Low- Field Transport

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.

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

Assumptions: low field
RTA
spherical parabolic bands

Low field solution (B=0) :

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

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: $f_S \gg f_A$

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

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

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

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

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

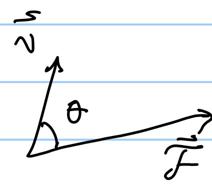
$$\begin{cases} \vec{\nabla}_r\theta = \dfrac{1}{k_B T_L}\left(\nabla_r E_c - \nabla_r F_n\right) + \left(E_c + E(p) - F_n\right)\nabla_r\left(\dfrac{1}{k_B T_L}\right) \\ \vec{\nabla}_p\theta = \dfrac{p}{m}\dfrac{1}{k_B T_L} = \vec{v}\,\dfrac{1}{k_B T_L} \end{cases}$$

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

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

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

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



$$\begin{cases} \text{Electric current: } \vec{J} = \dfrac{-q}{\Omega}\sum\limits_p \vec{v}\,(\underset{\text{even}}{\overset{\uparrow}{f_s}} + f_A) = \dfrac{-q}{\Omega}\sum\limits_p \vec{v} f_A \quad \checkmark \\[2em] \text{Heat current: } J_W = \dfrac{1}{\Omega}\sum\limits_p \underset{\text{heat is associated with kinetic energy}}{\underset{\downarrow}{E(\vec{p})}}\,\vec{v} f_A \quad \times \end{cases}$$

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 $J_Q \Rightarrow$

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

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

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

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

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

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

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

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

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:

$$\begin{bmatrix} \sigma_{ij} \\ B_{ij} \\ P_{ij} \\ K_{ij} \end{bmatrix} = \frac{1}{\Omega}\sum_{p}\left(-\frac{\partial f_s}{\partial\theta}\right)\tau\,\frac{v_i v_j}{k_B T_L}\begin{bmatrix} q^2 \\ -q T_L (E_c + E_p - F_n) \\ -q\,(E_c + E_p - F_n) \\ T_L\,(E_c + E_p - F_n)^2 \end{bmatrix}$$

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

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

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