

## The Drift-Diffusion model for semiconductors

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ABSTRACT: Some notes on Boltzmann Transport Equation (BTE) and the derivation of the Drift-Diffusion model (DD) from the 0<sup>th</sup> and 1<sup>st</sup> moment of BTE are presented.

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### 1 The Boltzmann's transport equation (BTE)

The BTE is essentially a continuity equation in the  $6^{th}$  dimensional space  $(\vec{x}, \vec{p}, t)$ . Assuming the motion of the particles is described by a Hamiltonian and that no collisions happen during the time interval  $dt$ , defining the vectors:

$$\vec{x} := \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} := \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ p_x \\ p_y \\ p_z \end{pmatrix}$$
$$\vec{Y} := \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \end{pmatrix} := \begin{pmatrix} \frac{\partial H}{\partial p_1} \\ \frac{\partial H}{\partial p_2} \\ \frac{\partial H}{\partial p_3} \\ -\frac{\partial H}{\partial q_1} \\ -\frac{\partial H}{\partial q_2} \\ -\frac{\partial H}{\partial q_3} \end{pmatrix}$$

the Hamilton's equations:

$$\begin{aligned} \frac{dq_r}{dt} &= \frac{\partial H}{\partial p_r} \\ \frac{dp_r}{dt} &= -\frac{\partial H}{\partial q_r} \end{aligned} \tag{1.1}$$

in vector form can be written as:

$$\frac{d\vec{x}}{dt} = \vec{Y} \tag{1.2}$$

Also:

$$\nabla \cdot \vec{Y} = \sum_{n=1}^6 \frac{\partial Y_i}{\partial x_i} = \sum_{n=1}^3 \frac{\partial^2 Y_i}{\partial p_i \partial q_i} + \sum_{n=1}^3 -\frac{\partial^2 Y_i}{\partial q_i \partial p_i} = 0 \quad (1.3)$$

The differential phase space volume  $dK$  after an infinitesimal interval  $dt$  from an initial phase space surface  $S$  of normal  $\vec{n}$  can be written as:

$$dK = \int_S d\vec{x} \cdot \vec{n} dS = dt \int_S \frac{d\vec{x}}{dt} \cdot \vec{n} dS \quad (1.4)$$

$$= dt \int_S \vec{Y} \cdot \vec{n} dS = dt \int_V (\nabla \cdot \vec{Y}) dV = 0 \quad (1.5)$$

which implies that the volume of the phase space is invariant when the system of particles is described by a Hamiltonian (1.1).

Writing  $\Phi = \Phi(\vec{r}, \vec{p}, t)$  as the number of particles in the sixth-dimensional phase space,  $\Phi dK$  represents the number of particles in the infinitesimal volume  $dK$  of the phase space around  $(\vec{r}, \vec{p}, t)$ . If the number of particles does not change, its variation can be written as  $\Phi(\vec{r} + d\vec{r}, \vec{p} + d\vec{p}, t + dt) dK' - \Phi(\vec{r}, \vec{p}, t) dK = 0$  because it is the same number of particles. Due to the invariance of the volume  $K' = K$ , it follows that :

$$\frac{d\Phi}{dt} = 0 \quad (1.6)$$

Writing (1.6) explicitly:

$$\frac{d\Phi}{dt} = \frac{\partial \Phi}{\partial t} + \sum_{n=1}^3 \frac{\partial \Phi}{\partial x_i} \frac{dx_i}{dt} + \sum_{n=1}^3 \frac{\partial \Phi}{\partial p_i} \frac{dp_i}{dt} = 0 \quad (1.7)$$

which can be written as:

$$\frac{\partial \Phi}{\partial t} + \vec{v}_g \cdot \nabla_r \Phi + \vec{F} \cdot \nabla_p \Phi = 0 \quad (1.8)$$

where  $\vec{v}_g$  represents the group velocity of the particle and its change in momentum is due to the applied force  $\vec{F}$ . Equation (1.8) includes only the change in the distribution function  $\Phi$  due to the motion of particles in coordinate space and due to momentum changes arising from applied forces. But particles can be transferred into or out of a region of phase space by collisions and/or recombination-generation mechanisms. Including such effects in (1.8), we can write:

$$\frac{\partial \Phi}{\partial t} + \vec{v}_g \cdot \nabla_r \Phi + \vec{F} \cdot \nabla_p \Phi = \frac{d\Phi}{dt} \Big|_{coll} + G(\vec{r}, \vec{p}, t) \quad (1.9)$$

where the two terms in the RHS represent the rate of change due to collisions and generation/recombination of particles. Equation 1.9 represents Boltzmann's transport equation (BTE), essentially a continuity equation in a six-dimensional phase space. It is valid under the assumption of semiclassical transport, i.e. :

- Born approximation
- effective mass approximation
- instantaneous collisions
- no memory effects

As the total number of particles is  $\Phi(\vec{r}, \vec{p}, t)d^3r d^3p = f(\vec{r}, \vec{k}, t)d^3r d^3k$  and using the  $p = \hbar k$  as the crystal momentum, (1.9) can be written as:

$$\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} + \vec{v}_g \cdot \nabla_r f(\vec{r}, \vec{k}, t) + \frac{1}{\hbar} \vec{F} \cdot \nabla_k f(\vec{r}, \vec{k}, t) = \left. \frac{df(\vec{r}, \vec{k}, t)}{dt} \right|_{coll} + G(\vec{r}, \vec{k}, t) \quad (1.10)$$

The RHS of (1.10) includes the scattering and recombination-generation effects. One often used approach to model these is via the relaxation time approximation (**RTA** [1]), where the distribution function is split into a symmetric and asymmetric term, i.e.  $f(\vec{r}, \vec{k}, t) = f_S(\vec{r}, \vec{k}, t) + f_A(\vec{r}, \vec{k}, t)$ . Under the assumption of non-degenerate semiconductor  $1 - f(\vec{r}, \vec{k}, t) \approx 1$  one gets:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \sum_{k'} [f_S(\vec{k}')S(\vec{k}', \vec{k}) - f_S(\vec{k})S(\vec{k}, \vec{k}')] + \sum_{k'} [f_A(\vec{k}')S(\vec{k}', \vec{k}) - f_A(\vec{k})S(\vec{k}, \vec{k}')] \quad (1.11)$$

Under equilibrium conditions the symmetric term  $f_S = f_0$  and the asymmetric term  $f_A = 0$ . In general in non-equilibrium conditions  $f_A \neq 0$ . In all cases of practical interests, for conditions not too far from equilibrium, a reasonable approximation is to assume:

$$\left. \frac{df}{dt} \right|_{coll} = -\frac{f_A}{\tau_f} \quad (1.12)$$

with  $\tau_f$  the characteristic time, assumed independent on the applied electric field, that describes the relaxation time of the distribution function to its equilibrium value, following scattering events. For near-equilibrium conditions, i.e low-field conditions and for non-degenerate semiconductors, (1.12) leads to a displaced Maxwellian form for the distribution function:

$$f(\vec{r}, \vec{k}, t) = \exp\left(\frac{E_{Fn} - E_{C0}}{k_B T}\right) \exp\left(\frac{-\hbar^2}{2m^* k_B T} |\vec{k} - \vec{k}_d|^2\right) \quad (1.13)$$

with  $\vec{k}_d = \frac{e\vec{E}\tau_f}{\hbar}$  the wave vector associated to the drift velocity  $\vec{v}_d$  due to the electric field,  $E_{Fn}$  the *quasi-Fermi* level,  $E_{C0}$  the energy level of the conduction band and  $m^*$  the effective mass. Once the distribution function is determined, the various moments of the distribution provide the values of quantity of interest, such as particle density, current density and energy density:

- particle density:

$$n(\vec{r}, t) = \frac{1}{V} \sum_{\vec{k}} f(\vec{r}, \vec{k}, t) \quad (1.14)$$

- current density:

$$J(\vec{r}, t) = -\frac{e}{V} \sum_{\vec{k}} v(\vec{k}) f(\vec{r}, \vec{k}, t) \quad (1.15)$$

- energy density:

$$W(\vec{r}, t) = \frac{1}{V} \sum_{\vec{k}} E(\vec{k}) f(\vec{r}, \vec{k}, t) \quad (1.16)$$

Formally, the scattering processes can be described using Fermi's golden rule, which accounts for energy and momentum conservation and provides the transition rate:

$$S(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar} |\langle \vec{k}, \vec{k}' \rangle|^2 \delta(E_{\vec{k}'} - E_{\vec{k}} \mp \hbar\omega) \quad (1.17)$$

The matrix element  $|\langle \vec{k}, \vec{k}' \rangle|$  is evaluated using plane wave electron wave functions, where the overlap integral due to the cell periodic part of the Bloch function is assumed to be unity in the case of spherical energy surfaces and parabolic dispersion relations:

$$|\langle \vec{k}, \vec{k}' \rangle| = \frac{1}{\Omega} \int_{-\infty}^{+\infty} \exp(-i\vec{k}' \cdot \vec{r}) V_s(\vec{r}) \exp(i\vec{k} \cdot \vec{r}) d^3r \quad (1.18)$$

Effects due to the finite collision time and collision broadening, i.e. the fact that the energy conservation part of (1.17) is valid only asymptotically or for times long after the collision is complete, can often be neglected ([2]).

## 2 Approximations of BTE: the Drift-Diffusion model

The moments of the BTE allow the description of charge carriers under the various influences of forces and gradients of concentration. The general expression:

$$\int_{\vec{k}} k_1^\alpha k_2^\beta k_3^\gamma f(\vec{r}, \vec{k}, t) d^3k, \quad (2.1)$$

$\alpha, \beta, \gamma \in \mathbb{N}$  provides different moments of the BTE, leading to different models for describing electronic devices. The moment of order 0, i.e.  $\alpha, \beta, \gamma = 0$ :

$$\int_{\vec{k}} f(\vec{r}, \vec{k}, t) d^3k \quad (2.2)$$

has a unique value and leads to the continuity equation.  
The moment of order 1:

$$\int_{\vec{k}} k_i f(\vec{r}, \vec{k}, t) d^3 k, \quad i = 1, 2, 3 \quad (2.3)$$

provides three different values and leads to the current density equations, which, with the inclusion of the continuity equation and Poisson's equation, constitute the drift-diffusion model. The moment of order 2:

$$\int_{\vec{k}} k_i k_j f(\vec{r}, \vec{k}, t) d^3 k, \quad (i, j) = 1, 2, 3 \quad (2.4)$$

gives 9 values, of which only 6 are independent ( $k_i k_j = k_j k_i$ ). In combination with the previous moments it leads to the hydrodynamic model.

In general, for devices of relatively large size, i.e.  $> 100$ 's nm, one should not expect an abrupt variation of the internal field or very steep doping gradients, which would require the use of the hydrodynamic model. Hence, in most cases of practical interest for HEP sensors, the DD model is adequate to describe the behaviour of the device. Such a model can be easily derived from the 0<sup>th</sup> and 1<sup>st</sup> moment of the BTE, as shown below.

Taking the 0<sup>th</sup> order of (1.10) provides:

$$\int_{\vec{k}} \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} d^3 k = \frac{\partial}{\partial t} \int_{\vec{k}} f(\vec{r}, \vec{k}, t) d^3 k = \frac{\partial n(\vec{r})}{\partial t}; \quad (2.5)$$

$$\begin{aligned} \int_{\vec{k}} \vec{v}_g \cdot \nabla_r f(\vec{r}, \vec{k}, t) d^3 k &= \nabla_r \int_{\vec{k}} \vec{v}_g f(\vec{r}, \vec{k}, t) d^3 k = \\ \nabla_r n(\vec{r}, t) \frac{\int_{\vec{k}} \vec{v}_g f(\vec{r}, \vec{k}, t) d^3 k}{n(\vec{r}, t)} &= \nabla_r (n(\vec{r}, t) \langle \vec{v}_g \rangle); \end{aligned} \quad (2.6)$$

$$-\frac{1}{\hbar} \int_{\vec{k}} \vec{F} \cdot \nabla_k f(\vec{r}, \vec{k}, t) d^3 k = -\frac{q}{\hbar} \int_{\vec{k}} (\vec{E} + \vec{v}_g \times \vec{B}) \cdot \nabla_k f(\vec{r}, \vec{k}, t) d^3 k = \mathbf{0}; \quad (2.7)$$

Equation (2.7) is a consequence of the asymptotic null behaviour of  $f(\vec{r}, \vec{k}, t)$ . Putting together (2.5), (2.6) and (2.7), equation (1.10) can be written as:

$$\frac{\partial n(\vec{r})}{\partial t} = \frac{1}{q} \nabla_r \cdot \vec{J}_n + U_n \quad (2.8)$$

where  $J_n$  represents the electron current density and  $U_n$  includes all the net generation-recombination rates for electrons. Equation (2.8) expresses the continuity equation for electrons, a similar expression can be derived for holes, by simply changing the sign for the charge  $q$ .

Taking the 1<sup>st</sup> order of (1.10) leads to the current density equation. Using  $\alpha = 1$  in (2.1) and multiplying (1.10) by  $\frac{\hbar}{m_i^*}$ , i.e. by integrating w.r.t. the group velocity rather than  $k_i$ , gives:

$$\int_{\vec{k}} \frac{\partial v_{gi} f(\vec{r}, \vec{k}, t)}{\partial t} d^3 k = \frac{\partial}{\partial t} \int_{\vec{k}} v_{gi} f(\vec{r}, \vec{k}, t) d^3 k = \frac{\partial (\langle v_{gi} \rangle n(\vec{r}))}{\partial t}; \quad (2.9)$$

$$\begin{aligned} -\frac{1}{\hbar} \int_{\vec{k}} v_{gi} \vec{F} \cdot \nabla_k f(\vec{r}, \vec{k}, t) d^3 k &= -\frac{q}{\hbar} \int_{\vec{k}} v_{gi} (\vec{E} \cdot \nabla_k f(\vec{r}, \vec{k}, t)) d^3 k = \\ &= -\frac{q}{\hbar} \frac{\hbar}{m_i^*} \sum_j E_j \int_{\vec{k}} k_i \left( \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial k_j} \right) d^3 k = \\ &= -\frac{q}{m_i^*} \sum_j E_j (-n \delta_{ij}) = \frac{q}{m_i^*} n E_i \end{aligned} \quad (2.10)$$

$$\begin{aligned} \int_{\vec{k}} v_{gi} (\vec{v}_g \cdot \nabla_r f(\vec{r}, \vec{k}, t)) d^3 k &= \sum_j \frac{\partial}{\partial x_j} \int_{\vec{k}} (v_{agi} + v_{rgi}) (v_{agj} + v_{rgj}) f(\vec{r}, \vec{k}, t) d^3 k = \\ \sum_j \frac{\partial}{\partial x_j} (v_{agi} v_{agj} \int_{\vec{k}} f(\vec{r}, \vec{k}, t) d^3 k + v_{agi} \int_{\vec{k}} v_{rgj} f(\vec{r}, \vec{k}, t) d^3 k + v_{agj} \int_{\vec{k}} v_{rgi} f(\vec{r}, \vec{k}, t) d^3 k + \\ & \int_{\vec{k}} v_{rgj} v_{rgi} f(\vec{r}, \vec{k}, t) d^3 k = \\ \sum_j \frac{\partial}{\partial x_j} (v_{agi} v_{agj} n + \int_{\vec{k}} v_{rgj} v_{rgi} f(\vec{r}, \vec{k}, t) d^3 k) &= \\ \nabla \cdot (v_{agi} n \vec{v}_g) + \nabla \cdot \left( \frac{n k_B \widehat{T}_i}{m_i^*} \right) &= \\ v_{agi} \nabla \cdot (n \vec{v}_g) + n \vec{v}_g \nabla (v_{agi}) + \nabla \cdot \left( \frac{n k_B \widehat{T}_i}{m_i^*} \right) & \end{aligned} \quad (2.11)$$

where, in the last term of (2.11), the average kinetic energy of the carrier due to thermal motion  $v_{rg}$ , i.e. the random component of the group velocity  $\vec{v}_g$ , written as the sum of an average plus a random term  $\vec{v}_g = \vec{v}_g + v_{rg}$ , has been written as  $k_B \widehat{T}_i$ , with  $\widehat{T}_i$  the temperature tensor for electrons. This temperature is not the lattice temperature  $T_L$ , which is defined only at equilibrium, but it allows us to describe the energy of the carriers out of equilibrium using a dimensionally correct form. At equilibrium, it can be shown that the temperature tensor becomes the lattice temperature ([3]).

The last term of (1.10) can be written as:

$$\int_{\vec{k}} v_{gi} \left( \frac{df(\vec{r}, \vec{k}, t)}{dt} \Big|_{coll} \right) d^3 k = C_{vi} \quad (2.12)$$

Putting together (2.9), (2.10), (2.11) and (2.12) one obtains:

$$va_{gi} \frac{\partial n}{\partial t} + n \frac{\partial va_{gi}}{\partial t} + va_{gi} \nabla \cdot (nv\vec{a}_g) + nv\vec{a}_g \nabla (va_{gi}) + \nabla \cdot \left( \frac{nk_B \widehat{T}_i}{m_i^*} \right) + \frac{q}{m_i^*} n E_i = C_{vi} \quad (2.13)$$

Equation (2.13) represents the 1<sup>st</sup> moment of BTE. It is clear that, by looking at the first four terms, (2.13) represents the conservation of  $n\vec{v}$ , i.e. density of velocity or, multiplying by the mass, density of momentum. A higher order of the BTE would then express the conservation of energy density.

The RHS of (2.13) expresses the change over time due to collisions of the velocity density. It can then be written as:

$$C_{vi} = va_{gi} \frac{dn}{dt} + n \frac{dva_{gi}}{dt} \quad (2.14)$$

The first and third terms in the LHS of (2.13) express the change of the number of particles, i.e the 0<sup>th</sup> moment of BTE, multiplied by  $va_{gi}$ , so they cancel with the first term of RHS of (2.14). Also, of the collision terms in (2.14), only those characterised by a very short time dominate, as they appear in the denominator. These are typically the collisions due to the intravalley scattering (in silicon they are  $\approx 10^{-12} - 10^{-13} s$ ) ([2]) that do not change the total number of particles. Using the approximation of the distribution function as in (1.12), equation (2.13) then becomes:

$$n \frac{\partial va_{gi}}{\partial t} + nv\vec{a}_g \nabla (va_{gi}) + \nabla \cdot \left( \frac{nk_B \widehat{T}_i}{m_i^*} \right) + \frac{q}{m_i^*} n E_i = -n \frac{va_{gi}}{\tau_p} \quad (2.15)$$

Summing over the indexes  $i = 1, 2, 3$ , (2.15) becomes:

$$n \frac{\partial v\vec{a}_g}{\partial t} + n(v\vec{a}_g \cdot \nabla) v\vec{a}_g + \frac{1}{m^*} \nabla \cdot nk_B \widehat{T}_n + \frac{q}{m^*} n \vec{E} = -n \frac{v\vec{a}_g}{\tau_p} \quad (2.16)$$

where  $(v\vec{a}_g \cdot \nabla)$  is the operator applied to  $v\vec{a}_g$  and  $\widehat{T}_n$  is the temperature tensor for electrons, which represents the kinetic energy of the particle associated with random motion. In equilibrium, this corresponds to the temperature  $T_L$  of the reticle, whereas under general conditions of non-equilibrium, the tensor should be assumed to have all its 9 components different.

Equation (2.16) can be further simplified, noticing that, due to the smallness of  $\tau_p$ , the first term in the LHS becomes negligible very rapidly, unless the characteristics times involved are of the order of ps or less.

The second term in the LHS of (2.16) can also be, in most cases, neglected ([4]). Equation (2.16) can then be approximated as:

$$\frac{1}{m^*} \nabla \cdot nk_B \widehat{T}_n + \frac{q}{m^*} n \vec{E} = -n \frac{v\vec{a}_g}{\tau_p} \quad (2.17)$$

Multiplying both sides of (2.17) by  $q\tau_p$  gives:



$$q\left(\frac{q\tau_p}{m^*}\right)\frac{k_B}{q}\nabla \cdot (n\widehat{T}_n) + q\left(\frac{q\tau_p}{m^*}\right)n\vec{E} = -qnv\vec{a}_g \quad (2.18)$$

with the RHS representing the current density. Equation (2.18) can then be written as:

$$q\widehat{\mu}_n\frac{k_B}{q}\nabla \cdot (n\widehat{T}_n) + q\widehat{\mu}_nn\vec{E} = \vec{J}_n \quad (2.19)$$

having introduced the electron mobility tensor  $\widehat{\mu}_n = \frac{q\tau_p}{m^*}$ . At equilibrium, the temperature tensor  $\widehat{T}$  converges to  $T_L\mathbb{I}$ , where the reticle's temperature is  $T_L$  and  $\mathbb{I}$  the identity matrix. Assuming a situation of near-equilibrium,  $\widehat{T}$  is approximated to  $T_L$ , which leads to:

$$q\widehat{D}_n\nabla(n) + q\widehat{\mu}_nn\vec{E} = \vec{J}_n \quad (2.20)$$

where  $\widehat{D}_n = \widehat{\mu}_n\frac{k_B T_L}{q}$  the electron diffusivity tensor.

Equation (2.20) is valid near an extremum (minimum) of the conduction band and has to be repeated for all the extrema of the band. In silicon, due to the diagonal form of the mass tensor, summing up over all the extrema makes the mass tensor become isotropic, i.e. a scalar. It is then possible to define an average mobility  $\mu_n = \frac{1}{3}q\tau_p\left(\frac{1}{m_l^*} + \frac{1}{m_t^*}\right)$  where  $\mu_l^*$ ,  $\mu_t^*$  represent the longitudinal and transverse effective mass respectively. The general expression of electron current density  $\vec{J}_n$  in BC then becomes:

$$qD_n\nabla(n) + q\mu_n n\vec{E} = \vec{J}_n \quad (2.21)$$

Repeating the same steps for holes, using the 0<sup>th</sup> and 1<sup>st</sup> moment of BTE and summing over the extrema (maximum) of the valence band, leads to the drift-diffusion (**DD**) model of semiconductor:

$$\frac{\partial n(\vec{r})}{\partial t} = \frac{1}{q}\nabla_r \cdot \vec{J}_n + U_n \quad (2.22)$$

$$\frac{\partial p(\vec{r})}{\partial t} = -\frac{1}{q}\nabla_r \cdot \vec{J}_p + U_p \quad (2.23)$$

$$qD_n\nabla(n) + q\mu_n n\vec{E} = \vec{J}_n \quad (2.24)$$

$$-qD_p\nabla(p) + q\mu_p p\vec{E} = \vec{J}_p \quad (2.25)$$

$$\nabla \cdot (\nabla\phi) = -\frac{q}{\epsilon}(p - n + N_D - N_A) \quad (2.26)$$

i.e. the four equations deduced from the 0<sup>th</sup> and 1<sup>st</sup> moment of BTE along with the Poisson's equation. The model consists of total of five equations in the five unknown  $(n, p, J_n, J_p, \phi)$ .

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