2 Semiclassical Transport Theory

Here, the classical theory of a kinetic gas is applied to the electron and hole ensembles in semiconductors with two quantum mechanical extensions. The particle kinetics are based on a position-dependent band structure calculated with the nonlocal empirical pseudopotential method [2.1–2.3] and scattering rates determined by Fermi's Golden Rule [2.4, 2.5]. In this theoretical framework the particle motion consists of a series of scattering events and accelerations by external forces, which is described by the semiclassical Boltzmann transport equation (BTE) [2.4–2.10].

In the first part of this section the distribution function, which characterizes the state of the particle gas, the evolution equation for the distribution function, the BTE, and the corresponding probability densities of the underlying stochastic process are introduced. In the next part balance equations for moments of the distribution function are analyzed, which are the basis of momentum-based models. In the third part the microscopic relaxation time is discussed, which allows to exactly solve the scattering integral of certain balance equations avoiding the macroscopic relaxation time approximation. In the last part of this section the theoretical background of fluctuations in the steady-state is given based on the Langevin-type Boltzmann transport equation, and corresponding balance equations are derived. The impact of the macroscopic relaxation time approximation is analyzed by comparison with exact solutions of the BTE for the velocity fluctuations in bulk systems.

2.1 The Boltzmann Transport Equation

The semiclassical Hamilton function of an electron in a conduction band is given by

\[ H_n(r, k, t) = E_c(r) + \epsilon_n(r, k) - q\Psi(r, t), \]  \hspace{1cm} (2.1)
2.1 The Boltzmann Transport Equation

where $E_c$ is the conduction band edge, which is the minimum energy of all conduction bands, $\varepsilon_n$ the energy of the $n$th band relative to the conduction band edge, $\Psi$ the electrostatic potential, $\mathbf{k}$ the wave vector, $\mathbf{r}$ a vector of the real space (RS), $t$ the time, and $q$ the positive electron charge. In the case of holes it reads

$$H_n(\mathbf{r}, \mathbf{k}, t) = -E_v(\mathbf{r}) + \varepsilon_n(\mathbf{r}, \mathbf{k}) + q\Psi(\mathbf{r}, t) ,$$

(2.2)

where $E_v$ is the valence band edge, which is the maximum energy of the valence bands in the electron picture. The relative band energy $\varepsilon$ is positive in the valence bands (hole picture). Electrons and holes are distinguished by the band index $n$.

The collisionless motion of the particles is described in the framework of semiclassical mechanics (Newton’s laws) by

$$\hbar \frac{\partial \mathbf{k}}{\partial t} = -\nabla_r H = \mathbf{F}$$

(2.3)

and

$$\frac{\partial \mathbf{r}}{\partial t} = \frac{1}{\hbar} \nabla_k H = \mathbf{v} ,$$

(2.4)

where $\hbar$ denotes Planck’s constant divided by $2\pi$, $\mathbf{v}$ the velocity, and $\mathbf{F}$ the force

$$\mathbf{F}_n(\mathbf{r}, \mathbf{k}, t) = \begin{cases} \nabla_r (E_v(\mathbf{r}) - q\Psi(\mathbf{r}, t) - \varepsilon_n(\mathbf{r}, \mathbf{k})) & \text{for holes} \\ \nabla_r (-E_c(\mathbf{r}) + q\Psi(\mathbf{r}, t) - \varepsilon_n(\mathbf{r}, \mathbf{k})) & \text{for electrons} \end{cases} .$$

(2.5)

The first and last terms on the right-hand side are due to the position-dependent band structure [2.11]. In the semiclassical theory the particle velocity is given by the group velocity of the particle’s wave packet defined as [2.4]

$$\mathbf{v}_n(\mathbf{r}, \mathbf{k}) = \frac{1}{\hbar} \nabla_k \varepsilon_n(\mathbf{r}, \mathbf{k}) .$$

(2.6)

The inverse mass tensor reads

$$\hat{m}^{-1}_n(\mathbf{r}, \mathbf{k}) = \frac{1}{\hbar} \nabla_k \mathbf{v}^T_n(\mathbf{r}, \mathbf{k}) = \frac{1}{\hbar^2} \nabla_k \nabla^T_k \varepsilon_n(\mathbf{r}, \mathbf{k}) .$$

(2.7)

The particles are scattered by various mechanisms (cf. Chap. 4) [2.9]. The scattering events are treated as local and instantaneous and they are characterized by a transition rate $S_{n',n}(\mathbf{k}'|\mathbf{k})(\mathbf{r}, t)$, which is the rate of particles that are scattered from the occupied state $(n, \mathbf{r}, \mathbf{k})$ into the empty state $(n', \mathbf{r}, \mathbf{k}')$. Since the final state is not uniquely defined, the particle scattering contains a certain degree of randomness making it impossible to calculate the exact particle trajectory in the phase space (PS). Instead, stochastic methods are used and the particle gas is described by a distribution function $f_n(\mathbf{r}, \mathbf{k}, t)$ being the particle density in the PS [2.4, 2.9, 2.12, 2.13]. The number of particles in an infinitesimal volume of the six-dimensional PS is given by

$$dN = \frac{2}{(2\pi)^3} f_n(\mathbf{r}, \mathbf{k}, t) d^3k d^3r .$$

(2.8)