Also, there is a $\hat{y}$-directed $\mathcal{E}_y$:

$$\mathcal{E}_y = -\alpha_1 B_z \frac{\partial T}{\partial x}$$

appearance an electric field normal to both the temperature gradient & B $\rightarrow$ Nernst effect.

This happens as the carriers that diffuse down ∇T are deflected by B.

$$\alpha_1 = |N| = \frac{-\mathcal{E}_y}{B_z \, dT/dx} = \frac{dv/dy}{B_z \, dT/dx}$$

Sign of N does not depend on e or h. This differs from S or the Hall effect. In Hall, we also have $\vec{\mathcal{E}} \perp \vec{B}$ which is caused by current flow. But in Nernst $\vec{\mathcal{E}} \perp \vec{B}$ is caused by carrier diffusion due to ∇T.

Ettingshausen Effect: $\vec{\nabla} T \perp \vec{B}$ is generated due to flow of current $\vec{J} \perp \vec{B}$:

Ettingshaussen Coefficient : $|P| = \dfrac{dT/dy}{i_x B_z}$

There is a thermodynamic relation between P and N:

$$P\kappa = NT$$

κ ↓ thermal conductivity

Righi-Leduc effect: (rē·gē lə´ dük)

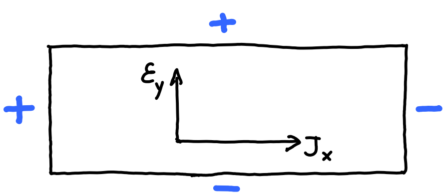
(Thermal Hall Effect)

A transverse temperature gradient caused from flow of longitudinal heat flow : $J_\varphi \Rightarrow \nabla T \perp B$

$$|R| = \frac{dT/dy}{B_z\, dT/dx}$$

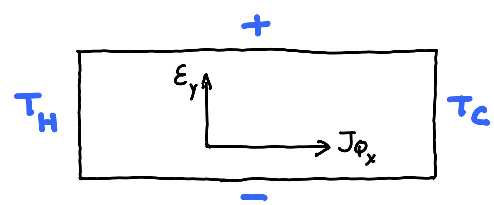
measurement of thermal conductivity in magnetic field is used to distinguish between the electronic & lattice thermal conductivity.

Hall :

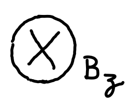


$$R_H = \frac{\mathcal{E}_y}{B_z J_x}$$

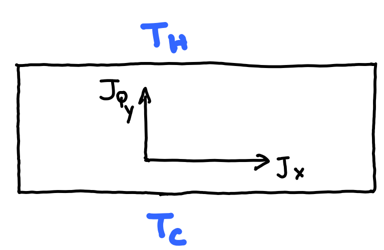
Nernst:



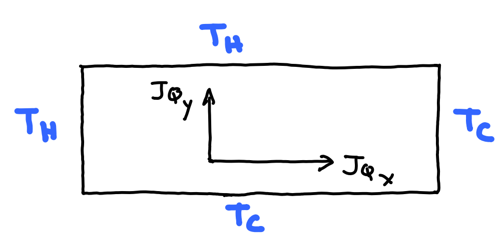
$$|N| = \frac{\mathcal{E}_y}{B_z\, dT/dx}$$



Ettingshaussen:



Righi-Leduc:



$$|P| = \frac{dT/dy}{B_z J_x}$$

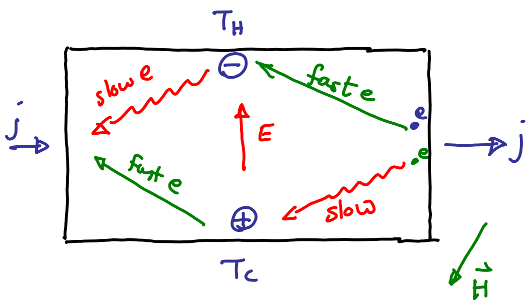
$$|P| = -\frac{\pi_1}{k_0} \rightarrow \pi_1 = -k_0 |P|$$

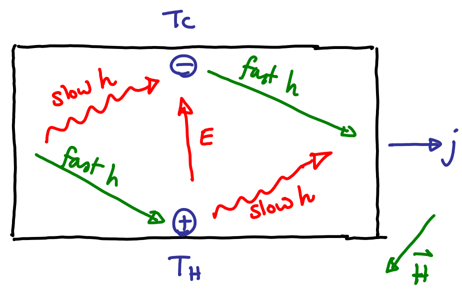
$$|R| = \frac{dT/dy}{B_z\, dT/dx}$$

when the effects are in the direction shown, the coefficients are ⊕ .

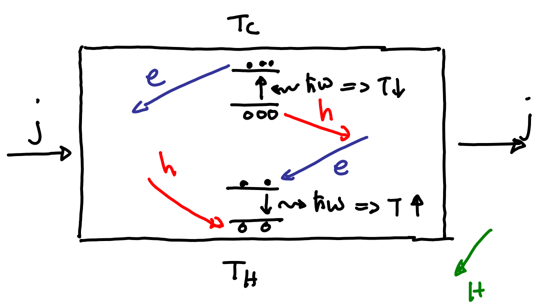
Ettingshaussen Effects:

Extrinsic:





Intrinsic:

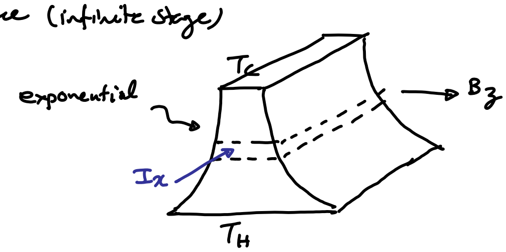


Ettingshausen vs. TE:

1) One material is sufficient

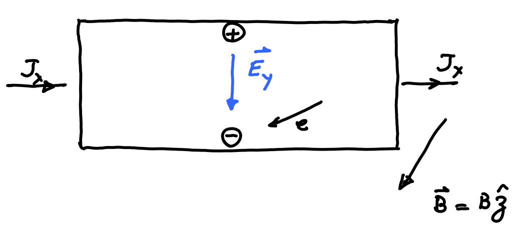
2) ΔT is normal to j. So current cross section can be small, but area for temperature can be large

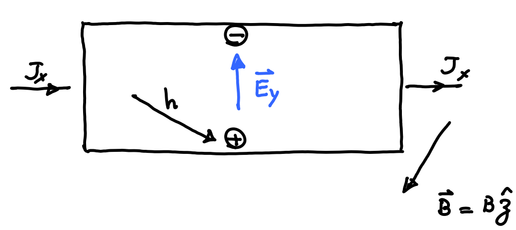
3) Cascade structure (infinite stage)



Galvanomagnetic Effects:

The best-known galvanomagnetic effect is the Hall Effect:





$\pi_1 = -k_0 |P| \qquad |P| = \frac{dT/dy}{J_x B_z}$

If isothermal and $\vec{J} = J_x \hat{x}$, $\vec{B} = B_z \hat{z}$

$$\mathcal{E}_i = \rho_0 J_i + \rho_0 \mu_H \epsilon_{ijk} J_j B_k + \rho_{ijkl} J_j B_k B_l + \underbrace{\alpha_0 \partial_i T + \alpha_1 \epsilon_{ijk} \partial_j T B_k + \alpha_{ijkl} \partial_j T B_k B_l}_{=0}$$

$$i=y \Rightarrow \quad \mathcal{E}_y = \overbrace{\rho_0 J_y}^{=0} + \rho_0 \mu_H \Big[\overbrace{\epsilon_{yxz}}^{-1} J_x B_z + \overbrace{\epsilon_{yzx} J_z B_x}^{=0} \Big] + \rho_{xxkl} \overbrace{J_x}^{=0} B_k B_l = -\rho_0 \mu_H J_x B_z$$

$$\Rightarrow \quad \boxed{-\rho_0 \mu_H = \frac{\mathcal{E}_y}{J_x B_z} \equiv R_H}$$

Hall Coefficient — we measure $\mathcal{E}_y$, J_x, B_z and calculate $-\rho_0 \mu_H$ from them $\Rightarrow n$

r_H Hall factor (1 to 2)

$$R_H = -\rho_0 \mu_H = -\frac{\mu_H}{qn\mu} = -\frac{r_H}{qn} \qquad \boxed{R_H = \frac{r_H}{-qn}} = \frac{\mathcal{E}_y}{J_x B_z}$$

r_H depends on the scattering rate. $\qquad R_H \Rightarrow n = \frac{r_H}{-qR_H}$ $\qquad$ also sign of $R_H \Rightarrow$ type (p or n)

We assumed isothermal. Experimentally, adiabatic condition (no heat in & out) may be easier to achieve. In this case:

$$J_{Q_i} = \pi_{ij}(\vec{B})\, \mathcal{E}_j + k_{ij}(\vec{B})\, \partial_j\left(\frac{1}{T}\right)$$ expand versus $\vec{B}$ similar to $\mathcal{E}_i \Rightarrow$

adiabatic

$$\underbrace{J_{Q_y}}_{=0} = \underbrace{\pi_{yx}}_{=0 \text{ diagonal}} J_x + \overbrace{\pi_{yxz}}^{\pi_1 \epsilon_{yxz}} J_x B_z - \overbrace{k_{yj}}^{k_0 \partial_y T} \partial_j T - \overbrace{k_{yjz}}^{k_1 \epsilon_{yxz}} \underbrace{\partial_j T}_{\partial_x T = 0} B_z$$ assume no $\partial_x T$

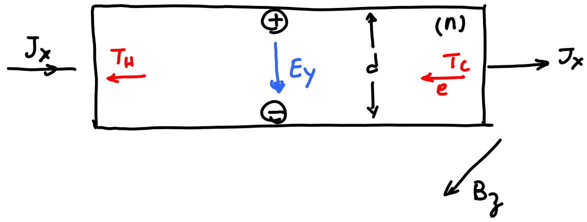
$|P| = \frac{\pi_1}{k_0}$ Ettingshausen

$$\Rightarrow \quad -\pi_1 J_x B_z - k_0 \partial_y T = 0 \Rightarrow \frac{\partial T}{\partial y} = -\frac{\pi_1}{k_0} J_x B_z$$ This $\frac{\partial T}{\partial y}$ produces a Seebeck voltage:

$$\Rightarrow \quad \mathcal{E}_y = \overbrace{-\rho_0 \mu_H J_x B_z}^{\text{Galvanomagnetic}} - \frac{\alpha_0 \pi_1}{k_0} J_x B_z = \left(-\rho_0 \mu_H - \frac{\alpha_0 \pi_1}{k_0}\right) J_x B_z \Rightarrow \boxed{R_H^Q = -\rho_0 \mu_H - \frac{\alpha_0 \pi_1}{k_0}}$$

In experiment it is difficult to know if isothermal or adiabatic condition exists and there is always an uncertainty in most measurements.

Thermomagnetic effect can also generate a voltage. For example if $\frac{\partial T}{\partial x} \neq 0$ perhaps due to heating caused by the Peltier effect associated with J_x:



$\Delta T = T_H - T_c \Rightarrow \mathcal{E}_{y_N} = -N\, B_z \dfrac{\partial T}{\partial x}$

$\Rightarrow \mathcal{E}_y = \mathcal{E}_{y_H} + \mathcal{E}_{y_N} = -\rho_0 \mu_H J_x B_z - N \dfrac{\partial T}{\partial x} B_z$

If $\vec{B}$ and $\vec{J}$ are reversed, $\mathcal{E}_{y_H}$ doesn't change sign: $\mathcal{E}_{y_H} = -\rho_0 \mu_H (-J_x)(-B_z)$ but $\mathcal{E}_{y_N}$ does: $\mathcal{E}_{y_N} = -N \dfrac{\partial T}{\partial x}(-B_z)$

assuming that the change is quick so $\dfrac{\partial T}{\partial x}$ doesn't change. So by averaging the two, we get $\mathcal{E}_{y_H}$.

Righi–Leduc & Ettingshausen effects can also affect the data. By reversing $\vec{J}$ & $\vec{B}$ we may eliminate Righi–Leduc effect, but it is impossible to eliminate Ettingshausen effect:

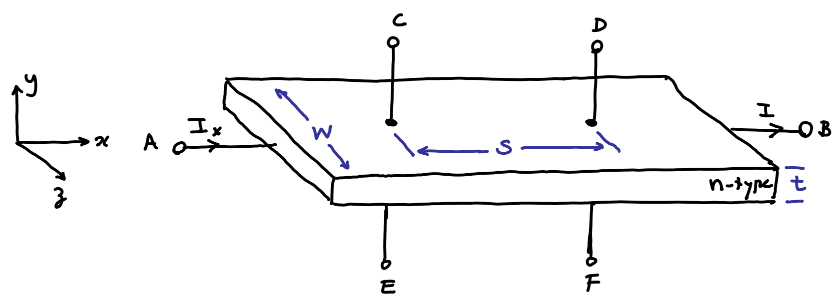
Ettingshausen: $\dfrac{\partial T}{\partial y} = -P J_x B_z = -P(-J_x)(-B_z)$

Righi–Leduc: $\dfrac{\partial T}{\partial y} = R \dfrac{\partial T}{\partial x} B_z = -R \dfrac{\partial T}{\partial x}(-B_z)$

Measurement of carrier concentration and mobility:

$-R_H = \rho_0 \mu_H = \dfrac{-\mathcal{E}_y}{B_z J_x} = \dfrac{+V_{CE}/t}{B_z I_x / wt} = \dfrac{w}{B_z} \dfrac{V_{CE}}{I_x}$

$\dfrac{r_H}{qn} = \dfrac{w}{B_z} \dfrac{V_{CE}}{I_x} \Rightarrow n = r_H \dfrac{B_z I_x}{q w V_{CE}}$



To find the mobility, we need to measure the resistivity:

$R = \dfrac{V_{CD}}{I} = \rho_0 \dfrac{s}{wt} \rightarrow \rho_0 = \dfrac{wt}{s} \dfrac{V_{CD}}{I} = \dfrac{1}{en\mu}$

we also had: $n = r_H \dfrac{B_z I}{q w V_{CE}}$

$$\mu = \frac{1}{r_H} \frac{s}{t B_z} \frac{V_{CE}}{V_{CD}}$$

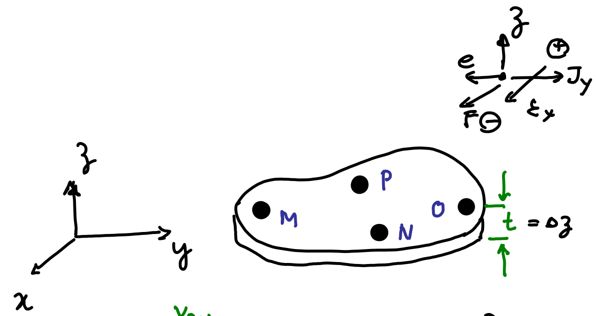
$\rightarrow$ we need to know r_H to find μ and n accurately.

So it is commonly taken $r_H = 1$ when reporting experimental results. So the actual μ is smaller than the reported μ_H by a factor of r_H. But actual n is larger: $\begin{cases} \mu < \mu_H \\ n > n_H \end{cases}$

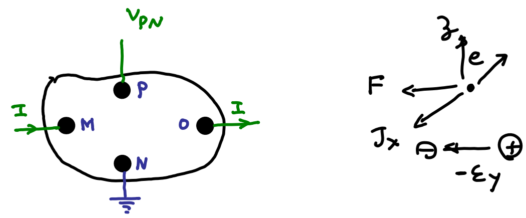
Van der Pauw method

Carrier Concentration:

For a general geometry:



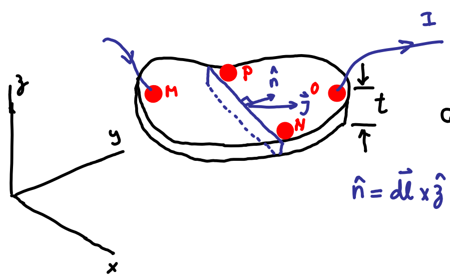
$$\begin{cases} \mathcal{E}_x = \rho_0 J_x + \rho_0 \mu_H B_z J_y \\ \mathcal{E}_y = -(\rho_0 \mu_H B_z) J_x + \rho_0 J_y \end{cases} \Rightarrow V_{PN} = ?$$



$$V_{PN}(B_z) = -\int_N^P \vec{\mathcal{E}}\cdot d\vec{l} = -\int_N^P \mathcal{E}_x dx + \mathcal{E}_y dy = -\int_{x_N}^{x_P} \mathcal{E}_x dx - \int_{y_N}^{y_P} \mathcal{E}_y dy = -\rho_0\int_{x_N}^{x_P} J_x dx - \rho_0 \mu_H B_z \int_{x_N}^{x_P} J_y dx + \rho_0 \mu_H B_z \int_{y_N}^{y_P} J_x dy - \rho_0 \int_{y_N}^{y_P} J_y dy$$

$$V_{PN}(-B_z) = -\rho_0\int_{x_N}^{x_P} J_x dx + \rho_0 \mu_H B_z \int_{x_N}^{x_P} J_y dx - \rho_0 \mu_H B_z \int_{y_N}^{y_P} J_x dy - \rho_0 \int_{y_N}^{y_P} J_y dy$$

Defining $V_H = \frac{1}{2}\left[V_{PN}(B_z) - V_{PN}(-B_z)\right] = \rho_0 \mu_H B_z \underbrace{\left[\int_{y_N}^{y_P} J_y dy - \int_{x_N}^{x_P} J_x dx\right]}_{I/t}$ which can be measured.



Conservation of current: $I = \int_N^P \vec{J}\cdot\hat{n}\, t\, dl = t\left(\int_{x_N}^{x_P} J_y dx - \int_{y_N}^{y_P} J_x dy\right)$

$\hat{n} = d\vec{l} \times \hat{z} = (dx\hat{x} + dy\hat{y})\times\hat{z} = -dx\hat{y} + dy\hat{x}$

$$V_H = \rho_0 \mu_H B_z \frac{I}{t} = \frac{\mu_H}{qn\mu} B_z \frac{I}{t} = \frac{r_H}{q\underbrace{nt}_{n_s}} B_z I$$

n_s sheet carrier density (cm^{-2})

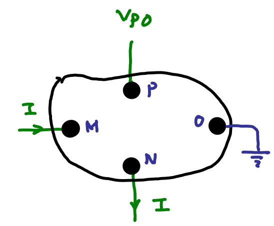
So the Hall measurement can give the sheet carrier density:

$$\boxed{V_H = \frac{r_H}{q n_s} B_z I} \qquad \text{where } n_s = \int_0^t n(z)\, dz$$

The location of the contacts doesn't need to be precise, but they should be small & on the boundary.

Mobility:

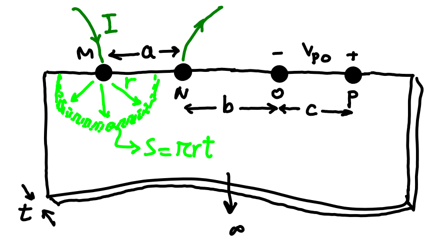
we must measure the resistivity to find the mobility. The measurement contacts are shown:



$$R_{MN,OP} = \frac{V_{PO}}{I}$$ how is this related to the resistivity?

It is easier to consider an infinite half-plane geometry: →

we will see the result is similar.



The current spreads radially into the film as: $J_r = \dfrac{I}{\pi r t} \rightarrow \mathcal{E}_r = \rho_o J_r = \dfrac{\rho_o I}{\pi r t}$

So the potential difference between any two radial distances is: $V(r) - V(r_o) = -\displaystyle\int_{r_o}^{r} \frac{\rho_o I}{\pi t r} = -\frac{\rho_o I}{\pi t} \ln \frac{r}{r_o}$

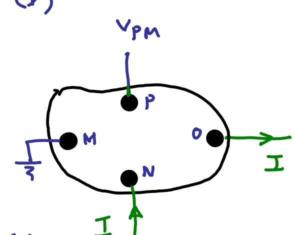
$$\Rightarrow \quad V_{PO}^{in} = V(P) - V(O) = -\frac{\rho_o I}{\pi t} \ln\left(\frac{a+b+c}{a+b}\right)$$ This is potential due to current flowing in at M.

There is another contribution with opposite sign due to current flowing out at contact N:

$$V_{PO}^{out} = +\frac{\rho_o I}{\pi t} \ln\left(\frac{b+c}{b}\right) \Rightarrow \quad V_{PO} = V_{PO}^{in} + V_{PO}^{out} = \frac{\rho_o I}{\pi t} \ln \frac{(a+b)(b+c)}{b(a+b+c)}$$

$$\Rightarrow \quad R_{MN,OP} = \frac{V_{PO}}{I_{MN}} = \frac{\rho_o}{\pi t} \ln \frac{(a+b)(b+c)}{b(a+b+c)} \rightarrow e^{-\frac{\pi t}{\rho_o} R_{MN,OP}} = \frac{b(a+b+c)}{(a+b)(b+c)} \quad (I)$$

Another resistance can be measured by I_{NO} and V_{PM}:



$$R_{NO,PM} = \frac{\rho_o}{\pi t} \ln \frac{(a+b)(b+c)}{ac} \rightarrow e^{-\frac{\pi t}{\rho_o} R_{NO,PM}} = \frac{ac}{(a+b)(b+c)} \quad (II)$$

$$(I), (II) \Rightarrow \quad e^{-\frac{\pi t}{\rho_o} R_{NO,PM}} + e^{-\frac{\pi t}{\rho_o} R_{MN,OP}} = \frac{ac + b(a+b+c)}{(a+b)(b+c)} = 1$$

Define $\boxed{R_S \equiv \frac{\rho_o}{t} \ (\Omega) \quad \text{sheet resistance}}$

$$\boxed{e^{-\pi \frac{R_{NO,PM}}{R_S}} + e^{-\pi \frac{R_{MN,OP}}{R_S}} = 1}$$

⇒ R_S can be solved numerically

With conformal mapping technique, we can map most geometries onto the infinite half-plane.

van der Pauw showed that the conditions for this mapping are:

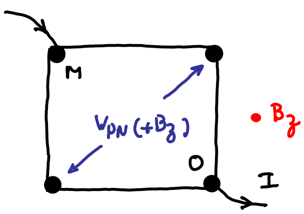
1) $\nabla \cdot J = \nabla \times J = 0$

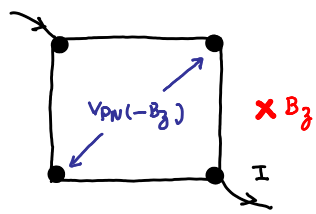
2) The region is simply-connected (i.e. no holes)

3) The region is homogeneous, isotropic, and of uniform thickness

4) The contacts are at the perimeter and are point contacts.

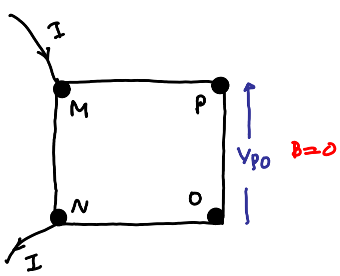
Sumary for van der Pauw method:

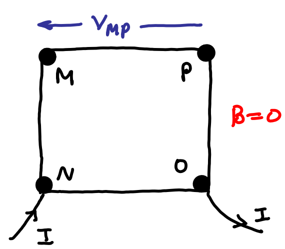




Measure: $V_H = \frac{1}{2}\left[V_{PN}(+B_z) - V_{PN}(-B_z)\right]$

Calculate n_s from: $V_H = \frac{r_H}{q n_s} B_z I$; $n = \frac{n_s}{t}$





Measure $R_{MN,OP} = \frac{V_{PO}}{I}$ and $R_{NO,PM} = \frac{V_{MP}}{I}$

Calculate R_s from: $e^{-\frac{\pi}{R_s} R_{MN,OP}} + e^{-\frac{\pi}{R_s} R_{NO,PM}} = 1$; $R_s = \frac{\rho_0}{t}$

Finally calculate μ_H from V_H and R_s : $\boxed{\mu_H = r_H \mu = \frac{V_H}{I R_s B_z}}$

Hydrodynamic Equations

- Simpler approach than BTE, less accurate than BTE
- More accurate than Drift & diffusion
- Gives the velocity overshoot that is not possible to get from D.D.
- Consists of balance equations for particle numbers, momentum and energy (two equ. for energy
- Drif-diffusion equ is only simplified form of the momentum balance equation

We can find the average value of a quantity that depends on momentum by $\Phi(p)$ by:

$$n_\phi \equiv \frac{1}{\Omega} \sum_p \phi(p) f(r,p,t)$$

Balance Equ. for n_ϕ:

BTE: $$\frac{\partial f}{\partial t} + \vec{v}\cdot\vec{\nabla}_r f + (-q)\,\vec{\mathcal{E}}\cdot\vec{\nabla}_p f = \Gamma(r,p,t) + \frac{\partial f}{\partial t}\Big|_{col}$$

does not depend on t

$$\times \frac{1}{\Omega}\sum_p \phi(\vec{p}) \Rightarrow \underbrace{\frac{1}{\Omega}\sum_p \phi(p)\frac{\partial f}{\partial t}}_{=\frac{\partial}{\partial t}\frac{1}{\Omega}\sum_p \phi f = \frac{\partial n_\phi}{\partial t}} + \underbrace{\frac{1}{\Omega}\sum_p \phi(p)\vec{v}\cdot\vec{\nabla}_r f}_{\vec{\nabla}\cdot \underbrace{\frac{1}{\Omega}\sum_p \phi\vec{v} f}_{F_\phi:\ \text{Flux}} = \vec{\nabla}\cdot\vec{F}_\phi} + \underbrace{\frac{1}{\Omega}\sum_p \phi(p)(-q)\,\vec{\mathcal{E}}\cdot\vec{\nabla}_p f}_{-q\vec{\mathcal{E}}\cdot\sum_p \phi(p)\vec{\nabla}_p f}$$

$$-q\vec{\mathcal{E}}\cdot\sum_p \phi(p)\vec{\nabla}_p f = \underbrace{-q\vec{\mathcal{E}}\cdot\sum_p \vec{\nabla}_p(\phi f)}_{\simeq 0} - \underbrace{(-q)\,\vec{\mathcal{E}}\cdot\sum_p f\vec{\nabla}_p\phi}_{\Omega G_\phi \;\equiv\; \text{generation rate}}$$

$$= \underbrace{\frac{1}{\Omega}\sum_p \phi(p)\Gamma(r,p,t)}_{S_\phi(r,t)} + \underbrace{\frac{1}{\Omega}\sum_p \phi(p)\frac{\partial f}{\partial t}\Big|_{col}}_{-R_\phi}$$

because this term increases with $\vec{\mathcal{E}}$ which increases n_ϕ.

we also have generation & recombination on the RHS.

$\phi=1 \to n_\phi$: carrier density $\to F_\phi$: carrier flux

$\phi=E \to n_\phi$: energy density $\to F_\phi$: energy flux

Collisions destroy momentum, so produce 'recombination'. They oppose deviation from equilibrium, so the rate of change from equilibrium depends on this term:

$$R_\phi = \left\langle\!\left\langle \frac{1}{\tau_\phi} \right\rangle\!\right\rangle \left(n_\phi(r,t) - n_\phi^0(r,t) \right)$$

$\langle\langle 1/\tau_\phi \rangle\rangle$: ensemble relaxation rate - NOT TO be confused with RTA.

there is no approximation here.

Ensemble relaxation time $\langle\langle \frac{1}{\tau_\phi} \rangle\rangle$:

Assume non-degenerate and expand the collision term:

$$\sum_{\vec{p}} \phi(\vec{p}) \left.\frac{\partial f}{\partial t}\right|_{coll} = \sum_{\vec{p}} \sum_{\vec{p}'} \phi(\vec{p}) \Gamma(\vec{p}', \vec{p}) f(\vec{p}') - \phi(\vec{p}) \Gamma(\vec{p}, \vec{p}') f(\vec{p})$$

dummy indices

$$= \sum_{\vec{p}} \sum_{\vec{p}'} \phi(\vec{p}') \Gamma(\vec{p}, \vec{p}') f(\vec{p}) - \phi(p) \Gamma(p, p') f(p)$$

$$= \sum_{\vec{p}} f(\vec{p}) \phi(\vec{p}) \underbrace{\sum_{p'} \left(\frac{\phi(\vec{p}')}{\phi(\vec{p})} - 1 \right) \Gamma(\vec{p}, \vec{p}')}_{\equiv -\frac{1}{\tau_\phi(p)}} \equiv - \sum_{\vec{p}} \frac{f(p)\phi(p)}{\tau_\phi(p)}$$

out scattering rate related to ϕ.

$$\frac{1}{\tau(\phi)} = \sum_{p'} \left(\frac{\phi(p')}{\phi(p)} - 1 \right) \Gamma(p, p')$$

Sum over transition rate from p to p' weighted by fractional change in ϕ

$$R_\phi = \frac{-1}{\Omega} \sum_{p} \phi(\vec{p}) \left.\frac{\partial f}{\partial t}\right|_{col} \equiv \langle\langle \frac{1}{\tau_\phi} \rangle\rangle \left(n_\phi(r,t) - n_\phi^0(r,t) \right) \Rightarrow$$

$$\langle\langle \frac{1}{\tau_\phi} \rangle\rangle = \frac{-\frac{1}{\Omega} \sum_{\vec{p}} \phi(\vec{p}) \frac{\partial f}{\partial t}}{n_\phi(r,t) - n_\phi^0(r,t)} = \frac{\frac{1}{\Omega} \sum_{\vec{p}} f(\vec{p}) \phi(\vec{p}) / \tau_\phi(\vec{p})}{n_\phi(r,t) - n_\phi^0(r,t)}$$

note: τ_ϕ depends only on scatterings. But $\langle\langle \frac{1}{\tau_\phi} \rangle\rangle$ depends both on out-scattering and on the distribution function f.

Putting all the terms in together, we get the balance eqn:

$$\boxed{\frac{\partial n_\phi(r,t)}{\partial t} = -\vec{\nabla} \cdot \vec{F}_\phi + G_\phi - R_\phi + S_\phi}$$

density — flux — Field gen. rate — Scatt recombination rate — particle gen-rec. rate

In Summary:

Density: $n_\phi(\vec{r},t) \equiv \frac{1}{\Omega}\sum_p f\phi(\vec{p})$

Flux : $\vec{F}_\phi(\vec{r},t) \equiv \frac{1}{\Omega}\sum_{\vec{p}} \vec{v} f \phi(\vec{p})$

Field gen rate: $G_\phi(\vec{r},t) \equiv -q\vec{\mathcal{E}}\cdot\frac{1}{\Omega}\sum_{\vec{p}} f \vec{\nabla}_p \phi(\vec{p})$

Scattering recombination rate: $R_\phi(\vec{r},t) \equiv \langle\langle \frac{1}{\tau_\phi} \rangle\rangle [n_\phi(\vec{r},t) - n_\phi^0(\vec{r},t)]$

Out scattering rate: $\frac{1}{\tau_\phi(\vec{p})} \equiv \sum_{\vec{p}'} \left(1 - \frac{\phi(\vec{p}')}{\phi(p)}\right) \Gamma(p, p')$

Particle gen-rec rate: $\Gamma_\phi(\vec{r},t) \equiv \frac{1}{\Omega}\sum_{\vec{p}} \phi(\vec{p})\Gamma(\vec{r},\vec{p},t)$

Ensemble relaxation rate: $\langle\langle \frac{1}{\tau_\phi} \rangle\rangle \equiv \dfrac{\frac{1}{\Omega}\sum_{\vec{p}} f(\vec{r},\vec{p},t)\phi(\vec{p})/\tau_\phi(\vec{p})}{n_\phi(\vec{r},t) - n_\phi^0(\vec{r},t)}$

Elaboration of $\langle\langle 1/\tau_\phi \rangle\rangle$:

If $\phi(P) = P_i$ => $n_\phi = \frac{1}{\Omega}\sum P_i f = \bar{P}_i$ average momentum density of the ensemble

$\bar{P}_i = n m \bar{v}_i$

$$\left.\frac{\partial n_\phi}{\partial t}\right|_{coll} = \frac{1}{\Omega}\sum_p \phi(p) \left.\frac{\partial f}{\partial t}\right|_{coll} = -\langle\langle \frac{1}{\tau_\phi} \rangle\rangle [n_\phi - n_\phi^0]$$

$\frac{\partial P_i}{\partial t} = -\langle\langle \frac{1}{\tau_m} \rangle\rangle P_i \qquad (P_i^0 = 0)$ So $\langle\langle \frac{1}{\tau_m} \rangle\rangle$ is the average momentum relaxation rate. It is not $\langle\langle \tau_f \rangle\rangle$ but related. we will see.

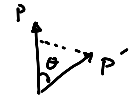
If $\phi(p) = E$ => $n_\phi = \bar{W}$ average kinetic energy $\bar{E_p} = n u$ u being the average kinetic energy of one particle

$\left.\frac{dW}{dt}\right|_{coll} = \langle\langle \frac{1}{\tau_E} \rangle\rangle (\bar{W} - \bar{W}^0)$ $\langle\langle \frac{1}{\tau_E} \rangle\rangle$ is the ensemble energy relaxation rate.

note that $\langle\langle \frac{1}{\tau_m} \rangle\rangle$ and $\langle\langle \frac{1}{\tau_E} \rangle\rangle$ are exact values with no approximation. But to evaluate them we need to know f. To avoid solving BTE, we often assume they are constant or depend only on average carrier energy. This will be the RTA.

The Outscattering Rate

$$\frac{1}{\tau_\phi(p)} = \sum_{p'} \left(1 - \frac{\Phi(\vec{p}')}{\Phi(p)}\right)\Gamma(p,p')$$



$p_z = p$

$p_z' = p\cos\theta$

$\Rightarrow p_z'/p_z = \cos\theta$

if $\Phi(\vec{p}) = p_z \rightarrow \frac{1}{\tau_\phi} = \frac{1}{\tau_m} = \sum_{p'} \Gamma(p,p')\left[1 - \frac{p_z'}{p_z}\right] = \sum_{p'} \Gamma(p,p')(1-\cos\theta)$

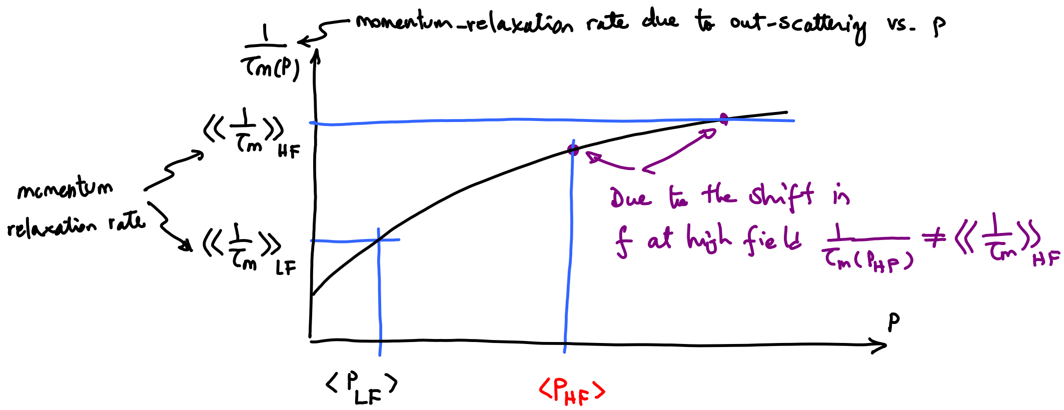
if $\Phi(\vec{p}) = E(p) \rightarrow \frac{1}{\tau_\phi} = \frac{1}{\tau_E} = \sum_{p'} \Gamma(p,p')\left[1 - \frac{E(\vec{p}')}{E(\vec{p})}\right] = \sum_{p'} \Gamma(p,p') \frac{E(\vec{p}) - E(\vec{p}')}{E(p)}$

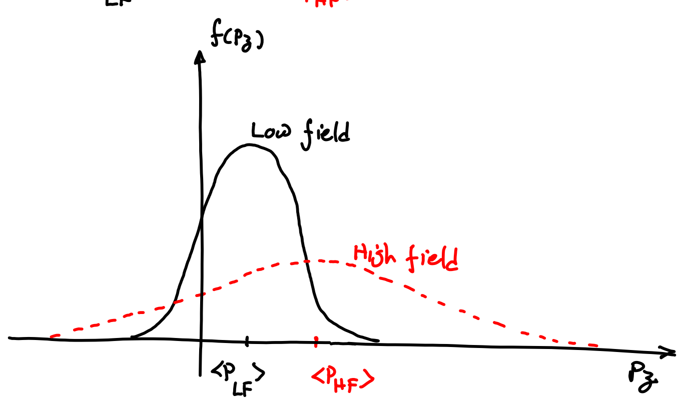
for phonon emission: $\frac{1}{\tau_E} = \sum_{p'} \Gamma(p,p')\frac{\hbar\omega_0}{E(p)} = \frac{\hbar\omega_0}{E(p)}\sum_{p'}\Gamma(p,p')$

$E(p') = E(p) - \hbar\omega_0$

These are the characteristic times describing the rate of loss of momentum or energy of electrons injected into the material. The probability of in-scattering is small.

Difference between the out-scattering & the ensemble momentum relaxation time:





The Balance Equations

Carrier Density Blance equ.

$\Phi(p) = 1 \Rightarrow n_\phi = n \Rightarrow F_\phi(r,t) = \frac{1}{\Omega}\sum_{\vec{p}} v f \Phi(\vec{p}) = \frac{1}{\Omega}\sum_{\vec{p}} \vec{v} f = n\vec{v}_d = \frac{J_n}{-q}$

$$G_\phi = -q\vec{\mathcal{E}} \cdot \frac{1}{\Omega}\sum_{p} f \underbrace{\nabla_p \Phi(\vec{p})}_{0} = 0$$

$R_\phi = \langle\langle \overbrace{\frac{1}{\tau_\phi}}^{0} \rangle\rangle [n_\phi - n_\phi^0] = 0$ because $\frac{1}{\tau_\phi(p)} = \frac{1}{\Omega}\sum_{p'}\Gamma(p,p')\left(\overbrace{1 - \frac{\Phi(p')}{\Phi(p)}}^{0}\right)$

$$\frac{\partial n}{\partial t} = -\underset{-J/q}{\nabla\cdot F_\phi} + \overbrace{G_\phi - R_\phi}^{0} + S_\phi$$

$$\Rightarrow \quad \boxed{\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\vec{J}_n + S_n}$$

which is our familiar continuity equation.

S_n is the particle generation–recom. rate $(G_n - R_n)$.

Momentum Balance equation

if $\phi(\vec{p}) = P_z \rightarrow n_\phi = \frac{1}{\Omega}\sum_{\vec{p}} p_z f = P_z = nmv_{dz}$

velocity × momentum => 2× kinetic energy

flux of momentum: $\vec{F}_\phi = \frac{1}{\Omega}\sum_{\vec{p}} \vec{v} p_z f \rightarrow F_{\phi_i} = \frac{1}{\Omega}\sum_{\vec{p}} \overbrace{v_i p_z}^{} f \equiv 2W_{iz}$

$$G_\phi(r,t) = -q\vec{\mathcal{E}}\cdot\frac{1}{\Omega}\sum_{\vec{p}} f\vec{\nabla}_p\phi(\vec{p}) = -q\vec{\mathcal{E}}\cdot\frac{1}{\Omega}\sum_{\vec{p}} f\underbrace{\vec{\nabla}_p P_z}_{\hat{z}} = -q\underbrace{\vec{\mathcal{E}}\cdot\hat{z}}_{\mathcal{E}_z}\underbrace{\frac{1}{\Omega}\sum_{\vec{p}} f}_{n} = -qn\mathcal{E}_z$$

$$R_\phi = \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle[\overbrace{n_\phi}^{P_z} - \overbrace{n_\phi^0}^{=0}] = \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle P_z$$

$$\frac{\partial n_\phi}{\partial t} = -\vec{\nabla}\cdot\vec{F}_\phi + G_\phi - R_\phi + \overbrace{S_\phi}^{=0}$$

since the source is assumed to inject carrier at random derection. So it doesn't generate ensemble momentum.

$$\frac{\partial P_z}{\partial t} = -\frac{\partial}{\partial x_i}(2W_{iz}) + n(-q)\mathcal{E}_z - \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle P_z$$

Similarly for other two components of x & y => $\frac{\partial P_j}{\partial t} = -\frac{\partial}{\partial x_i}(2W_{ij}) + n(-q)\mathcal{E}_j - \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle P_j$

Or in symbolic form: $\boxed{\frac{\partial\vec{P}}{\partial t} = -2\vec{\nabla}\cdot\overleftrightarrow{W} + n(-q)\vec{\mathcal{E}} - \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle\vec{P}}$

$\overleftrightarrow{W}$ is a tensor: $W_{ij} \equiv \frac{1}{2\Omega}\sum_{\vec{p}} v_i p_j f$ The dot product is: $\vec{\nabla}\cdot\overleftrightarrow{W}\cdot\hat{x}_j = \frac{\partial}{\partial x_i}W_{ij}$ which is a vector.

Note the trace of $\overleftrightarrow{W}$ is: $W_{ii} = \sum_i \frac{1}{2\Omega}\sum_{\vec{p}} v_i p_i f = \sum_i \frac{1}{\Omega}\sum_{\vec{p}} \frac{1}{2}mv_i^2 f(\vec{p}) = W = nu$

average kinetic energy per particle

average kinetic energy density

For simple spherical, parabolic energy bands:

$$\vec{J}_n = -qn\vec{v}_d = -q\frac{\vec{P}}{m} \rightarrow \boxed{\frac{\partial\vec{J}}{\partial t} = \frac{-2(-q)\nabla\cdot\overleftrightarrow{W}}{m} + \frac{q^2 n\vec{\mathcal{E}}}{m} - \left\langle\!\left\langle\frac{1}{\tau_m}\right\rangle\!\right\rangle\vec{J}_n}$$

We will see that this can be simplified to Drift Diffusion Equation.

The Energy Balance Equation

$\Phi(p) = E(p) \rightarrow n_\phi = \frac{1}{\Omega}\sum_{\vec{p}} E(\vec{p}) f = W$ kinetic energy density $\Rightarrow \vec{F}_\phi = \frac{1}{\Omega}\sum_{\vec{p}} \vec{v} E(\vec{p}) f = \vec{F}_W$ energy flux

Energy is supplied to the carriers by the electric field $\Rightarrow G_\phi$

$$G_\phi = (-q)\vec{\mathcal{E}}\cdot\frac{1}{\Omega}\sum_{\vec{p}} f \vec{\nabla}_p \Phi(\vec{p}) = (-q)\vec{\mathcal{E}}\cdot\frac{1}{\Omega}\sum_{\vec{p}} [\overbrace{\vec{\nabla}_p E(\vec{p})}^{\vec{v}}] f = -q\vec{\mathcal{E}}\cdot v_d = \vec{J}_n\cdot\vec{\mathcal{E}}$$

input power density as expected

Energy is lost by collision $\Rightarrow R_\phi$

$$R_\phi = \langle\langle \frac{1}{\tau_E} \rangle\rangle (W - W^0)$$

energy density in thermal equilibrium

$$\Rightarrow \boxed{\frac{\partial W}{\partial t} = -\nabla\cdot\vec{F}_W + \vec{J}_n\cdot\vec{\mathcal{E}} - \langle\langle\frac{1}{\tau_E}\rangle\rangle (W - W^0) + S_E}$$

energy flowing in — Field acceleration — lost by collision

It is possible to re-write this equation for energy flux (Problem 5.6 in book):

$$\boxed{\frac{\partial \vec{F}_W}{\partial t} = -\vec{\nabla}\cdot\overleftrightarrow{X} + \frac{(-q)W}{m}\vec{\mathcal{E}} + 2(-q)\frac{\vec{\mathcal{E}}\cdot\overleftrightarrow{W}}{m} - \langle\langle\frac{1}{\tau_{FW}}\rangle\rangle \vec{F}_W}$$

where : $X_{ij} \equiv \frac{1}{\Omega}\sum_{\vec{p}} v_i v_j E(\vec{p}) f$

Summary of Balance Equations:

Unknowns

(i) Carrier density $\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\vec{J}_n + S_n \rightarrow n, J_n$

(ii) momentum density $\frac{\partial \vec{J}_n}{\partial t} = \frac{-2(-q)\nabla\cdot\overleftrightarrow{W}}{m} + \frac{q^2 n\vec{\mathcal{E}}}{m} - \langle\langle\frac{1}{\tau_m}\rangle\rangle\vec{J}_n \rightarrow J_n$ $\quad W_{ij} = \frac{1}{2\Omega}\sum v_i p_j f$, $\vec{J} = -q\frac{\vec{p}}{m} = -q\vec{v}_d$

(iii) energy density $\frac{\partial W}{\partial t} = -\vec{\nabla}\cdot\vec{F}_W + \vec{J}_n\cdot\vec{\mathcal{E}} - \langle\langle\frac{1}{\tau_E}\rangle\rangle(W - W^0) + S_E \rightarrow W$ $\quad \vec{F}_W = \frac{1}{\Omega}\sum_{\vec{p}} v E(p) f$

(iv) energy flux $\frac{\partial \vec{F}_W}{\partial t} = -2\vec{\nabla}\cdot\overleftrightarrow{X} + \frac{(-q)W}{m}\vec{\mathcal{E}} - \langle\langle\frac{1}{\tau_{FW}}\rangle\rangle\vec{F}_W \rightarrow F_W$ $\quad X_{ij} = \frac{1}{\Omega}\sum_{\vec{p}} v_i v_j E(p) f$

4 equation & 5 unknowns! This always happens with balance equations. No matter how many balance equations we write, there is always one more unknown than the number of equations. The solution to these infinite number of equations is the solution to the BTE itself.

These equations were derived from the BTE without simplifying approximation. However, to solve this set of balance equations, it must be truncated and simplified.

Let's rewrite these equations in a more convenient form:

Carrier temperature and heat flux

Carrier temperature : T_c

Lattice temperature : T_L

Electric field $\Rightarrow T_c > T_L$ Collision $\Rightarrow T_c \to T_L$

Let's look at the kinetic energy density:

$$W_{ii} = \frac{1}{2\Omega}\sum_{\vec{p}} p_i v_i f = \frac{m}{2\Omega}\sum_{\vec{p}} v^2 f = \frac{nm}{2}\langle v^2\rangle$$

$\langle\cdot\rangle \Rightarrow$ average over the distribution function $\langle \frac{1}{\tau}\rangle = \frac{1}{\Omega}\sum \frac{f}{\tau}$

$\langle\langle\cdot\rangle\rangle \Rightarrow$ specially defined ensemble average $\langle\langle \frac{1}{\tau_\phi}\rangle\rangle = \frac{1}{\Omega}\sum \frac{f}{\tau_\phi}\phi(p)/(n_\phi - n_\phi^0)$

Carrier velocity $\vec{v} = \vec{v}_d + \vec{c}$

$\vec{v}_d$: average comp. due to electric field

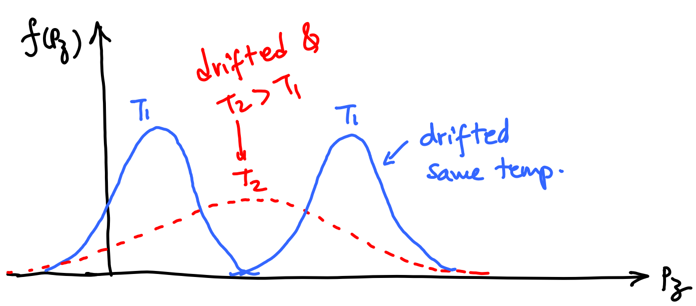
$\vec{c}$: random component due to collision

$$\Rightarrow W_{ii} = \frac{m}{2\Omega}\sum_{\vec{p}} v_i v_i f = \frac{m}{2\Omega}\sum_{\vec{p}}\sum_i v_i^2 f = \frac{m}{2\Omega}\sum_p\sum_i (v_{d_i} + c_i)^2 f$$

$$= \frac{m}{2\Omega}\sum_p\sum_i v_{d_i}^2 f + \frac{m}{2\Omega}\sum_p \overbrace{\sum_i c_i^2}^{c^2} f + \frac{m}{2\Omega}\overbrace{\sum_p\sum_i v_{d_i} c_i f}^{=0 \text{ random } \vec{c}}$$

$$= \underbrace{\frac{m}{2}\sum_i v_{d_i}^2 \overbrace{\frac{1}{\Omega}\sum f}^{n}}_{n v_d^2} + \frac{m}{2}\underbrace{\frac{1}{\Omega}\sum_p c^2 f}_{\langle c^2\rangle} = \underbrace{\frac{1}{2} n m v_d^2}_{\text{Drift energy}} + \underbrace{\frac{1}{2} n m \langle c^2\rangle}_{\text{Thermal motion energy}} = \frac{3}{2} n k_B T$$

$\frac{3}{2} n k_B T_c \equiv \frac{1}{2} m n \langle c^2\rangle \longrightarrow$ temperature tensor $\boxed{\frac{1}{2} n k_B T_{ij} = \frac{1}{2} m n \langle c_i c_j\rangle}$



Heat flux