# **Computational Electronics**

# **Choice of a Distribution Function**

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# **Semiclassical Transport Theory**

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 the carriers is to solve Newton's equations

$$\frac{d\mathbf{p}}{dt} = -e\mathbf{E} + R(\mathbf{r}, \mathbf{p}, t) \quad \text{and} \quad \mathbf{v}(t) = \frac{d\mathbf{r}}{dt},$$
(1)

where  $R(\mathbf{r}, \mathbf{p}, t)$  is a random force function due to impurities or lattice vibrations or other imperfections in the system. Alternative approach would be to calculate the probability of finding a carrier with crystal momentum **k** at position **r** at time *t*, given by the distribution function  $f(\mathbf{r}, \mathbf{k}, t)$ , obtained by solving the Boltzmann transport equation (BTE) [1,2,3]. It is important to note that this theory is based on the following assumptions:

- Electrons and holes are independent particles.
- The system is described by a set of Bloch functions [4,5].
- Particles do not interact with each other, but may be scattered by impurities, phonons, etc.
- The number of electrons in an elementary volume  $\Delta V$  centered around **r**, that have wavevectors in the range of  $d^3k$  centered around **k** is given by  $2 \times \frac{\Delta V}{8\pi^3} f(\mathbf{r}, \mathbf{k}, t) d^3k$

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

$$n(\mathbf{r},t) = \frac{1}{V} \sum_{k} f(\mathbf{r},\mathbf{k},t), \text{ particle density}$$
(2)

$$\mathbf{J}(\mathbf{r},t) = -\frac{e}{V} \sum_{k} \mathbf{v}(\mathbf{k}) f(\mathbf{r},\mathbf{k},t), \text{ current density}$$
(3)

$$W(\mathbf{r},t) = \frac{1}{V} \sum_{k} E(\mathbf{k}) f(\mathbf{r},\mathbf{k},t), \text{ energy density}$$
(4)

A full quantum-mechanical view to this problem is rather difficult [6,7]. 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 specified within a macroscopic volume, and momenta are also specified

within some interval. If one tries to go straightforwardly and construct  $f(\mathbf{r}, \mathbf{k}, t)$  from the quantummechanical wavefunctions, difficulties arise since *f* is not necessarily positive definite.

## Approximations made for the distribution function

The most difficult problem in device analysis is to calculate the distribution function  $f(\mathbf{r}, \mathbf{k}, t)$ . 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.

#### (A) Quasi-Fermi level concept

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

$$f_n(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}, \quad f_p(E) = 1 - f_n(E) = \frac{1}{1 + \exp\left(\frac{E_F - E}{k_B T}\right)}.$$
 (5)

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

$$f_{n}(E) = \frac{1}{1 + \exp\left(\frac{E - E_{Fn}}{k_{B}T}\right)} \qquad f_{p}(E) = 1 - f_{n}(E) = \frac{1}{1 + \exp\left(\frac{E_{Fp} - E}{k_{B}T}\right)} \quad \text{and} \quad (6)$$

Therefore, under non-equilibrium conditions and assuming non-degenerate statistics, we will have

$$n = N_C \exp\left(\frac{E_{Fn} - E_C}{k_B T}\right), \text{ and } p = N_V \exp\left(\frac{E_V - E_{Fp}}{k_B T}\right),$$
 (7)

where  $N_C$  and  $N_V$  are the effective density of states of the conduction and valence band, respectively [8,9]. The product

$$np = n_i^2 \exp\left(\frac{E_{Fn} - E_{Fp}}{k_B T}\right)$$
(8)

suggests that the difference  $E_{Fn} - E_{Fp}$  is a measure for the deviation from the equilibrium. 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  $\sqrt{2k_BT/m^*} \approx 10^7 \text{ cm/s}$  for  $m^* = m_0$  (free electron mass).



Figure 1. Energy band profile of a pn-diode under equilibrium and non-equilibrium conditions. Note that to get the excess electron density (bottom right panel) the electron quasi-Fermi level must move up (top right panel), thus increasing the probability of state occupancy. The same is true for the excess hole concentration, where the hole quasi-Fermi level moves downward.

#### (B) Displaced Maxwellian Approximation

A better guess for the distribution function  $f(\mathbf{r}, \mathbf{k}, t)$  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 [10]



Figure 2. Displaced Maxwellian distribution function.

Using this form of the distribution function gives

$$n(\mathbf{r},t) = \frac{1}{V} \sum_{k} f(\mathbf{r},\mathbf{k},t) = N_{C} \exp\left(\frac{E_{Fn} - E_{C0}}{k_{B}T}\right).$$
(10)

In the same manner, one finds that the kinetic energy density per carrier is given by

$$u(\mathbf{r},t) = \frac{1}{2}m * v_d^2 + \frac{3}{2}k_B T$$
(11)

The first term on the RHS represents the drift energy due to average drift velocity, and the second term is the well known thermal energy term due to collisions of carriers with phonons [11].

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 [12]. This necessitates the solution of the Boltzmann transport equation that is introduced in the following section.

## **Boltzmann transport equation**

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  $(x-v_xdt, y-v_ydt, z-v_zdt, p_x-F_xdt, p_y-F_ydt, p_z-F_zdt)$  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 to the fact that force fields acting on the particles tend to move them from one region to another in momentum space is [13]:

$$df = f(x - v_x dt, y - v_y dt, z - v_z dt, p_x - F_x dt, p_y - F_y dt, p_z - F_z dt) - f(x, y, z, p_x, p_y, p_z)$$
(12)

Using Taylor series expansion, we get

$$\frac{df}{dt} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f - \mathbf{F} \cdot \nabla_{\mathbf{p}} f$$
(13)

So far, only the change in the distribution function due to the motion of 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 transferred into or out of a given region in phase space by collisions or scattering interactions involving other particles of the distribution or scattering centers external 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

$$\frac{df}{dt} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f - \mathbf{F} \cdot \nabla_{\mathbf{p}} f + \frac{\partial f}{\partial t} \Big|_{coll} + s(r, p, t)$$
(14)

i.e.

$$\frac{df}{dt} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = \frac{\partial f}{\partial t} \Big|_{coll} + s(r, p, t)$$
(15)

The last term on the RHS of Eqs. (3.14) and (3.15) occurs when generation-recombination processes play significant role. Eq. (3.15) represents the Boltzmann transport equation, which is nothing more but a book-keeping equation for the particle flow in the phase space.



Figure 3. A cell in two-dimensional phase space. The three processes, namely drift, diffusion, and scattering, that affect the evolution of f(r,p,t) with time in phase space are shown.

The various terms that appear in Eq. (15) represent

•  $(\partial f / \partial t)_{forces} = -\mathbf{F} \cdot \nabla_{\mathbf{p}} f$ , where  $\mathbf{F} = \frac{d\mathbf{p}}{dt} = \hbar \frac{d\mathbf{k}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ , the total force equals the sum of the force due to the electric field and the Lorentz force due to the magnetic

flux density, **B**.

- $(\partial f/\partial t)_{diff} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f$ . This term arises if there is a spatial variation in the distribution function due to concentration or temperature gradients, both of which will result in a diffusion of carriers in coordinate space.
- $(\partial f / \partial t)_{coll}$  is the collision term which equals the difference between the in-scattering and the out-scattering processes, i.e.

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{k'} \left\{ S(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') \left[1 - f(\mathbf{k})\right] - S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) \left[1 - f(\mathbf{k}')\right] \right\} = \widehat{C}f$$
(16)

The presence of  $f(\mathbf{k})$  and  $f(\mathbf{k'})$  in the collision integral makes the BTE rather complicated integro-differential equation for  $f(\mathbf{r}, \mathbf{k}, t)$ , whose solution requires a number of simplifying assumptions. In the absence of perturbing fields and temperature gradients, the distribution function must be the Fermi-Dirac function. In this case, the collision term must vanish and the principle of detailed balance gives for all  $\mathbf{k}$  and  $\mathbf{k'}$  and all scattering mechanisms

$$\frac{S(\mathbf{k},\mathbf{k}')}{S(\mathbf{k}',\mathbf{k})} = \frac{f_0(\mathbf{k}')[1-f_0(\mathbf{k})]}{f_0(\mathbf{k})[1-f_0(\mathbf{k}')]}$$
(17)

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

$$\frac{S(\mathbf{k},\mathbf{k}')}{S(\mathbf{k}',\mathbf{k})} = \exp\left(\frac{E_{\mathbf{k}} - E_{\mathbf{k}'}}{k_B T}\right).$$
(18)

This relation must be satisfied regardless of the origin of the scattering forces. If, for example, we assume  $E_{\mathbf{k}} > E_{\mathbf{k}'}$ , then  $S(\mathbf{k}, \mathbf{k}')$  which involves emission must exceed  $S(\mathbf{k}', \mathbf{k})$  which involves absorption. Note that the BTE is valid under assumptions of semi-classical transport: effective mass approximation (which incorporates the quantum effects due to the periodicity of

the crystal); Born approximation for the collisions, in the limit of small perturbation for the electron-phonon interaction and instantaneous collisions; no memory effects, i.e. no dependence on initial condition terms. The phonons are usually treated as in equilibrium, although the condition of non-equilibrium phonons may be included through an additional equation [14].

## **Scattering Processes**

Free carriers (electrons and holes) interact with the crystal and with each other through a variety of scattering processes which relax the energy and momentum of the particle. Based on first order, time-dependent perturbation theory, the transition rate from an initial state  $\mathbf{k}$  in band n to a final state  $\mathbf{k}'$  in band m for the *j*th scattering mechanism is given by Fermi's Golden rule [15]

$$\Gamma_{j}[n,\mathbf{k};m,\mathbf{k}'] = \frac{2\pi}{\hbar} \left| \left\langle m,\mathbf{k}' \middle| V_{j}(\mathbf{r}) \middle| n,\mathbf{k} \right\rangle \right|^{2} \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \mp \hbar \omega)$$
(19)

where  $V_j(\mathbf{r})$  is the scattering potential of this process,  $E_{\mathbf{k}}$  and  $E_{\mathbf{k}'}$  are the initial and final state energies of the particle. The delta function describes conservation of energy, valid for long times after the collision is over, with  $\hbar\omega$  the energy absorbed (upper sign) or emitted (lower sign) during the process. The total rate used to generate the free flight, discussed previously, is then given by

$$\Gamma_{j}[n,\mathbf{k}] = \frac{2\pi}{\hbar} \sum_{m,\mathbf{k}'} \left| \left\langle m,\mathbf{k}' \middle| V_{j}(\mathbf{r}) \middle| n,\mathbf{k} \right\rangle \right|^{2} \delta(E_{\mathbf{k}'} - E_{\mathbf{k}} \mp \hbar \omega) .$$
<sup>(20)</sup>

There are major limitations to the use of the Golden rule due to effects such as *collision* broadening and finite collision duration time. The energy conserving delta function is only valid asymptotically for times long after the collision is complete. The broadening in the final state energy is given roughly by  $\Delta E \approx \hbar/\tau$ , where  $\tau$  is the time after the collision, which implies that the normal  $E(\mathbf{k})$  relation is only recovered at long times. Attempts to account for such collision broadening in Monte Carlo simulation have been reported in the literature [16,17], although this is still an open subject of debate. Inclusion of the effects of finite collision duration in Monte Carlo simulation have also been proposed [18,19]. Beyond this, there is still the problem of

dealing with the quantum mechanical phase coherence of carriers, which is neglected in the scatter free-flight algorithm of the Monte Carlo algorithm, and goes beyond the semi-classical BTE description.



Figure 4. Scattering mechanisms in a typical semiconductor.

**Figure 4** lists the scattering mechanisms one should in principle consider in a typical Monte Carlo simulation. They are roughly divided into scattering due to crystal defects, which is primarily elastic in nature, lattice scattering between electrons (holes) and lattice vibrations or phonons, which is inelastic, and finally scattering between the particles themselves, including both single particle and collective type excitations. Phonon scattering involves different modes of vibration, either acoustic or optical, as well as both transverse and longitudinal modes. Carriers may either emit or absorb quanta of energy from the lattice, in the form of phonons, in individual scattering events. The designation of inter- versus intra-valley scattering comes from the multi-valley band-structure model of semiconductors discussed earlier, and refers to whether the initial and final states are in the same valley or in different valleys. The scattering rates  $\Gamma_j[n, \mathbf{k}; m, \mathbf{k'}]$  and  $\Gamma_j[n, \mathbf{k}]$  are calculated using time dependent perturbation theory using Fermi's rule, and the calculated rates are then tabulated in a scattering table in order to select the type of scattering and final state after scattering as discussed earlier.

# References

- C. Jacoboni and L. Reggiani, "The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials", *Rev. Mod. Phys.*, Vol. 55, pp. 645–705 (1983).
- 2 P.J. Price, "Monte Carlo calculation of electron transport in solids," *Semiconductors and Semimetals*, Vol. 14, pp. 249-334 (1979).
- 3 C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation* (Springer-Verlag, Wien New York).
- 4 C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1986, sixth edition).
- 5 N. W. Aschroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, 1976).
- 6 D. J. Griffits, *Introduction to Quantum Mechanics* (Prentice Hall Inc., Englewood Cliffs, NewJersey, 1995).
- 7 D. K. Ferry, *Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers* (Institute of Physics Publishing, London, 2001).
- 8 R. F. Pierret, *Semiconductor Device Fundamentals* (Addison-Wesley, 1996).
- 9 S. M. Sze, *Physics of Semiconductor Devices* (John Wiley & Sons, Inc., 1981).
- 10 M. Lundstrom, *Fundamentals of Carrier Transport* (Cambridge University Press, Cambridge, 2000)
- B. K. Ridley, *Quantum Processes in Semiconductors* (Oxford University Press, Oxford, 1988).
- 12 D. K. Ferry, *Semiconductor Transport* (Taylor & Francis, London, 2000).
- 13 J. P. McKelvey, Solid State and Semiconductor Physics (Krieger Pub. Co., 1982).
- J. M. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids* (Oxford University Press, New York, 2001).

- 15 L. I. Schiff, *Quantum Mechanics*, McGraw-Hill Inc., New York (1955).
- 16 Y.-C. Chang, D. Z.-Y. Ting, J. Y. Tang and K. Hess, Appl. Phys. Lett. 42, 76 (1983).
- 17 L. Reggiani, P. Lugli and A. P. Jauho, Phys. Rev. B 36, 6602 (1987).
- 18 D. K. Ferry, A. M. Kriman, H. Hida and S. Yamaguchi, Phys. Rev. Lett. 67, 633 (1991).
- 19 P. Bordone, D. Vasileska and D. K. Ferry, Phys. Rev. B 53, 3846 (1996).