BOLTZMANN TRANSPORT EQUATION - INTRODUCTION

- To completely specify the operation of a device, one must know the state of each carrier within the device. If carriers are treated as classical particles, one way of specifying the state of carriers is to solve Newton's equations:

$$\frac{d\vec{p_i}}{dt} = -e\vec{\mathcal{E}} + R(\vec{r},\vec{p},t) \quad \text{and} \quad \vec{v_i}(t) = \frac{d\vec{r_i}}{dt},$$

where $R(\vec{r},\vec{p},t)$ is a random force function due to impurities or lattice vibrations.

- Alternative approach would be to calculate the probability of finding a carrier with crystal momentum $\vec{k}$ at position $\vec{r}$ at time t, given by the distribution function $f(\vec{r},\vec{k},t)$, obtained by solving BTE.

It is important to note that this theory is based on the following assumptions:
(1) Electrons and holes are independent particles.
(2) The system is described by a set of Bloch functions.
(3) Particles do not interact with each other, but may be scattered by impurities, phonons, etc.
(4) The number of electrons in an elementary volume ΔV centered around $\vec{r}$, that have wave vectors in a range of d^3k centered around $\vec{k}$ is given by:

$$2 \times \frac{\Delta V}{8u^3} \, f(\vec{r},\vec{k},t) \, d^3k$$

Therefore, once the distribution function is specified, various moments of the distribution function can give us particle density, current density, energy density, etc. More precisely:

$$n(\vec{r},t) = \frac{1}{V}\sum_{k} f(\vec{r},\vec{k},t) \qquad \rightarrow \text{particle density}$$

$$J(\vec{r},t) = -\frac{e}{V}\sum_{k} \vec{v}(\vec{k})\, f(\vec{r},\vec{k},t) \quad \rightarrow \text{current density}$$

$$W(\vec{r},t) = \frac{1}{V}\sum_{k} E(\vec{k})\, f(\vec{r},\vec{k},t) \quad \rightarrow \text{energy density}$$

• A full quantum mechanical view to this problem is rather difficult. The uncertainty principle states, for example, that we can not specify simultaneously the position and the momentum of the particle. Hence, one needs to adopt a coarse-grained average point of view, in which positions are only specified within a macroscopic volume element, and momenta are also within some interval. If one tries to go straightforwardly and constructs $f(\vec{r}, \vec{k}, t)$ from the quantum-mechanical wave functions, difficulties arise since f cannot be positive everywhere.

(A) APPROXIMATIONS USED FOR $f(\vec{r}, \vec{p}, t)$

The most difficult problem in device analysis is to calculate the distribution function $f(\vec{r}, \vec{k}, t)$. To overcome these difficulties, reasonable guess for the distribution function is often made. Two most commonly used approaches are:
- quasi-Fermi level concept
- displaced Maxwellian approximation for the distribution function

Quasi-Fermi levels

Under equilibrium conditions $np = n_i^2$, where n_i is the intrinsic carrier concentration; which follows from the use of the equilibrium distribution functions for electrons and holes, i.e.

$$f_n = \frac{1}{1+\exp\left(\frac{E-E_F}{k_B T}\right)} \quad \text{and} \quad f_p(E) = 1 - f_n(E) = \frac{1}{1+\exp\left(\frac{E_F-E}{k_B T}\right)}$$

Under non-equilibrium conditions, it may still be useful to represent the distribution functions for electrons and holes as:

$$f_n(E) = \frac{1}{1+\exp\left(\frac{E-E_{Fn}}{k_B T}\right)} \quad \text{and} \quad f_p(E) = \frac{1}{1+\exp\left(\frac{E_{FP}-E}{k_B T}\right)}$$

Therefore, under nonequilibrium conditions and assuming non-degenerate sc, we will have:

$$n = N_c \exp\left(\frac{E_{Fn}-E_c}{k_B T}\right) \quad \text{and} \quad p = N_v \exp\left(\frac{E_v-E_{FP}}{k_B T}\right).$$

The product $np = n_i^2 \exp\left(\frac{E_{Fn} - E_{FP}}{k_B T}\right)$ suggests that the difference $E_{Fn} - E_{FP}$ is a measure for the deviation from the equilibrium.

excess electron density is zero

excess hole density is zero
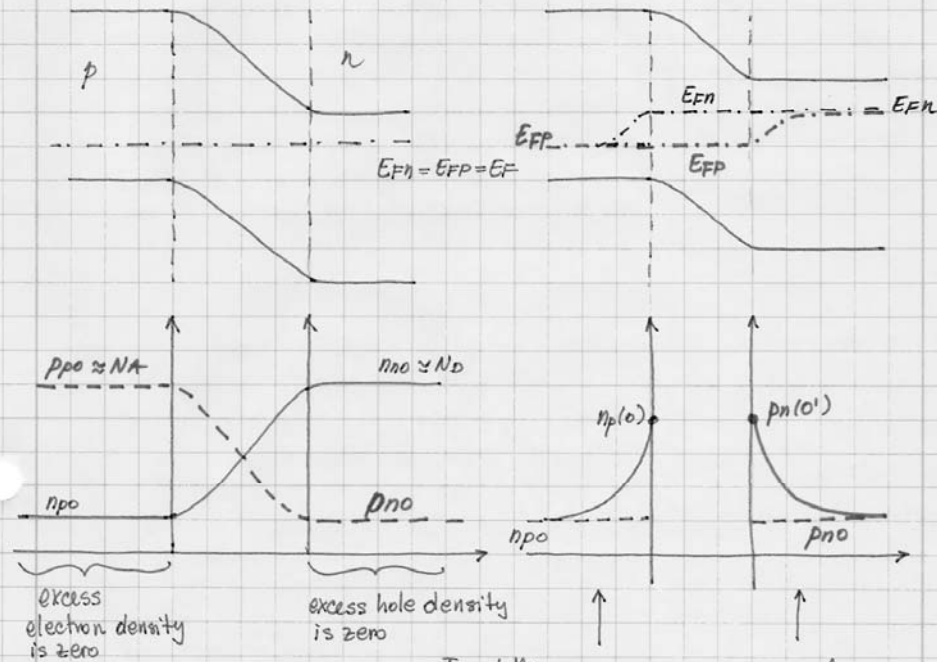
To get this excess electron density the electron quasi-Fermi level must move up, thus increasing the probability of state occupancy

Same here. To get excess hole density, hole quasi-Fermi level moves downward.

• However, this can not be correct distribution function since it is even in k, which means that it suggests that current can never flow in a device. The fact that makes it not so unreasonable is that average carrier velocities are usually much smaller than the spread in velocity, given by:

$$\sqrt{\frac{2k_B T}{m^*}} \approx 10^7 \text{ cm/s} \quad \text{for } m^* = m_0 \text{ (free-electron mass)}$$

DISPLACED MAXWELLIAN DISTRIBUTION FUNCTION

- Better guess for $f(\vec{r},\vec{k},t)$ is to assume that the distribution function retains its shape, but that its average momentum is displaced from the origin. For example, particularly suitable form to use is:

$$f(\vec{r},\vec{k},t) = \exp\left(\frac{E_{Fn}-E_{c0}}{k_B T}\right) \exp\left[-\frac{\hbar^2}{2m^* k_B T}\,|\vec{k}-\vec{k}_d|^2\right]$$
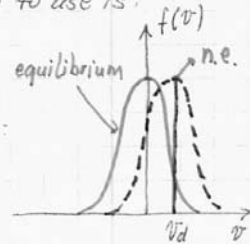
- Using this form of the distribution function gives:

$$n(\vec{r},t) = \frac{1}{V}\sum_{\vec{k}} f(\vec{r},\vec{k},t) = N_c \exp\left(\frac{E_{Fn}-E_{c0}}{k_B T}\right)$$

$$w(\vec{r},t) = \frac{1}{V}\frac{V}{4\bar{u}^3}\int_0^{2\bar{u}} d\varphi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} k^2 dk\ \frac{\hbar^2 k^2}{2m^*}\exp\left[\frac{E_{Fn}-E_{c0}}{k_B T}\right]\exp\left[\frac{-\hbar^2|\vec{k}-\vec{k}_d|^2}{2m^* k_B T}\right]$$

using variable change: $\vec{k}-\vec{k}_d = \vec{k}'$ => $\vec{k} = \vec{k}_d + \vec{k}'$, we get:

$$w(\vec{r},t) = \frac{1}{2\bar{u}^2}\int_0^{\infty} k^2 dk'\int_{-1}^{1} d(\cos\theta)\frac{\hbar^2}{2m^*}\underbrace{|\vec{k}'+\vec{k}_d|^2}_{k'^2 + 2k_d k'\cos\theta + k_d^2}\exp\left[\frac{E_{Fn}-E_{c0}}{k_B T}\right]\exp\left[-\frac{\hbar^2 k'^2}{2m^* k_B T}\right]$$

$$= \frac{1}{2\bar{u}^2}\int_0^{\infty} k'^2 dk'\int_{-1}^{1} d(\cos\theta)\ \frac{\hbar^2 k'^2}{2\mu^*}\exp\left(\frac{E_{Fn}-E_{c0}}{k_B T}\right)\exp\left(-\frac{\hbar^2 k'^2}{2m^* k_B T}\right)$$

$$+ \frac{\hbar^2}{2m^*}k_d^2\ \frac{1}{2\bar{u}^2}\int_0^{\infty} k'^2 dk'\int_{-1}^{1} d(\cos\theta)\exp\left(\frac{E_{Fn}-E_{c0}}{k_B T}\right)\exp\left(-\frac{\hbar^2 k'^2}{2m^* k_B T}\right)$$

$$+ \frac{\hbar^2 k_d}{m^*}\ \frac{1}{2\bar{u}^2}\int_0^{\infty} k'^2 dk'\underbrace{\int_{-1}^{1} d(\cos\theta)\ k'\cos\theta\exp\left(\frac{E_{Fn}-E_{c0}}{k_B T}\right)\exp\left(-\frac{\hbar^2 k'^2}{2m^* k_B T}\right)}_{\text{integration gives } 0}$$

$$w(\vec{r},t) = \frac{3}{2}n k_B T + \frac{1}{2}n\frac{\hbar^2 k_d^2}{m^*} = \left(\frac{3}{2}k_B T + \frac{\hbar^2 k_d^2}{2m^*}\right)n$$

The kinetic energy density per carrier is then given by:

$$u(\vec{r},t) = \frac{w(\vec{r},t)}{n} = \underbrace{\frac{1}{2}m^* v_d^2}_{\substack{\text{drift energy due to average} \\ \text{drift velocity}}} + \underbrace{\frac{3}{2}k_B T}_{\substack{\text{thermal energy due to collisions} \\ \text{of carriers with phonons}}}$$

Since in both cases, the guess for the non-equilibrium distribution has been guided by the form of the equilibrium, they are only valid in near-equilibrium conditions. For far-from-equilibrium conditions, the shape of the distribution function can be rather different. This requires the solution of the BTE that is introduced below.

(B) THE BOLTZMANN TRANSPORT EQUATION (BTE)

○ To derive the BTE, consider a region of phase space about the point (x, y, z, p_x, p_y, p_z). The number of particles entering this region in time dt is equal to the number which were in the region of phase space at: $(x - v_x dt, y - v_y dt, z - v_z dt, p_x - F_x dt, p_y - F_y dt, p_z - F_z dt)$ at a time dt earlier. If $f(x, y, z, p_x, p_y, p_z)$ is the distribution function, which expresses the number of particles per quantum state in the region, then the change df which occurs during time dt due to the motion of the particles in coordinate space and due the fact that force fields acting on the particles tend to move them from one region to another in momentum space is.

$$df = f(x - v_x dt, y - v_y dt, z - v_z dt, p_x - F_x dt, p_y - F_y dt, p_z - F_z dt) - f(x, y, z, p_x, p_y, p_z)$$

Using taylor series expansion, we get:

$$df = \left[-v_x \frac{\partial f}{\partial x} - v_y \frac{\partial f}{\partial y} - v_z \frac{\partial f}{\partial z} - F_x \frac{\partial f}{\partial p_x} - F_y \frac{\partial f}{\partial p_y} - F_z \frac{\partial f}{\partial p_z} \right] dt$$

i.e.

$$\frac{df}{dt} = -\vec{v} \cdot \nabla_r f - F \cdot \nabla_p f$$

○ So far, only the change in the distribution function due to the motion of the particles in coordinate space and due to the momentum changes arising from the force fields acting on the particles have been accounted for. Particles may also be transfered into or out of a given region of phase space by collisions or scattering interactions involving

other particles of the distribution or scattering centers exter-nal to the assembly of particles under consideration. If the rate of change of the distribution function due to collisions or scattering is denoted by $(\partial f/\partial t)_{coll}$, the total rate of change of f becomes:

$$\frac{df}{dt} = -\vec{v}\cdot\nabla_r f - \vec{F}\cdot\nabla_p f + \frac{\partial f}{\partial t}\Big|_{coll}$$

i.e.

$$\boxed{\frac{df}{dt} + \vec{v}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f = \frac{\partial f}{\partial t}\Big|_{coll.} + s(\vec{r},\vec{p},t)}$$

due to generation-recombination processes.

The above equation represents the Boltzmann Transport equation, which is nothing more but a book-keeping equation for the particle flow in the phase space. The various terms that appear represent:

(a) $\dfrac{\partial f}{\partial t}\Big|_{Forces} = -F\nabla_p f$, where $\vec{F} = \dfrac{d\vec{p}}{dt} = \hbar\dfrac{d\vec{k}}{dt} = -e(\vec{E} + \vec{v}\times\vec{B})$

Electrostatic   Lorentz force

(b) $\dfrac{\partial f}{\partial t}\Big|_{diff} = -\vec{v}\cdot\nabla_r f \rightarrow$ this term arises if there is a spatial variation in the distribution function due to concentration gradient or temperature gradient, both of which will result in a diffusion of carriers in coordinate space.

(c) $\dfrac{\partial f}{\partial t}\Big|_{coll} \rightarrow$ This is the collision term which equals the difference between the in-scattering and out-scattering processes, i.e.

$$\frac{\partial f}{\partial t}\Big|_{coll} = \sum_{k'}\left\{s(\vec{k}',\vec{k})f(\vec{k}')[1-f(\vec{k})] - s(\vec{k},\vec{k}')f(\vec{k})[1-f(\vec{k}')]\right\} = \hat{c}f$$

The presence of $f(\vec{k})$ and $f(\vec{k}')$ in the collision integral, makes

the BTE rather complicated integro-differential equation for $f(\vec{r}, \vec{k}, t)$, whose solution requires a number of simplifying assumptions.
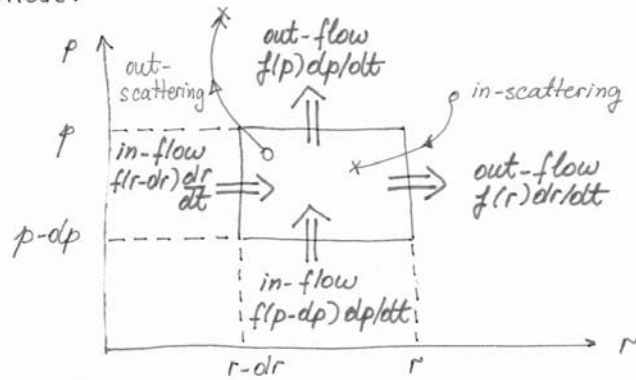
Cell in two-dimensional position-momentum space.

- In the absence of perturbing fields and temperature gradients, the distribution function must be the Fermi-Dirac function f_0. In this case, the collision term must vanish and the PRINCIPLE OF DETAILED BALANCE gives for all $\vec{k}$ and $\vec{k}'$ and all scattering mechanisms:

$$S(\vec{k}', \vec{k}) \, f_0(\vec{k}') \, [1 - f_0(\vec{k})] = S(\vec{k}, \vec{k}') \, f_0(\vec{k}) \, [1 - f_0(\vec{k}')]$$

i.e. $$\frac{S(\vec{k}, \vec{k}')}{S(\vec{k}', \vec{k})} = \frac{f_0(\vec{k}') \, [1 - f_0(\vec{k})]}{f_0(\vec{k}) \, [1 - f_0(\vec{k}')]} .$$

Now, using equilibrium Fermi-Dirac statistics, we get:

$$\frac{f_0(\vec{k})}{1 - f_0(\vec{k})} = \frac{\dfrac{1}{1 + \exp[(E_c + E_k - E_F)/k_B T]}}{1 - \dfrac{1}{1 + \exp[(E_c + E_k - E_F)/k_B T]}} = \frac{1}{1 + \exp[(E_c + E_k - E_F)/k_B T] - 1}$$

i.e. $$\frac{f_0(\vec{k})}{1 - f_0(\vec{k})} = \exp[-(E_c + E_k - E_F)/k_B T]$$

Therefore, if the phonons interacting with the electrons are in thermal equilibrium, we get:

$$\frac{S(\vec{k}, \vec{k}')}{S(\vec{k}', \vec{k})} = \frac{\exp(-E_{k'}/k_B T)}{\exp(-E_k/k_B T)} = \exp\left(\frac{E_k - E_{k'}}{k_B T}\right)$$

This relation must be satisfied regardles of the origin of the scattering fores. Let assume $E_K > E_{K'}$. $S(k, k')$ which involves emission must exceed $S(k', k)$ which involves absorption.