BALANCE EQUATIONS MODEL

In this section we will first describe the prescription for generating balance equations from the BTE, which in its most general form is given by:

$$\frac{\partial f}{\partial t} + \nabla_r \cdot (\vec{v} f) - \frac{e}{\hbar} \vec{\mathcal{E}} \cdot \nabla_k f = S_{op} f + S(\vec{r}, \vec{p}, t)$$

We define a quantity $\phi(\vec{p})$ that can have values $1, p, \ldots$ etc, and the total value (averaged) of the quantity associated with $\phi(\vec{p})$ is

$$n_\phi(\vec{r}, t) = \frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r}, \vec{p}, t)$$

where n_ϕ can represent carrier density, current density, etc. To find the balance equation for n_ϕ, we need to multiply the BTE by $\phi(\vec{p}) \frac{1}{V}$ and to integrate over $\vec{p}$. Then, the various terms that appear in the BTE become:

$$\frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) \frac{\partial f}{\partial t} = \frac{\partial}{\partial t} \left[\frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r}, \vec{p}, t) \right] = \frac{\partial n_\phi}{\partial t}$$

$$\frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) \nabla_r \cdot (\vec{v} f) = \nabla_r \cdot \frac{1}{V} \sum_{\vec{p}} \vec{v} \phi(\vec{p}) f(\vec{r}, \vec{p}, t) = \nabla_r \cdot F_\phi$$

where $F_\phi = \frac{1}{V} \sum_{\vec{p}} \vec{v} \phi(\vec{p}) f(\vec{r}, \vec{p}, t)$ is the flux associated with n_ϕ. For example, if $\phi(\vec{p}) = 1$, then F_ϕ is carrier flux, and if $\phi(p) = E_p$, then F_ϕ is the energy flux. The third term is then given by:

$$-e \sum_{\vec{p}} \phi(\vec{p}) \vec{\mathcal{E}} \cdot \nabla_p f = -e \vec{\mathcal{E}} \cdot \sum_{\vec{p}} \phi(\vec{p}) \nabla_p f$$

where:

$$\sum_{\vec{p}} \phi(\vec{p}) \nabla_p f = \underbrace{\phi(\vec{p}) f(\vec{r}, \vec{p}, t) \Big|_{\vec{p} = -\infty}^{+\infty}}_{0} - \sum_{\vec{p}} f(\vec{r}, \vec{p}, t) \nabla_p \phi(\vec{p})$$

which leads to:

$$-e\sum_{\vec{p}}\phi(\vec{p})\,\vec{\mathcal{E}}\cdot\nabla_p f = e\,\vec{\mathcal{E}}\cdot\sum_{\vec{p}} f(\vec{r},\vec{p},t)\,\nabla_p\phi(\vec{p}) = -G_\phi$$

and is called a generation term since electric field increases momentum and the quantity n_ϕ. Besides the electric field term, there is another term $s(\vec{r},\vec{p},t)$ that leads to increase/decrease of n_ϕ (generation or recombination processes). The contribution of this term is:

$$S_\phi = \frac{1}{V}\sum_{\vec{p}}\phi(\vec{p})\,s(\vec{r},\vec{p},t)$$

The collision events, for example, destroy momentum and, thus, represent a recombination term:

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

where $\langle\langle 1/\tau_\phi\rangle\rangle$ is ensemble relaxation rate. To find the definition of this term, we assume non-degenerate semiconductor, for which:

$$\left.\frac{\partial f}{\partial t}\right|_{coll.} = \sum_{\vec{p}'}\left[f(\vec{r},\vec{p}',t)\,s(\vec{p}',\vec{p}) - f(\vec{r},\vec{p},t)\,s(\vec{p},\vec{p}')\right]$$

Then:

$$\frac{1}{V}\sum_{\vec{p}}\phi(\vec{p})\left.\frac{\partial f}{\partial t}\right|_{coll.} = \frac{1}{V}\sum_{\vec{p}}\sum_{\vec{p}'}\phi(\vec{p})\left[f(\vec{r},\vec{p}',t)\,s(\vec{p}',\vec{p}) - f(\vec{r},\vec{p},t)\,s(\vec{p},\vec{p}')\right]$$

$$= \frac{1}{V}\sum_{\vec{p}}\sum_{\vec{p}'}\left[\phi(\vec{p}')\,f(\vec{r},\vec{p},t)\,s(\vec{p},\vec{p}') - \phi(\vec{p})\,f(\vec{r},\vec{p},t)\,s(\vec{p},\vec{p}')\right]$$

$$= \frac{1}{V}\sum_{\vec{p}}\sum_{\vec{p}'}\left[\phi(\vec{p}') - \phi(\vec{p})\right]f(\vec{r},\vec{p},t)\,s(\vec{p},\vec{p}')$$

$$= -\frac{1}{V}\sum_{\vec{p}}\phi(\vec{p})\,f(\vec{r},\vec{p},t)\underbrace{\sum_{\vec{p}'}\left[1-\frac{\phi(\vec{p}')}{\phi(\vec{p})}\right]s(\vec{p},\vec{p}')}_{\frac{1}{\tau_\phi(\vec{p})}\ =\ \text{total out-scattering rate associated with } \phi.}$$

Therefore:

$$\left\langle\!\left\langle \frac{1}{\tau_\phi} \right\rangle\!\right\rangle \left[n_\phi - n_\phi^0 \right] = - \frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) \left. \frac{\partial f}{\partial t} \right|_{coll} = \frac{1}{V} \sum_{\vec{p}} \frac{\phi(\vec{p}) f(\vec{r},\vec{p},t)}{\tau_\phi(\vec{p})}$$

which gives:

$$\left\langle\!\left\langle \frac{1}{\tau_\phi} \right\rangle\!\right\rangle = \frac{\frac{1}{V} \sum_{\vec{p}} \frac{f(\vec{r},\vec{p},t)\phi(\vec{p})}{\tau_\phi(\vec{p})}}{n_\phi(\vec{r},t) - n_\phi^0(\vec{r},t)}$$

This ensemble relaxation rate depends upon the type of the scattering mechanism and how carriers are distributed in momentum. In summary, when $\phi(\vec{p}) = p_i$, then $n_\phi = P_i$ and

$$\left. \frac{dP_i}{dt} \right|_{coll} = - P_i \left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle$$

Also, when $\phi(\vec{p}) = E(\vec{p})$, then $n_\phi = W$ (average kinetic energy density) given by $W = nu$ (u is average energy density per electron) and then:

$$\left. \frac{dW}{dt} \right|_{coll} = - \left\langle\!\left\langle \frac{1}{\tau_E} \right\rangle\!\right\rangle (W - W_0)$$

The above results are exact. NO RTA approximation is made.

- Summarizing all these results, we arrive at the Balance equation for the quantity n_ϕ:

$$\boxed{\frac{\partial n_\phi}{\partial t} = - \nabla \cdot F_\phi + G_\phi - R_\phi + S_\phi} \qquad (*)$$

The various quantities that appear in (*) are calculated using:

$$n_\phi = \frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) f(\vec{r},\vec{p},t) \qquad G_\phi = - e \vec{\mathcal{E}} \cdot \sum_{\vec{p}} f(\vec{r},\vec{p},t) \nabla_p \phi(\vec{p})$$

$$\vec{F}_\phi = \frac{1}{V} \sum_{\vec{p}} \vec{v} \phi(\vec{p}) f(\vec{r},\vec{p},t) \qquad R_\phi = - \frac{1}{V} \sum_{\vec{p}} \phi(\vec{p}) \left. \frac{\partial f}{\partial t} \right|_{coll} = \left\langle\!\left\langle \frac{1}{\tau_\phi} \right\rangle\!\right\rangle \left[n_\phi(\vec{r},t) - n_\phi^0(\vec{r},t) \right]$$

(A) CARRIER-DENSITY BALANCE EQUATION

when $\phi(\vec{p}) = 1$ then:

$$n_\phi = n$$

$$F_\phi = \frac{1}{V}\sum_{\vec{p}} \vec{v} f(\vec{r},\vec{p},t) = -\frac{1}{e}\vec{J}_n(\vec{r},t)$$

$G_\phi = R_\phi = 0$ → scattering mechanisms and the electric field redistribute carriers among states but do not generate or destroy carriers.

This then leads to the continuity equation for the electrons:

$$\boxed{\frac{\partial n}{\partial t} = \frac{1}{e}\nabla\cdot J_n + S_n} \quad (1) \qquad \text{conservation of particles}$$

(B) The momentum balance equation

The momentum balance equation is obtained by assuming $\phi(\vec{p}) = p_z$, for example. Then:

$$n_\phi = \frac{1}{V}\sum_{\vec{p}} p_z f(\vec{r},\vec{p},t) = P_z \quad \text{(total momentum density along } z\text{)}$$

$$\vec{F}_\phi = \frac{1}{V}\sum_{\vec{p}} \vec{v}\, p_z f(\vec{r},\vec{p},t) \Rightarrow F_{\phi i} = \frac{1}{V}\sum_{\vec{p}} v_i p_z f = \frac{1}{V}\sum_{\vec{p}} m^* v_z v_i f$$

$$F_{\phi i} = 2W_{iz} \quad \text{(kinetic energy density tensor)}$$

$$G_\phi = -e\vec{\mathcal{E}}\cdot\sum_p f(\vec{r},\vec{p},t)\nabla_p p_z = -e\mathcal{E}_z n$$

$$R_\phi = \left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle P_z$$

Then:

$$\frac{\partial P_z}{\partial t} = -\nabla\cdot\vec{F}_\phi - en\mathcal{E}_z - \left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle P_z = -\sum_i 2\frac{\partial W_{iz}}{\partial x_i} - en\mathcal{E}_z - \left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle P_z$$

The trace of the tensor $\overleftrightarrow{W}$ is:

$$tr(\overleftrightarrow{W}) = \sum_i W_{ii} = \sum_i \frac{1}{2V}\sum_{\vec{p}} m^* v_i^2 f = \frac{1}{V}\sum_{\vec{p}} f(\vec{r},\vec{p},t)\sum_i \frac{1}{2}m^* v_i^2 = W = nu$$

For simple parabolic bands, we have:

$$\vec{p} = n m^* \vec{v}_d = -\frac{1}{e}(-en\vec{v}_d)m^* = -\vec{J}m^*/e$$

which gives:

$$\vec{J} = -\frac{e}{m^*}\vec{p}$$

or:

$$\boxed{\frac{\partial J_z}{\partial t} = \frac{2e}{m^*}\sum_i \frac{\partial W_{iz}}{\partial x_i} + \frac{ne^2}{m^*}\mathcal{E}_z - \langle\!\langle \frac{1}{\tau_m} \rangle\!\rangle J_z} \quad (2) \quad \textbf{flow of mass}$$

With appropriate simplifications, the balance equation for the current density reduces to the drift-diffusion equation.

(c) <u>Energy balance equation</u>

The energy balance equation is obtained from the prescription that $\phi(p) = \varepsilon_p$.

Then: $n_\phi = \frac{1}{V}\sum_{\vec{p}} E(\vec{p}) f(\vec{r},\vec{p},t) = W$

$$F_\phi = \frac{1}{V}\sum_{\vec{p}} \vec{v}\, E(\vec{p}) f(\vec{r},\vec{p},t) = \vec{F}_W \quad \text{(energy flux)}$$

$$G_\phi = -\frac{e\vec{\mathcal{E}}}{V}\cdot\sum_{\vec{p}} f(\vec{r},\vec{p},t)\,\vec{v} = \vec{\mathcal{E}}\cdot\left(-\frac{e}{V}\right)\cdot\sum_{p}\vec{v}\, f(\vec{r},\vec{p},t) = \vec{\mathcal{E}}\cdot\vec{J}_n$$

$$R_\phi = \langle\!\langle \frac{1}{\tau_E} \rangle\!\rangle (W - W_0) \rightarrow \text{loss of energy to phonons}$$

The energy balance equation is, thus,

$$\boxed{\underbrace{\frac{\partial W}{\partial t}}_{\text{increase in energy}} = \underbrace{-\nabla\cdot\vec{F}_W}_{\text{energy flowing into the volume}} + \underbrace{\vec{\mathcal{E}}\cdot\vec{J}}_{\text{energy increase due to field accelerating the carriers}} - \underbrace{\langle\!\langle \frac{1}{\tau_E} \rangle\!\rangle [W - W_0]}_{\text{energy loss due to collisions.}}} \quad (3) \quad \textbf{conservation of energy}$$

To summarize:

$$\frac{\partial n}{\partial t} = \frac{1}{e}\nabla\cdot J_n + S_n$$ carrier density balance equation

$$\frac{\partial J_z}{\partial t} = \frac{2e}{m^*}\sum_i \frac{\partial W_{iz}}{\partial x_i} + \frac{ne^2}{m^*}\mathcal{E}_z - \left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle J_z$$ momentum density (current density balance equation).

$$\frac{\partial W}{\partial t} = -\nabla\cdot\vec{F}_W + \vec{\mathcal{E}}\cdot\vec{J} - \left\langle\!\left\langle \frac{1}{\tau_E} \right\rangle\!\right\rangle [W - W_0]$$ energy density balance equation

The balance equation for carrier density introduces the current density, which balance equation introduced the kinetic energy density. The balance equation for the kinetic energy density, on the other hand, introduced the energy flux. Therefore, a new variable appears in the hierarchy of balance equations and the set of infinite balance equations is actually the solution of the BTE.

- The balance equations can be reformulated in a more convenient form by separating the carrier temperature (T_c) from the lattice temperature (T_L). To achieve this, we will work on the kinetic energy density tensor and write the carrier velocity as:

$$\vec{v} = \underbrace{\vec{v}_d}_{\text{average drift velocity}} + \underbrace{\vec{c}}_{\text{random (thermal) component}}$$

Then:

$$\langle v_i v_z \rangle = \langle (v_{di} + c_i)(v_{dz} + c_z) \rangle = \langle v_{di} v_{dz} + c_i v_{dz} + c_z v_{di} + c_i c_z \rangle$$

where the brackets $\langle\ \rangle$ represent an average over the distribution function. Now, since $\langle c_i \rangle = 0$, we have:

$$\langle v_i v_z \rangle = \langle v_{di} v_{dz} \rangle + \langle c_i c_z \rangle$$

The kinetic energy tensor component W_{iz} is, thus, given by:

$$W_{iz} = \frac{1}{2} n m^* \langle v_i v_z \rangle = \underbrace{\frac{1}{2} n m^* \langle v_{di} v_{dz} \rangle}_{\substack{\text{drift energy} \\ K_{iz}}} + \underbrace{\frac{1}{2} n m^* \langle c_i c_z \rangle}_{\text{thermal energy due to the random thermal motion}}$$

The kinetic energy density equals the trace of the tensor $\overleftrightarrow{W}$, i.e.

$$W = \sum_{i=x,y,z} W_{ii} = \frac{1}{2} nm^* \sum_i \langle v_{di}^2 \rangle + \frac{1}{2} nm^* \sum_i \langle c_i^2 \rangle$$

$$= \frac{1}{2} nm^* \langle v_d^2 \rangle + \frac{1}{2} nm^* \langle c^2 \rangle$$

For the thermal carrier energy, we have:

$$\frac{1}{2} nm^* \langle c^2 \rangle = \frac{1}{2} nm^* \sum_i \langle c_i^2 \rangle = \frac{3}{2} nk_B T_c = 3 \frac{1}{2} nm^* \langle c_i^2 \rangle$$

Therefore: $\frac{1}{2} nm^* \langle c_i^2 \rangle = \frac{1}{2} nk_B T_c$, which gives: $\langle c_i c_j \rangle = \frac{k_B}{m^*} T_{ij}$

$$W_{iz} = \frac{1}{2} nm^* \langle v_{di} v_{dz} \rangle + \frac{1}{2} nm^* \langle c_i c_z \rangle = \frac{1}{2} nm^* \langle v_{di} v_{dz} \rangle + \frac{1}{2} nm^* T_{iz} \frac{k_B}{m^*}$$

where T_{iz} is a component of the temperature tensor.

- We now want to express the energy flux in terms of the temperature tensor. The energy flux $\vec{F}_W$ was defined as:

$$\vec{F}_W = \frac{1}{V} \sum_{\vec{p}} \vec{v} E(\vec{p}) f(\vec{r}, \vec{p}, t)$$

which means that the i-th component of this vector equals to:

$$F_{Wi} = \frac{1}{V} \sum_{\vec{p}} v_i \frac{m^* v^2}{2} f(\vec{r}, \vec{p}, t) = \frac{nm^*}{2} \langle v_i v^2 \rangle$$

where:

$$\langle v_i v^2 \rangle = \langle (v_{di} + c_i) v^2 \rangle = v_{di} \langle v^2 \rangle + \langle c_i v^2 \rangle$$

$$= v_{di} \sum_j \langle (v_{dj} + c_j) \cdot (v_{dj} + c_j) \rangle + \sum_j \langle c_i (v_{dj} + c_j)^2 \rangle$$

$$= v_{di} \sum_j \langle v_{dj}^2 + 2 c_j v_{dj} + c_j^2 \rangle + \sum_j \langle c_i (v_{dj}^2 + 2 v_{dj} c_j + c_j^2) \rangle$$

$$= v_{di} \sum_j [\langle v_{dj}^2 \rangle + \langle c_j^2 \rangle] + 2 \sum_j v_{dj} \langle c_i c_j \rangle + \sum_j \langle c_i c_j^2 \rangle$$

The energy flux vector component with these simplifications becomes:

$$F_{Wi} = v_{di} \frac{nm^*}{2} \sum_j [\langle v_{dj}^2 \rangle + \langle c_j^2 \rangle] + 2 \frac{nm^*}{2} \sum_j v_{dj} \langle c_i c_j \rangle + \underbrace{\frac{1}{2} nm^* \sum_j \langle c_i c_j^2 \rangle}_{Q_i}$$

$$= v_{di} W + \cancel{n} m^* \sum_j v_{dj} \frac{k_B}{m^*} T_{ij} + Q_i$$

$$F_{wi} = v_{di} W + n k_B \sum_j T_{ij} v_{dj} + Q_i$$

where $Q_i = \frac{1}{2} n m^* \sum_j \langle c_i c_j^2 \rangle$ is the component of the heat flux vector which describes loss of energy due to flow of heat out of the volume.

To summarize:

$$\vec{F_w} = \vec{v} W + \underbrace{n k_B \overleftrightarrow{T} \cdot \vec{v}} + \underbrace{\vec{Q}}$$

kinetic energy flux

energy density times velocity

velocity times pressure, which actually represents the work to push the volume

loss of energy due to flow of heat out

- With the above representation, the momentum and the energy balance equations become:

$$\frac{\partial J_z}{\partial t} = \frac{2e}{m^*} \sum_i \frac{\partial}{\partial x_i} \left[K_{iz} + \frac{1}{2} n k_B T_{iz} \right] + \frac{ne^2}{m^*} \mathcal{E}_z - \langle\langle \frac{1}{\tau_m} \rangle\rangle J_z$$

$$\frac{\partial W}{\partial t} = -\nabla \cdot \left(\vec{v} W + \vec{Q} + n k_B \overleftrightarrow{T} \cdot \vec{v} \right) + \vec{\mathcal{E}} \cdot \vec{J_n} - \langle\langle \frac{1}{\tau_E} \rangle\rangle [W - W_0]$$

DISPLACED-MAXWELLIAN APPROXIMATION

- Most common way to solve the balance equations is to guess a form for the distribution function and use the balance equations to solve for the parameters in this functional form. Most commonly used form is Displaced-Maxwellian:

$$f(\vec{p}) \sim \exp\left[-|\vec{p} - m^* \vec{v_d}|^2 / 2 m^* k_B T_c \right]$$

This is a good model for cases when electron-electron interactions thermalize the distribution function. For a displaced-Maxwellian, the temperature tensor is diagonal, i.e. $T_{ij} = T_c \delta_{ij}$. With these

approximations: $\sum_i \frac{\partial}{\partial x_i}\left(\frac{1}{2} n k_B T_c \delta_{iz}\right) = \frac{1}{2}\frac{\partial}{\partial x_z}(n k_B T_c)$. The current density (momentum) balance equation becomes:

$$\frac{\partial J_z}{\partial t} = \frac{2e}{m^*}\sum_i \frac{\partial K_{iz}}{\partial x_i} + \frac{\cancel{2}e}{m^*}\frac{1}{\cancel{2}}\frac{\partial}{\partial x_z}(n k_B T_c) + \frac{ne^2}{m^*}\mathcal{E}_z - \langle\langle \frac{1}{\tau_m} \rangle\rangle J_z$$

$$\boxed{\frac{\partial J_z}{\partial t} = \frac{2e}{m^*}\sum_i \frac{\partial K_{iz}}{\partial x_i} + \frac{e}{m^*}\frac{\partial}{\partial x_z}(n k_B T_c) + \frac{ne^2}{m^*}\mathcal{E}_z - \langle\langle \frac{1}{\tau_m} \rangle\rangle J_z}$$

The momentum balance equation can be immediately obtained by multiplying the above result by $(-e/m^*)^{-1}$ to get:

$$\boxed{\frac{\partial P_z}{\partial t} = -\sum_i 2\frac{\partial K_{iz}}{\partial x_i} - \frac{\partial}{\partial x_z}(n k_B T_c) - en\mathcal{E}_z - \langle\langle \frac{1}{\tau_m} \rangle\rangle P_z}$$

Therefore, to solve the balance equation for P_z (or equivalently J_z), one needs to know the carrier temperature:

(a) under low-field conditions, the carrier temperature T_c can be assumed to be equal to the lattice temperature T_L.

(b) under high-field conditions, the carrier temperature T_c is larger than the lattice temperature, and under these circumstances one needs to solve the energy balance equation that is discussed next.

- For displaced-Maxwellian approximation for the distribution function, the heat flux $Q=0$. However, Blotekjaer has pointed out that this term must be significant for non-Maxwellian distributions, so that a phenomenological description for the heat flux, of the form

$$\vec{Q} = -\varkappa \nabla T_c ,$$

where $\varkappa$ is the thermal conductivity, is usually introduced. The above description for $\vec{Q}$ actually leads to a closed set of equations, in which the energy balance equation is of the form:

$$\boxed{\frac{\partial W}{\partial t} = -\nabla\cdot(\vec{v}W - \varkappa\nabla T_c + n k_B T_c \vec{v}) + \vec{\mathcal{E}}\cdot\vec{J_n} - \langle\langle \frac{1}{\tau_E} \rangle\rangle [W - W_0]}$$

Now using:

$$\frac{\partial}{\partial x_i}\left(2K_{iz}\right) = \frac{\partial}{\partial x_i}\left(nm^* v_{di} v_{dz}\right) = nm^* \frac{\partial}{\partial x_i}\left(v_{di} v_{dz}\right) = nm^*\left[\frac{\partial v_{di}}{\partial x_i} v_{dz} + v_{di}\frac{\partial v_{dz}}{\partial x_i}\right]$$

$$= nm^*\left[\frac{\partial v_{di}}{\partial x_i} v_{dz} + v_{di}\frac{\partial v_{dz}}{\partial x_z}\delta_{iz}\right] = nm^*\left[\frac{\partial v_{di}}{\partial x_i} v_{dz} + v_{dz}\frac{\partial v_{dz}}{\partial x_z}\right]$$

and assuming that the spatial variations are confined along the z-direction, we have:

$$\frac{\partial}{\partial x_z}\left(2K_{iz}\right) = nm^*\left[\frac{\partial v_{dz}}{\partial x_z} v_{dz} + v_{dz}\frac{\partial v_{dz}}{\partial x_z}\right] = \frac{\partial}{\partial x_z}\left(nm^* v_{dz}^2\right)$$

- To summarize, the balance equations for the drifted-Maxwellian distribution function simplify to:

Hydrodynamic model

$$\begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{1}{e}\nabla\cdot J_n + S_n \\[2ex] \dfrac{\partial J_z}{\partial t} = \dfrac{e}{m^*}\dfrac{\partial}{\partial x_z}\left(nm^* v_{dz}^2 + nk_B T_c\right) + \dfrac{ne^2}{m^*}\mathcal{E}_z - \left\langle\!\left\langle\dfrac{1}{\tau_m}\right\rangle\!\right\rangle J_z \\[2ex] \dfrac{\partial W}{\partial t} = -\dfrac{\partial}{\partial x_z}\left[\left(W + nk_B T_c\right)v_{dz} - \kappa\dfrac{\partial T_c}{\partial x_z}\right] + J_z\mathcal{E}_z - \left\langle\!\left\langle\dfrac{1}{\tau_E}\right\rangle\!\right\rangle\left[W - W_0\right] \end{cases}$$

where:

$$\begin{cases} J_z = -env_{dz} = -\dfrac{e}{m^*}nm^* v_{dz} = -\dfrac{e}{m^*}P_z \\[2ex] W = \dfrac{1}{2}nm^* v_{dz}^2 + \dfrac{3}{2}nk_B T_c \end{cases}$$

- The next task is to calculate the momentum and energy relaxation rates, which in this case are ensemble averaged quantities. For simple scattering mechanisms, one can utilize the drifted-Maxwellian form of the distribution function, but for cases where several scattering mechanisms are important, one

must use bulk Monte Carlo simulations to calculate these quantities.

MOMENTUM AND ENERGY RELAXATION RATES

(a) using Drifted-Maxwellian form for the D.F.

Assume that the distribution function is of the form:

$$f(\vec{p}) = \exp\left[-\frac{|\vec{p} - m^* \vec{v}_d|^2}{2m^* k_B T_c}\right]$$

where:

$T_c \Rightarrow$ carrier temperature

$\vec{v}_d = v_{dz}\,\vec{i_z} \rightarrow$ carrier drift velocity

expanding the distribution function gives:

$$f(\vec{p}) \approx \exp\left(-\frac{p^2}{2m^* k_B T_c}\right)\left[1 + \frac{1}{2m^* k_B T_c} 2m^* v_{dz} p_z\right]$$

$$\approx \exp\left(-\frac{p^2}{2m^* k_B T_c}\right)\left[1 + \frac{p_z v_{dz}}{k_B T_c}\right] = f_S + f_A$$

- The ensemble averaged momentum relaxation time is then:

$$\left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle = \frac{1}{V} \frac{\sum_{\vec{p}} f(\vec{r},\vec{p},t)\, p_z / \tau_m(p)}{\sum_{\vec{p}} p_z f(\vec{r},\vec{p},t)}$$

For homogeneous systems: $f(\vec{r},\vec{p},t) = f(\vec{p})$ (steady-state).
Since $\tau_m(p)$ is generally even function of p_z, we therefore have contribution from the asymmetric term only, which gives:

$$\left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle = \frac{\frac{1}{V}\sum_{\vec{p}} \frac{p_z^2 v_{dz}}{k_B T_c} \frac{1}{\tau_m(E)} f_S(E)}{\frac{1}{V}\sum_{\vec{p}} \frac{p_z^2 v_{dz}}{k_B T_c} f_S(E)} = \frac{\frac{1}{V}\sum_{\vec{p}} p_z^2 \frac{1}{\tau_m(E)} f_S(E)}{\frac{1}{V}\sum_{\vec{p}} p_z^2 f_S(E)}$$

Now, if θ is the angle between $\vec{p}$ and the electric field $\vec{\mathcal{E}} = \mathcal{E}_z \vec{i_z}$, we have $p_z = p\cos\theta$, which then gives:

$$\left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle = \frac{\int_0^{2\pi} d\varphi \int_{-1}^{1} \cos^2\theta \, d(\cos\theta) \int_0^\infty p^2 dp \; p^2 \frac{1}{\tau_m(E)} f_s(E)}{\int_0^{2\pi} d\varphi \int_{-1}^{1} \cos^2\theta \, d(\cos\theta) \int_0^\infty p^2 dp \; p^2 f_s(E)}$$

$$= \frac{\int_0^\infty p^2 dp \; E(p) \frac{1}{\tau_m(E)} f_s(E)}{\int_0^\infty p^2 dp \; E f_s(E)}$$

For parabolic band structure, for which $E(p) = p^2/2m^*$, we have $p^2 dp = a\sqrt{E}\, dE$. Therefore:

$$\left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle = \frac{\int E^{3/2} \frac{1}{\tau_m(E)} f_s(E)\, dE}{\int E^{3/2} f_s(E)\, dE}$$

For the case when the energy-dependent momentum relaxation rate is of the form:

$$\tau_m(E) = \tau_0 \left(E/k_B T_L\right)^s \quad \text{, we have :}$$

$$\left\langle\!\left\langle \frac{1}{\tau_m} \right\rangle\!\right\rangle = \frac{\int_0^\infty E^{3/2} \frac{1}{\tau_0} E^{-s} (k_B T_L)^s f_s(E)\, dE}{\int_0^\infty E^{3/2} f_s(E)\, dE} =$$

$$= (k_B T_L)^s \frac{1}{\tau_0} \frac{\int_0^\infty E^{3/2-s} f_s(E)\, dE}{\int_0^\infty E^{3/2} f_s(E)\, dE} =$$

$$= (k_B T_L)^s \frac{1}{\tau_0} \frac{\int_0^\infty (E/k_B T_c)^{3/2-s} f_s(E)\, d(E/k_B T_c) \cdot (k_B T_c)^{3/2-s}}{\int_0^\infty (E/k_B T_c)^{3/2} f_s(E)\, d(E/k_B T_c) \, (k_B T_c)^{3/2}}$$

$$= \frac{1}{\tau_0} \left(\frac{T_L}{T_c}\right)^s \frac{\Gamma(5/2 - s)}{\Gamma(5/2)}$$

For low fields, the momentum relaxation rate was given by: $\langle \tau_m \rangle = \tau_0 \dfrac{\Gamma(s+3/2)}{\Gamma(3/2)}$ (very different behavior)

For acoustic deformation potential scattering, $s=-1/2$, which then gives:

$$\langle\langle \frac{1}{\tau_m} \rangle\rangle = \frac{1}{\tau_0}\sqrt{\frac{T_c}{T_L}} \; \frac{\Gamma(3/2+1/2)}{\Gamma(3/2)} = A\sqrt{\frac{T_c}{T_L}}$$

- Similarly, for acoustic deformation potential scattering, the ensemble averaged energy relaxation rate is given by:

$$\langle\langle \frac{1}{\tau_E} \rangle\rangle = B\,\frac{1}{T_L}\sqrt{\frac{T_L}{T_c}}$$

- Now, under steady-state conditions and for homogeneous systems, the momentum and energy balance equations become:

$$\left.\begin{aligned} \frac{ne^2}{m^*}\mathcal{E}_z &= \langle\langle \frac{1}{\tau_m} \rangle\rangle J_z \\ J_z \mathcal{E}_z &= \langle\langle \frac{1}{\tau_E} \rangle\rangle (W - W_0) \end{aligned}\right\} \Rightarrow \frac{ne^2}{m^*}\mathcal{E}_z^2 = \langle\langle \frac{1}{\tau_m} \rangle\rangle \langle\langle \frac{1}{\tau_E} \rangle\rangle \frac{3}{2} k_B (T_c - T_L) n$$

which then leads to:

$$T_c = T_L + \frac{2e^2}{3m^* k_B} \cdot \frac{\mathcal{E}_z^2}{\langle\langle 1/\tau_m \rangle\rangle \langle\langle 1/\tau_E \rangle\rangle}$$

$$\boxed{\frac{T_c}{T_L} = 1 + \left(\mathcal{E}_z / \mathcal{E}_{crit}\right)^2}$$, where $\mathcal{E}_{crit.}$ is some critical field.

(b) Using bulk monte Carlo simulations

- An alternative way of deriving the momentum relaxation rate (ensemble averaged) is to use steady-state Monte Carlo simulation for bulk materials under uniform electric fields. Under these conditions, the momentum balance equation simplifies to:

$$\frac{\cancel{n}e^{\cancel{2}}}{m^*}\mathcal{E}_z = \langle\!\langle \frac{1}{\tau_m} \rangle\!\rangle J_z = -\frac{\cancel{e}}{\cancel{n}\cancel{m^*}} \langle\!\langle \frac{1}{\tau_m} \rangle\!\rangle \cancel{n}\cancel{m^*} v_{dz}$$

which then gives:

$$\langle\!\langle \frac{1}{\tau_m} \rangle\!\rangle = -\frac{e\,\mathcal{E}_z}{m^* v_{dz}}$$

- Similarly, the energy relaxation rate is calculated from the steady-state energy balance equation for bulk materials, which is of the form:

$$J_z\,\mathcal{E}_z = \langle\!\langle \frac{1}{\tau_E} \rangle\!\rangle (W - W_0)$$

which gives:

$$\langle\!\langle \frac{1}{\tau_E} \rangle\!\rangle = \frac{J_z\,\mathcal{E}_z}{W - W_0} = \frac{-en\,v_{dz}\,\mathcal{E}_z}{\frac{3}{2}k_B(T_c - T_L)} = -\frac{en\,v_{dz}\,\mathcal{E}_z}{W - W_0}$$

- Note that the as-calculated momentum and energy relaxation rates are electric field, i.e. energy-dependent quantities.

Simplifications that Lead to the Drift-Diffusion model

- We rewrite the momentum balance equation in the following form:

$$\frac{\partial J_z}{\partial t} + \langle\!\langle \frac{1}{\tau_m} \rangle\!\rangle J_z = \frac{e}{m^*}\frac{\partial}{\partial x_z}\left(nm^* v_{dz}^2 + nk_B T_c\right) + \frac{ne^2}{m^*}\mathcal{E}_z$$

or: $$J_z + \frac{1}{\langle\!\langle 1/\tau_m \rangle\!\rangle}\cdot\frac{\partial J_z}{\partial t} = \frac{e/m^*}{\langle\!\langle 1/\tau_m \rangle\!\rangle}\frac{\partial}{\partial x_z}\left(nm^* v_{dz}^2 + nk_B T_c\right) + ne\frac{e}{m^*\langle\!\langle 1/\tau_m \rangle\!\rangle}\mathcal{E}_z$$

Defining the carrier mobility as: $\mu_n = \dfrac{e}{m^*\langle\!\langle 1/\tau_m \rangle\!\rangle}$, we first have for acoustic deformation potential scattering:

$$\mu_n = \frac{e}{m^* A\sqrt{T_c/T_L}} = \frac{\mu_0}{\sqrt{1 + (\mathcal{E}_z/\mathcal{E}_{crit})^2}}$$ $\longrightarrow$ decrease in mobility with increase in electric field.

For general case, we have:

$$J_z + \frac{1}{\langle\langle 1/\tau_m \rangle\rangle} \frac{\partial J_z}{\partial t} = \mu_n \frac{\partial}{\partial x_z}\left(n m^* v_{dz}^2 + n k_B T_c\right) + n e \mu_n \mathcal{E}_z$$

<u>Approximation</u>: Assume that the carrier drift energy is much smaller than the thermal energy. This approximation is valid for low-field conditions and leads to kinetic energy density of the form:

$$W = \frac{1}{2} n m^* v_{dz}^2 + \frac{3}{2} n k_B T_c \approx \frac{3}{2} n k_B T_c$$

Hence:

$$n k_B T_c \approx \frac{2}{3} W$$

Under steady-state conditions this then leads to:

$$J_z = \mu_n \frac{\partial}{\partial x_z}\left(\frac{2}{3} W\right) + n e \mu_n \mathcal{E}_z = n e \mu_n \mathcal{E}_z + \underbrace{\frac{2}{3} \mu_n \frac{\partial}{\partial x_z}(W)}$$

The above expression suggests that diffusion is associated with gradients in the kinetic energy density.

The simplified expression for J_z can also be written as:

$$J_z = k_B T_c \mu_n \frac{\partial n}{\partial x_z} + n k_B \mu_n \frac{\partial T_c}{\partial x_z} + n e \mu_n \mathcal{E}_z$$

$$= e D_n \frac{\partial n}{\partial x_z} + e S_n \frac{\partial T_c}{\partial x_z} + e n \mu_n \mathcal{E}_z$$

where: $D_n = \frac{k_B T_c}{e} \mu_n$ is the diffusion coefficient

$S_n = n k_B \mu_n / e$ is the Soret coefficient

- As a further simplification to the drift-diffusion equations, we assume that there are no temperature gradients in the system. Then,

the set of equations that one solves using, for example, in Silvaco's ATLAS, is of the form:

$$\begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{1}{e} \nabla \cdot \vec{J_n} + \underbrace{G_n - R_n}_{S_n} \\ \vec{J_n} = e n \mu_n \vec{\mathcal{E}} + e D_n \nabla n \end{cases}$$

Note that in the above expressions, D_n and μ_n are low-field quantities. To extend the validity of this model for high-field conditions, one usually uses field-dependent models for the mobility and the diffusion coefficient. A variety of models have been developed for this purpose.

(1) Closure:

To close the Balance - Hydrodynamic equations, one needs to use some kind of a model for the heat flux:

(a) Ignore the heat flux altogether
(b) Use the Franz-Wiedemann law, which states that:

$$n\vec{q} = -\kappa \nabla T$$

where κ is the heat conductivity of the electron gas. In Silicon, the experimental value of κ is 1.4 W/cmK. It has been recognized in recent years that this approach is not correct for semiconductors in the junction regions, where high and unphysical velocity peaks are established by the Franz-Wiedemann law.

(c) Stettler, Alam and Lundstrom have suggested a new form for practical applications:

$$\vec{Q} = -\kappa \nabla T + \frac{5}{2}(1-r)\frac{k_B T_0}{q}\vec{J}$$

where:

$T_0 \Rightarrow$ lattice temperature
$\vec{J} \Rightarrow$ current density
$r \Rightarrow$ tunnable parameter less than unity.

(*) Important thing to notice here is that for a truly a displaced Maxwellian distribution function of the form:

$$f(p) \sim \exp\left[-|\vec{p} - m^*\vec{v}_d|^2/2m^* k_B T_c\right]$$

the heat flux is $\vec{Q} = 0$. Since the heat flux is often important in devices, it is better to abandon the displaced Maxwellian when evaluating $\vec{Q}$ and to use the phenomenological expressions given in (b) and (c).

(2) Ensemble rates calculation

The momentum and energy ensemble relaxation rates can be calculated in two different ways:

(1) Assuming displaced Maxwellian distribution function to obtain analytic results for the ensemble relaxation rates
(2) Using bulk Monte Carlo calculations to obtain the energy dependence of the ensemble relaxation rates.