Energy-transport models for charge carriers involving impact ionization in semiconductors

Isabelle Choquet * Pierre Degond † Christian Schmeiser ‡

April 20, 2000

Abstract

Energy-transport models taking into account impact ionization are derived from a kinetic framework by formal asymptotic methods. The derivation is based on a system of Boltzmann transport equations governing the distribution functions of conduction electrons and holes in a semiconductor. The charge carriers are assumed to obey a degenerate gas statistics. The energy exchanged during collisions between a charge carrier and a phonon is supposed to be weak. Ionization collisions and elastic phonon collisions are retained at leading order to carry out a rigorous diffusion limit of the system of Boltzmann equations. The resulting set of diffusion equations are balance laws for the total charge and for a shifted total kinetic energy, rather than for the densities and for the temperature of charge carriers. The diffusion limit is also investigated by a detour through an intermediate Spherical Harmonics Expansion model. Simpler expressions for the diffusion matrix are obtained leading to explicit formulas in some limiting cases.

1 Introduction

This paper is devoted to the derivation of Energy Transport (ET) models for semiconductors from a system of Boltzmann Transport Equations (BTE) where impact ionization is a predominant collision process.

Let us first recall that impact ionization takes place in semiconductors under relatively high electric fields. For example: The order of magnitude is above around 1.5 eV cm^{-1} in Silicon or GaliumArsenide devices [1]-[3]. A charge carrier accelerated by such an electric

*Institut für Techno- und Wirtschaftsmathematik, Erwin-Schrödinger-Straße, Gebäude 49, D-67663 Kaiserslautern.

†MIP, UMR CNRS 9974, Université Paul Sabatier, 118 rue de Narbonne, F-31062 Toulouse Cedex.

‡Institut für Angewandte und Numerische Mathematik, TU Wien, Wiedner Hauptstr. 8-10, A-1040 Wien.

field can reach a kinetic energy larger than the ionization threshold of lattice atoms, i.e. the width of the band gap between valence band and conduction band. Ionization can thus occur by the interaction of a carrier with a lattice atom. This leads to the generation of two new charge carriers: a negative one (a conduction electron) and a positive one (a hole).

This generation process can be observed in submicron devices used in the design of transistors for integrated circuits. In High Electron Mobility Transistors and Metal Semiconductor Field Effect Transistors for instance [4], it causes a gate current. In Metal-Oxide Semiconductor Field Effect Transistors it creates a substrate current [5]. These currents limit the performances of the transistors and shorten their lifetime. With regards to Avalanche PhotoDiodes and IMPact ionization Avalanche Transit Time diodes [8]-[9], the situation turns out to be completely different since impact ionization is the mechanism of operation. It induces luminescence at the gate edge, allowing to amplify weak optical signals. The control of this process is therefore an important challenge concerning both transistors and diodes.

Impact ionization has indeed been widely investigated since the last five decades. Up to now, most of the studies are focussed on one aspect of the problem: the characterization of the ionization reaction rates. To that purpose, various experimental techniques are developed, cf. [10]-[12] for instance. They are intended to evaluate the influence of parameters such as the electric field, the crystallographic directions [11] or the temperature [12]. A great spread in experimental data is observed, however, due to the complexity inherent to the operating regime. This spread is accordingly reflected by the parameters involved in the phenomenological models, cf. [13]-[16]. The first one was proposed by Wolff [13] to model ionization reaction rates in the limit of very high fields. The lower fields domain was investigated by Shockley [14]. These two limiting cases are included in models developed later on, by Baraff [15] for instance. Their adjustable parameters (such as the phonon mean free path and the ionization threshold energy) are set to fit experimental data valid for specific materials. Next, it turned out that a more realistic description of the band structure was generally necessary to obtain further improvements. This evolution is associated with a switch from phenomenological models to numerical ones, based on simulations of the BTE. Hess and co-workers [8]-[9], and later Fischetti and Laux [17], have thus included details of the band structure and the density of states of semiconductors in conventional Monte Carlo methods. These numerical methods allow to fix the parameters of previous phenomenological models with a higher accuracy, to investigate various materials (as in Refs. [17]-[20] applied to Keldysh's model [16]), and to take into account additional properties such as the anisotropy [21].

The present study is devoted to a different aspect of the problem: the description of charge carrier transport. Opting for a kinetic approach, through the use of the Boltzmann equation, the transport description is also mostly based on Monte Carlo and particle methods [2]. This is however highly time consuming and often too costly to design devices for industrial purposes.

This drawback is not met by the Drift-Diffusion (DD) model, as it involves a lower space dimension than the BTE. This macroscopic model is widely used in solid-state electronics since half a century [22]. It can be rigorously derived from the BTE by means of a perturbation approach, cf. Refs. [23]-[25]. It has been employed to handle impact ionization in semiconductors [27], although it cannot describe the related non local effects. The DD model is indeed developed assuming that charge carriers and lattice atoms (i.e., the phonon gas) are at thermal equilibrium. The momentum relaxation is however much faster than the temperature relaxation. An intermediate scale, at which charge carriers reach an equilibrium that differs from the lattice temperature, can thus be introduced. This allows to propose improved DD models, such as the Spherical Harmonics Expansion (SHE) model and the ET model.

Originally, the SHE model has been developed as an approximation of the BTE by a numerical procedure [28]-[29]. This mesoscopic model remains valid when a single temperature parameter is not sufficient for a complete description of the distribution function, and the distribution of particles in terms of kinetic energy must be considered. It has been derived from the Boltzmann equation through a diffusion limit (first in [30] and then in [31] in an extended form) retaining elastic phonon collisions at the leading order. The modeling of impact ionization based on a spherical harmonic expansion of the BTE was derived by Gnudi and co-authors in Ref. [32]. As we shall see in a forthcoming section, impact ionization can cover a larger operating domain than the one corresponding to elastic phonon collisions at leading order.

The ET model was derived from the Boltzmann equation, through a macroscopic limit, by Stratton [33]. A mathematical foundation of this derivation, based on asymptotic analysis, can be found in [34]. Besides elastic electron-phonon collisions, the dominating collisional process investigated in [34] also includes electron-electron collisions, and the present paper proposes another example. The ET model for conduction electrons (without hole coupling) consists of a system of partial differential equations governing the evolution of the density and temperature of electrons. It can also be derived through the SHE model, as shown in [31], leading to simpler expressions for the diffusion matrix that can be computed explicitly in some particular cases. Besides, this model can be interpreted as an hydrodynamic model with a simplified momentum transport equation (i.e., without terms involving the electron mass), cf. [34].

The ET models developed up to now do not take into account the impact ionization process. The purpose of the present paper is to derive ET models from a system of BTE when impact ionization is a dominating process.

This paper is organized as follows: the system of BTE for conduction electrons and holes is presented in section 2. The various collisional processes concomitant to impact ionization are specified within the general framework of a degenerate gas statistics. The appropriate scaling, assuming weak energy exchange during collisions between a charge carrier and a phonon, is introduced in section 3. The relative orders of magnitude of the involved collisional processes are also discussed. The ionization collision operator is then studied in section 4. Its properties needed for performing the diffusion approximation by a Hilbert expansion, are established. The remaining sections are concerned with the formal diffusion limit of the system of BTE to ET models. Two cases are successively investigated, depending on the relative order of magnitude of the elastic phonon and ionization collision frequencies. The first one, presented in Section 5, deals with similar orders of magnitude. The resulting set of diffusion equations governs the total charge and a shifted total kinetic energy. Its properties as a hydrodynamic model, also possessing a macroscopic entropy, are underlined. Section 6 corresponds to elastic phonon collisions dominating impact ionization. A second diffusion limit is then investigated doing a multiple scaling, through a SHE model. The same set of diffusion equations is obtained, but with simpler expressions for the diffusion matrix. Under certain assumptions, the diffusion matrix can then be computed explicitly, which allows to discuss limiting problems and to recover results available in the literature.

2 A System of Boltzmann Transport Equations

Hot electron and hole transport in semiconductors involves several scattering mechanisms: i) scattering with lattice-defects, ii) phonon scattering, iii) carrier-carrier interactions, and iv) carrier generation and recombination. The collision mechanisms i) to iii) are taken into account in Refs. [31], [34], to derive ET models from the BTE for conduction electrons. Assuming that carrier-carrier interactions only involve particles of identical charge, these first three mechanisms allow omitting the Boltzmann equation for holes. This simplification no longer applies to the present study since the collision mechanisms iv) are also considered. The transport equations for electrons and holes are then coupled through source terms of generation and recombination. We will thus consider the following coupled system of Boltzmann transport equations:

$$\begin{aligned} \frac{\partial f_n}{\partial t} + \frac{1}{\hbar}\nabla_k \varepsilon_n(k) \cdot \nabla_x f_n + \frac{q}{\hbar}\nabla_x V(x,t) \cdot \nabla_k f_n = Q_n(f_n, f_p) \ , \\ \frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\nabla_k \varepsilon_p(k) \cdot \nabla_x f_p - \frac{q}{\hbar}\nabla_x V(x,t) \cdot \nabla_k f_p = Q_p(f_n, f_p) \ , \end{aligned} \tag{1}$$

governing the distribution functions for conduction electrons $f_n = f_n(x,k,t)$, and holes $f_p = f_p(x,k,t)$. Hereafter, quantities associated with the negative and positive carriers will be denoted by the subscript n and p, respectively. The position variable x belongs to $\mathbb{R}^3$ since we concentrate on the behaviour of bulk material. The pseudo wave-vector k belongs to the first Brillouin zone denoted by B and the time $t \geq 0$. B is the elementary cell of the dual crystal lattice $\mathbb{L}^*$ of period L^*. Functions of k are thus periodic functions on $\mathbb{R}^3$ of period L^*. The kinetic energies $(\varepsilon_n, \varepsilon_p) : \ B \times B \to \mathbb{R} \times \mathbb{R}$ are given by the energy band diagrams. We assume that they do not depend on the space variable. $\hbar$ is the reduced Planck constant and q the positive elementary charge. The electric potential $V(x,t)$ will be considered as a given function since its coupling to the BTE through the Poisson equation is of no relevance for the subsequent analysis. The collision operators Q_n for electrons and Q_p for holes comprise the scattering mechanisms i) to iv):

$$\begin{aligned} Q_n(f_n,f_p) =&\ Q_{n,ld}(f_n) + Q_{n,ph}(f_n) + Q_{n,c}(f_n,f_p) + Q_{n,gr}(f_n,f_p)\ , \\ Q_p(f_n,f_p) =&\ Q_{p,ld}(f_p)\ + Q_{p,ph}(f_p) + Q_{p,c}(f_n,f_p)\ + Q_{p,gr}(f_n,f_p)\ , \end{aligned} \tag{2}$$

where $Q_{n,ld}$ and $Q_{p,ld}$ model scattering with lattice-defects, $Q_{n,ph}$ and $Q_{p,ph}$ phonon scattering, $Q_{n,c}$ and $Q_{p,c}$ carrier-carrier interactions, and $Q_{n,gr}$ and $Q_{p,gr}$ generation-recombination processes.

2.1 Scattering with Lattice Defects

Collisions of carriers with lattice-defects, such as dislocations or neutral impurities, include intra and intervalley scatterings concerning electrons, respectively intra and interband scatterings concerning holes; cf. Ref. [2] for instance. They share the common property of being elastic. Consequently, $Q_{n,ld}$ and $Q_{p,ld}$ remain the same for a degenerate and non-degenerate gas statistics since the Pauli exclusion terms vanish:

$$Q_{n,ld}(f_n) = \int_B \phi_{n,ld}(k;k')\ \delta(\varepsilon_n' - \varepsilon_n)\,(f_n' - f_n)\,dk'\ , \tag{3}$$

where the apostrophes indicate evaluation at k' instead of k, and δ is the delta measure. The scattering matrix element $\phi_{n,ld}(k;k') = \phi_{n,ld}(k';k)$ is the sum of the transition rates associated with the various types of lattice-defects. $Q_{p,ld}$ is inferred from (3) replacing the subscript n by p.

2.2 Phonon Scattering

Phonon scattering can involve acoustic or optical phonons, both longitudinal or transverse, cf. [2]. Hereafter, we will consider only one of these carrier-phonon collision operators since they have the same mathematical structure

$$\begin{aligned} Q_{n,ph}\ (f_n) = \int_B &\phi_{n,ph}(k;k') \\ \times\Big\{&\Big[(N_{ph}+1)\,\delta(\varepsilon_n - \varepsilon_n' + \varepsilon_{ph}) + N_{ph}\ \delta(\varepsilon_n - \varepsilon_n' - \varepsilon_{ph})\Big] f_n'\ (1-f_n) \\ -&\Big[(N_{ph}+1)\,\delta(\varepsilon_n' - \varepsilon_n + \varepsilon_{ph}) + N_{ph}\ \delta(\varepsilon_n' - \varepsilon_n - \varepsilon_{ph})\Big] f_n\ (1-f_n')\Big\}\ dk'\ , \end{aligned} \tag{4-a}$$

where $\phi_{n,ph}(k;k') = \phi_{n,ph}(k';k)$ and ε_{ph} is the phonon energy. Notice that ε_{ph} is a constant concerning optical phonons while it is a non-constant function of $|k-k'|$ concerning acoustic phonons. The phonon occupation number N_{ph} is given by the Bose-Einstein statistics

$$N_{ph} = \Big(\exp[\varepsilon_{ph}/(k_B T_L)] - 1\Big)^{-1}, \tag{4-b}$$

where T_L is the lattice temperature and k_B the Boltzmann constant. $Q_{p,ph}$ is deduced from (4-a) replacing the subscript n by p.

2.3 Carrier-Carrier Interaction

The carrier-carrier binary collision integral $Q_{n,c}$, cf. [2], includes collisions between identical carriers $Q^n_{n,c}$ plus another term modeling collisions between electrons and holes $Q^p_{n,c}$:

$$Q_{n,c}(f_n, f_p) = Q^n_{n,c}(f_n) + Q^p_{n,c}(f_n, f_p)\ , \tag{5-a}$$

with

$$\begin{aligned} Q^n_{n,c}(f_n) = \int_{B^3} &\phi^n_{n,c}(k, k^*; k', k^{*\prime})\ \delta^c_{\varepsilon_n}\delta^c_k \\ &\times\Big[f'_n f^{*\prime}_n(1-f_n)(1-f^*_n) - f_n f^*_n(1-f'_n)(1-f^{*\prime}_n)\Big]\ dk^* dk' dk^{*\prime}\ , \end{aligned} \tag{5-b}$$

and

$$\begin{aligned} Q^p_{n,c}(f_n, f_p) = \int_{B^3} &\phi^p_{n,c}(k, k^*; k', k^{*\prime})\ \delta^c_{\varepsilon_{np}}\delta^c_k \\ &\times\Big[f'_n f^{*\prime}_p(1-f_n)(1-f^*_p) - f_n f^*_p(1-f'_n)(1-f^{*\prime}_p)\Big]\ dk^* dk' dk^{*\prime}\ , \end{aligned} \tag{5-c}$$

where $\delta^c_{\varepsilon_n} = \delta(\varepsilon'_n + \varepsilon^{*\prime}_n - \varepsilon_n - \varepsilon^*_n)$ and $\delta^c_{\varepsilon_{np}} = \delta(\varepsilon'_n + \varepsilon^{*\prime}_p - \varepsilon_n - \varepsilon^*_p)$. The delta function δ^c_k is defined as follows, to preserve the periodic structure in k:

$$\delta^c_k = \delta_k(k' + k^{*\prime} - k - k^*) = \sum_{g\in \mathbb{L}^*} \delta(k' + k^{*\prime} - k - k^* + g)\ .$$

The terms with $g \neq 0$ account for umklapp processes. Their number is finite since the wave vectors only vary in the bounded Brillouin zone B. In the particular case of a parabolic band model, the first Brillouin zone is extended to $\mathbb{R}^3$ and there is no umklapp process (i.e., $g \equiv 0$).

Notice that the factor 1/2 coming from the indistinguishability of electrons (resp. holes) is supposed to be already included in $\phi^n_{n,c}$ (resp. $\phi^p_{p,c}$). Moreover, due to the indistinguishability and detailed-balance properties, $\phi^n_{n,c}$ and $\phi^p_{n,c}$ satisfy the following symmetry relations:

$$\begin{aligned} \phi^n_{n,c}(k, k^*; k', k^{*\prime}) = \phi^n_{n,c}(k', k^*; k, k^{*\prime}) = \phi^n_{n,c}(k^*, k; k^{*\prime}, k')\ , \\ \phi^p_{n,c}(k, k^*; k', k^{*\prime}) = \phi^p_{n,c}(k', k^*; k, k^{*\prime}) = \phi^p_{n,c}(k^*, k; k^{*\prime}, k')\ . \end{aligned} \tag{6}$$

$Q_{p,c}$ is derived from (5-a) to (6) exchanging n and p.

2.4 Carrier Generation and Recombination

The generation of carriers from lattice atoms, as well as the recombination of a conduction electron with a hole, requires an additional particle to satisfy the energy conservation (i.e., take off or give the ionization energy). Most of the time, this additional particle can be a phonon, a photon or a carrier; cf. [1], [3].

The phonon transition, frequently called Shockley-Read-Hall generation (recombination), takes place in two steps via traps, with absorption (emission) of a phonon at each step. The traps are impurities that differ from dopants since they are effective for generation (recombination) if their energy is roughly in the middle of the band gap (gold in Silicon devices for instance). A mathematical study of this problem can be found in [35]. We assume that the devices studied in the present work do not contain trap impurities.

The photon transition mechanism is a direct (one-step) generation (recombination) process, with the absorption (emission) of a photon. This process, also called optical generation (radiative recombination), is important for narrow gap semiconductors. Although observed in GaAs devices, whose specific band structure allows direct transitions contrary to Si devices, it is not considered here.

The carrier transition mechanisms considered in this work, can be schematized by the following reactions:

$$n \ \overset{\phi^d_{n,gr}}{\longrightarrow} \ n + n + p \ , \qquad\qquad p \ \overset{\phi^d_{p,gr}}{\longrightarrow} \ p + p + n \ , \tag{7-a}$$

$$p \ \overset{\phi^r_{p,gr}}{\longleftarrow} \ p + p + n \ , \qquad \text{and} \qquad n \ \overset{\phi^r_{n,gr}}{\longleftarrow} \ n + n + p \ , \tag{7-b}$$

where n represents a conduction electron, p a hole, and the neutral atoms of the underlying lattice are not mentioned. $\phi^d_{n,gr}$ and $\phi^d_{p,gr}$ ($\phi^r_{n,gr}$ and $\phi^r_{p,gr}$) denote the direct (reverse) reaction rates. For high carrier concentrations, the reactions (7-a) and (7-b) are usually called Auger generation-recombination. For a large current density, the recombination reactions (7-b) get negligible compared with the generation mechanisms (7-a). When reduced to the generation reactions, these processes are generally called impact ionization.

Electrons can be created through ionization reactions initiated by electrons as well as holes. The generation-recombination collision integral for electrons $Q_{n,gr}$, thus, involves the two corresponding terms:

$$Q_{n,gr}(f_n, f_p) = Q^n_{n,gr}(f_n, f_p) + Q^p_{n,gr}(f_n, f_p) \ , \tag{8}$$

where the superscripts n and p indicate the additional carrier allowing to satisfy the energetic requirement of the reaction. From the principle of detailed balance, we assume in the sequel that the direct and reverse reaction rates are linked through

$$\phi^d_{n,gr} = \mathcal{F}_0^2 \ \phi^r_{n,gr} \quad \text{and} \quad \phi^d_{p,gr} = \mathcal{F}_0^2 \ \phi^r_{p,gr} \ , \tag{9}$$

where $\mathcal{F}_0^2$ is a constant. Then $Q^n_{n,gr}$, which contains the electron gain and loss terms due to ionization and recombination initiated by an electron, reads

$$\begin{aligned} &Q^n_{n,gr}(f_n, f_p) = \\ &\int_{B^3} \phi^r_{n,gr}\ \delta^{gr}_{\varepsilon_n} \left[\mathcal{F}_0^2 f_n'(1-f_n)(1-f_n^*)(1-f_p^+) - f_n f_n^* f_p^+ (1-f_n')\right] dk'dk^*dk^+ \\ +\tfrac{1}{2} &\int_{B^3} \phi^{r\ \prime}_{n,gr}\ \delta^{gr\prime}_{\varepsilon_n} \left[f_n' f_n^* f_p^+ (1-f_n) - \mathcal{F}_0^2 f_n (1-f_n')(1-f_n^*)(1-f_p^+)\right] dk'dk^*dk^+ \ , \end{aligned} \tag{10-a}$$

where $\delta^{gr}_{\varepsilon_n} = \delta(\varepsilon_n + \varepsilon_n^* + \varepsilon_p^+ + \Delta - \varepsilon_n')$, $\delta^{gr\prime}_{\varepsilon_n} = \delta(\varepsilon_n' + \varepsilon_n^* + \varepsilon_p^+ + \Delta - \varepsilon_n)$. The ionization energy Δ can be position dependent. For consistency purposes, we will however consider it constant (otherwise, one should also take into account position dependent kinetic energies). The Delta-distributions reflect the energy balance of a generation-recombination event. In the literature, Monte Carlo simulations of impact ionization are reported neglecting [17] and enforcing [21] momentum conservation. Here it is not assumed that generation-recombination events conserve momentum. The consequences of adding a momentum conservation assumption to the model are investigated in [40]. $Q^p_{n,gr}$ contains the electron gain and loss terms due to generation initiated by a hole and the corresponding recombination reaction,

$$\begin{aligned} &Q^p_{n,gr}(f_n, f_p) = \\ &\frac{1}{2}\int_{B^3} \phi^r_{p,gr}\ \delta^{gr}_{\varepsilon_p} \left[\mathcal{F}_0^2 f_p'(1-f_p^+)(1-f_p^*)(1-f_n) - f_p^+ f_p^* f_n (1-f_p')\right] dk'dk^*dk^+ \ . \end{aligned} \tag{10-b}$$

The abbreviations $\phi^r_{n,gr}$, $\phi^{r\ \prime}_{n,gr}$ and $\phi^r_{p,gr}$ stand for $\phi^r_{n,gr}(k, k^*, k^+; k')$, $\phi^r_{n,gr}(k', k^*, k^+; k)$, and $\phi^r_{p,gr}(k^+, k^*, k; k')$ respectively. The factor $1/2$ is a consequence of the indistinguishability of particles. Moreover, this indistinguishability implies that

$$\phi^r_{n,gr}(k'; k, k^*, k^+) = \phi^r_{n,gr}(k'; k^*, k, k^+) \ . \tag{11}$$

The generation-recombination collision kernel for holes $Q_{p,gr}$ can be immediately inferred from (8) to (10-b) by exchanging n and p.

For bounded Brillouin zones, electron and hole energies vary in bounded intervals $[0, \overline{\varepsilon}_n]$ and $[0, \overline{\varepsilon}_p]$, respectively. It is then a simple consequence of the energy balance relations of generation-recombination events that an electron can participate in an electron triggered event, only if its energy is either not smaller than Δ or not bigger than $\overline{\varepsilon}_n - \Delta$. On the other hand, an electron participating in a hole triggered event has an energy not bigger than $\overline{\varepsilon}_p - \Delta$. This shows that, if $\max\{\overline{\varepsilon}_n, \overline{\varepsilon}_p\} - \Delta < \Delta$, then all electrons with energies between these two values are excluded from generation-recombination events. An analogous argument is valid for holes. Therefore, we make the assumption

$$2\Delta \le \max\{\overline{\varepsilon}_n, \overline{\varepsilon}_p\} \ , \tag{12}$$

implying that carriers of all possible energies are eligible for participation in generation-recombination events.

3 Scaled System of Boltzmann Equations

In this section the system (1) is scaled in accordance with hot-electron transport in semiconductors. The potential scale V_0 is thus associated with a typical temperature $T_0 = qV_0/k_B$ of the charge carriers much bigger than the lattice temperature T_L:

$$\alpha^2 = \frac{T_L}{T_0} \ll 1\,.$$

Typically, the phonon energy ε_{ph} is of the same order of magnitude as the lattice thermal energy $k_B T_L$, which will be used for the nondimensionalization of ε_{ph}. Thus, the small parameter α^2 can also be interpreted as a typical ratio between phonon energy and carrier energy. The characteristic kinetic energy that electrons and holes can gain in the device is equal to $\varepsilon_0 = qV_0\,(= k_B T_0)$. When ε_0 varies between 1 eV and 5 eV, and $T_L = 300$K, the order of magnitude of α^2 lies between 6.10^{-2} and 10^{-2} for Silicon and between 4.10^{-2} and 7.10^{-3} for Gallium Arsenide. Let us precise that α^2 is evaluated here for intervalley phonons, cf. [2].

The typical norm k_0 of pseudo wave-vectors is chosen such that the scaled band diagrams $\varepsilon_n(k_0 k)/\varepsilon_0$ and $\varepsilon_p(k_0 k)/\varepsilon_0$ take moderate values for moderate values of their (nondimensionalized) argument k. The choice of a common value k_0 for both electrons and holes contains an implicit assumption on the band diagrams. For parabolic band models $\varepsilon_n(k) = \hbar^2 k^2/(2m_n^*)$, $\varepsilon_p(k) = \hbar^2 k^2/(2m_p^*)$, for example, it means that the effective masses m_n^* of electrons and m_p^* of holes are of the same order of magnitude. A reasonable choice for k_0 in this case is given by $k_0 = (m_n^* m_p^*)^{1/4}\sqrt{\varepsilon_0}\,/\hbar$, leading to the scaled band diagrams $\gamma|k|^2/2$ and $|k|^2/(2\gamma)$ for electrons and holes, respectively, with $\gamma = \sqrt{m_p^*/m_n^*}$.

The velocity scale is given by $v_0 = \varepsilon_0/(\hbar k_0)$. The time and space scales, t_0 and x_0, respectively, are assumed to satisfy $v_0 = x_0/t_0$, with t_0 specified below.

A typical charge carrier density n_0 is considered as given. The according distribution function scale,

$$\eta = \frac{4\pi^3 n_0}{k_0^3}$$

measures the level of degeneracy of the electron and hole gases. The classical non-degenerate statistics is recovered when η tends to zero.

Typical values of the collision frequencies of the different scattering mechanisms are introduced by

$$\nu_{ld} = \frac{\phi_{ld}^0 k_0^3}{\varepsilon_0}\,, \qquad \nu_{ph} = \frac{\phi_{ph}^0 k_0^3}{\varepsilon_0}\,, \qquad \nu_c = \frac{n_0 \phi_c^0 k_0^3}{\varepsilon_0}\,, \qquad \nu_{gr} = \frac{\phi_{gr}^0 k_0^9}{\varepsilon_0}\,.$$

The numbers ϕ_{ld}^0, ϕ_{ph}^0, ϕ_c^0, and ϕ_{gr}^0 are typical values of the transition rates $\phi_{i,ld}$, $\phi_{i,ph}$, $\phi_{j,c}^i$ and $\phi_{i,gr}^r$, respectively, with $i,j = n,p$. We assume that the transition rates corresponding to one type of scattering are of the same order of magnitude.

A typical value of the phonon collision frequency ν_{ph} is 10^{14} s^{-1} in Si (cf. Refs. [2], [21]) when considering the above mentioned values of ε_0 and $k_B T_L$. Under the same conditions, it lies within the range 10^{12} to 10^{14} s^{-1} in GaAs (cf. Ref. [2]). The order of magnitude of the lattice defect frequency (cf. Ref. [2]) ν_{ld} is always much smaller than ν_{ph}; scattering with lattice defects is thus often neglected. Referring to [33], [36], we know that the carrier-carrier collision frequency ν_c is small compared to ν_{ph} for low carrier densities and can reach the order of magnitude of ν_{ph} for high densities. A mathematical study of these two cases can be found in [34], [31]. Contrary to ν_c, the ionization collision frequency ν_{gr} does not depend on the carrier density. It is nearly equal to zero as long as the characteristic carrier energy ε_0 is smaller than the ionization energy Δ (typical value: 1.5 eV). Above that value, it increases strongly to reach 10^{16} s^{-1} in Silicon when $\varepsilon_0 \simeq 5$ eV (cf. Refs. [37], [21] and references within). A similar behavior is observed in GalliumArsenide (cf. Ref. [9]). Thus, the two different cases $\nu_{gr} << \nu_{ph}$ and $\nu_{gr} \approx \nu_{ph}$ successively occur when increasingly high applied biases are considered. Superimposed on this, $\nu_c << \nu_{ph}$ or $\nu_c \approx \nu_{ph}$, depending on the carrier concentrations.

The above discussion shows that phonon collisions always belong to the dominating scattering effects, except for very high carrier energies (when generation-recombination effects dominate). This last case will be excluded here and is deferred to future work [40]. Therefore the time scale is chosen as $t_0 = \nu_{ph}^{-1}$. The dimensionless parameters $\alpha_c^2 = \nu_c/\nu_{ph}$ and $\alpha_{gr}^2 = \nu_{gr}/\nu_{ph}$ will appear below.

The scaled phonon collision operators contain the small parameter α^2, the typical ratio between phonon energies and carrier energies. An expansion in powers of α^2 (cf. Refs. [30]-[31], [34]) produces an elastic contribution at the leading order and an inelastic $O(\alpha^2)$ correction. In this expansion we include the scattering with lattice defects:

$$Q_{i,ph}(f_i) + Q_{i,ld}(f_i) = Q_i^0(f_i) + \alpha^2 Q_i^1(f_i)\,, \tag{13-a}$$

with

$$Q_i^0(f_i) = \int_B \phi_i^0(k;k')\delta(\varepsilon_i' - \varepsilon_i)(f_i' - f_i)dk'\,, \tag{13-b}$$

and $i = n, p$. Note that here and in the following, dimensionless quantities are denoted by the same symbols as their dimensional counterparts. The dimensionless version of the Boltzmann equations (1) can then be written as

$$\begin{aligned}
&\frac{\partial f_n}{\partial t} + \nabla_k \varepsilon_n \cdot \nabla_x f_n + \nabla_x V \cdot \nabla_k f_n \\
&\qquad\qquad = Q_n^0(f_n) + \alpha_c^2 Q_{n,c}(f_n, f_p) + \alpha_{gr}^2 Q_{n,gr}(f_n, f_p) + \alpha^2 Q_n^1(f_n)\,, \\
&\frac{\partial f_p}{\partial t} + \nabla_k \varepsilon_p \cdot \nabla_x f_p - \nabla_x V \cdot \nabla_k f_p \\
&\qquad\qquad = Q_p^0(f_p) + \alpha_c^2 Q_{p,c}(f_n, f_p) + \alpha_{gr}^2 Q_{p,gr}(f_n, f_p) + \alpha^2 Q_p^1(f_p)\,.
\end{aligned} \tag{14}$$

The scaled collision operator for carrier-carrier interaction in the electron equation $Q_{n,c} = Q^n_{n,c} + Q^p_{n,c}$ reads

$$
\begin{aligned}
Q^n_{n,c}\,(f_n) &= \int_{B^3} \phi^n_{n,c}\ \delta^c_{\varepsilon_n}\ \delta^c_k \\
&\quad\times\Big[f'_n\ f^{*\prime}_n\ (1-\eta f_n)(1-\eta f^*_n) - f_n\ f^*_n\ (1-\eta f'_n)(1-\eta f^{*\prime}_n)\Big]\ dk^* dk' dk^{*\prime}\ , \\
Q^p_{n,c}\,(f_n, f_p) &= \int_{B^3} \phi^p_{n,c}\ \delta^c_{\varepsilon_{np}}\ \delta^c_{k_{np}} \\
&\quad\times\Big[f'_n f^{*\prime}_p(1-\eta f_n)(1-\eta f^*_p) - f_n f^*_p(1-\eta f'_n)(1-\eta f^{*\prime}_p)\Big]\ dk^* dk' dk^{*\prime}\ .
\end{aligned}
$$

The generation-recombination operator in the electron equation reads $Q_{n,gr} = Q^n_{n,gr} + Q^p_{n,gr}$ where

$$
\begin{aligned}
Q^n_{n,gr}(f_n, f_p) &= \int_{B^3} \phi^r_{n,gr}\ \delta^{gr}_{\varepsilon_n}\ \Big[\mathcal{F}^2_0\ f'_n\ (1-\eta f_n)(1-\eta f^*_n)(1-\eta f^+_p) \\
&\qquad\qquad -f_n\ f^*_n\ f^+_p\ (1-\eta f'_n)\Big]\ dk' dk^* dk^+ \\
&\quad+\tfrac{1}{2}\int_{B^3} \phi^{r\ \prime}_{n,gr}\delta^{gr\prime}_{\varepsilon_n}\ \Big[f'_n\ f^*_n\ f^+_p\ (1-\eta f_n) \\
&\qquad\qquad -\mathcal{F}^2_0\ f_n\ (1-\eta f'_n)(1-\eta f^*_n)(1-\eta f^+_p)\Big]\ dk' dk^* dk^+\ , \\
Q^p_{n,gr}(f_n, f_p) &= \tfrac{1}{2}\int_{B^3} \phi^r_{p,gr}\ \delta^{gr}_{\varepsilon_p}\ \Big[\mathcal{F}^2_0\ f'_p\ (1-\eta f^+_p)(1-\eta f^*_p)(1-\eta f_n) \\
&\qquad\qquad -f^+_p\ f^*_p\ f_n\ (1-\eta f'_p)\Big]\ dk' dk^* dk^+\ .
\end{aligned}
$$

The collision operators $Q_{p,c}$ and $Q_{p,gr}$ for holes are obtained from the previous expressions by interchanging the subscripts n and p.

Following the discussion above, we shall only consider cases where the parameters α_c and α_{gr} are at most of the order of magnitude of 1. For definiteness, we allow for the significant cases where they are set equal to 1 or equal to α:

1. $\alpha_c = \alpha$, $\alpha_{gr} = 1$,
2. $\alpha_c = 1$, $\alpha_{gr} = 1$,
3. $\alpha_c = \alpha$, $\alpha_{gr} = \alpha$,
4. $\alpha_c = 1$, $\alpha_{gr} = \alpha$.

In the following sections, energy transport models are derived for situations where the carrier distributions are in equilibrium relative to the generation-recombination mechanisms. Different scalings lead to different routes to this aim with the resulting models all having the same basic structure, only differing in the way the transport coefficients are computed. In cases 1 and 2, the derivation just amounts to carrying out the limit $\alpha \to 0$, since in these cases the generation-recombination operator is of leading order. The formal asymptotic analysis for case 1 is carried out in section 5. The procedure for case 2 is analogous and is deferred to a remark at the end of section 5. For cases 3, the limit $\alpha \to 0$ is already available in the literature, cf., e.g., [31]. It leads to SHE-models for electrons and holes coupled by source terms coming from carrier-carrier collisions and generation-recombination. A second macroscopic limit, assuming dominance of generation-recombination, then leads to the desired ET-model. This route is taken in section 6. It is attractive compared to the direct limit, since it leads to simpler formulas for the transport coefficients. Similarly, case 4 leads to a detour via (instead of the SHE-model) an ET-model with the individual macroscopic carrier densities and a common carrier temperature as unknowns. This is a slight modification of the ET-model for the individual carriers [34] since the electron-hole scattering leads to a thermalization with a common temperature. This last route is not considered here.

4 Properties of the leading order collision operator

In this section, the analysis of section 5 is prepared by deriving some useful properties of the sum of the elastic collision operators and the generation-recombination operators. The first lemma recalls from [31] the basic symmetry property and the collision invariants of the elastic operators.

Lemma 4.1:

(i) $$\int_B Q_q^0(f)\ \psi dk = -\frac{1}{2}\int_{B^2} \phi_q^0\ \delta(\varepsilon_q' - \varepsilon_q)\ (f'-f)\ (\psi'-\psi)\ dk'\ dk\ ,$$

(ii) $$\int_B Q_q^0(f)H(f)dk = -\frac{1}{2}\int_{B^2} \phi_q^0\delta(\varepsilon_q' - \varepsilon_q)(f'-f)(H(f')-H(f))dk'dk \le 0\ ,$$

for every increasing H.

(iii) $$\text{If} \quad \psi = \psi(\varepsilon_q) \quad \text{then} \quad \int_B Q_q^0(f)\psi dk = 0\ .$$

The subscript q can be replaced by n and p.

The following properties of the generation-recombination operators apply to the electron-hole system. Corresponding results for the individual operators are not available.

Lemma 4.2: For any pair of regular test functions (ψ_n, ψ_p),

$$\begin{aligned}
\int_B Q_{n,gr}(f_n,f_p)\ \psi_n dk &+ \int_B Q_{p,gr}(f_n,f_p)\psi_p dk \\
&= \tfrac{1}{2}\int_{B^4} \phi_{n,gr}^r \delta_{\varepsilon_n}^{gr}[\mathcal{F}_0^2 f_n'(1-\eta f_n)(1-\eta f_n^*)(1-\eta f_p^+) - f_n f_n^* f_p^+(1-\eta f_n')] \\
&\qquad\qquad \times[\psi_n + \psi_n^* + \psi_p^+ - \psi_n']dk^4 \\
&+\tfrac{1}{2}\int_{B^4} \phi_{p,gr}^r \delta_{\varepsilon_p}^{gr}[\mathcal{F}_0^2 f_p'(1-\eta f_p^+)(1-\eta f_p^*)(1-\eta f_n) - f_p^+ f_p^* f_n(1-\eta f_p')] \\
&\qquad\qquad \times[\psi_p^+ + \psi_p^* + \psi_n - \psi_p']dk^4\ ,
\end{aligned}$$

holds, where $dk^4 = dk\ dk'\ dk^*\ dk^+$.

Proof: The proof is straightforward using the symmetry property (11) of the scattering cross sections. ∎

Corollary 4.3: (H-Theorem)
Let $H(f) = \log\left[f\mathcal{F}_0^{-1}(1-\eta f)^{-1}\right]$, and let $\phi^r_{n,gr}$, $\phi^r_{p,gr}$ be positive. Then

$$
\begin{aligned}
&\int_B Q_{n,gr}(f_n,f_p)H(f_n)dk + \int_B Q_{p,gr}(f_n,f_p)H(f_p)dk = \\
&\quad \tfrac{1}{2}\int_{B^4} \phi^r_{n,gr}\ \delta^{gr}_{\varepsilon_n}\ \left[\mathcal{F}_0^2\ f'_n\ (1-\eta f_n)(1-\eta f^*_n)(1-\eta f^+_p) - f_n\ f^*_n\ f^+_p\ (1-\eta f'_n)\right] \\
&\qquad \times\left[\log\Big(f_n\ f^*_n\ f^+_p\ (1-\eta f'_n)\Big) - \log\Big(\mathcal{F}_0^2\ f'_n\ (1-\eta f_n)(1-\eta f^*_n)(1-\eta f^+_p)\Big)\right]\ dk^4 \\
&\quad + \tfrac{1}{2}\int_{B^4} \phi^r_{p,gr}\ \delta^{gr}_{\varepsilon_p}\ \left[\mathcal{F}_0^2\ f'_p\ (1-\eta f_p)(1-\eta f^*_p)(1-\eta f^+_n) - f_p\ f^*_p\ f^+_n\ (1-\eta f'_p)\right] \\
&\qquad \times\left[\log\Big(f_p\ f^*_p\ f^+_n\ (1-\eta f'_p)\Big) - \log\Big(\mathcal{F}_0^2\ f'_p\ (1-\eta f_p)(1-\eta f^*_p)(1-\eta f^+_n)\Big)\right]\ dk^4 \le 0\ .
\end{aligned}
$$

Lemma 4.4: Assume that ϕ^0_n, ϕ^0_p, $\phi^r_{n,gr}$, and $\phi^r_{p,gr}$ are positive and that (12) holds. Then

$$
\int_B \left[Q^0_n(f_n) + Q_{n,gr}(f_n,f_p)\right]\psi_n\ dk + \int_B \left[Q^0_p(f_p) + Q_{p,gr}(f_n,f_p)\right]\psi_p\ dk = 0
$$

holds for all f_n, f_p and for a pair (ψ_n,ψ_p) of continuous functions, iff there exist real constants a and c such that

$$
\begin{aligned}
\psi_n(k) &= \ \ a + c\ (\varepsilon_n(k) + \Delta/2) \\
\psi_p(k) &= -a + c\ (\varepsilon_p(k) + \Delta/2)
\end{aligned}
\quad .
$$

Proof: ($\Longleftarrow$) is a simple computation.

Let $f_n = \mathcal{F}_0\exp(\psi_n)\left[1+\eta\mathcal{F}_0\exp(\psi_n)\right]^{-1}$ and $f_p = \mathcal{F}_0\exp(\psi_p)\left[1+\eta\mathcal{F}_0\exp(\psi_p)\right]^{-1}$. Then the positivity of the collision cross sections, corollary 4.3, and lemma 4.1 imply that

$$
\int_B [Q^0_{n,lp}(f_n) + Q_{n,gr}(f_n,f_p)]\psi_n\ dk + \int_B [Q^0_{p,lp}(f_p) + Q_{p,gr}(f_n,f_p)]\psi_p\ dk = 0
$$

is satisfied, iff $\psi_n(k) = \psi_n(\varepsilon_n(k))$, $\psi_p(k) = \psi_p(\varepsilon_p(k))$, and

$$
\psi_n(\varepsilon_n) + \psi_n(\varepsilon^*_n) + \psi_p(\varepsilon_p) = \psi_n(\varepsilon'_n) \quad \text{with} \quad \varepsilon_n + \varepsilon^*_n + \varepsilon_p + \Delta = \varepsilon'_n, \tag{14}
$$

$$
\psi_p(\varepsilon_p) + \psi_p(\varepsilon^*_p) + \psi_n(\varepsilon_n) = \psi_p(\varepsilon'_p) \quad \text{with} \quad \varepsilon_p + \varepsilon^*_p + \varepsilon_n + \Delta = \varepsilon'_p\ , \tag{15}
$$

whenever $\varepsilon_n, \varepsilon^*_n, \varepsilon'_n \in [0,\overline{\varepsilon}_n]$ and $\varepsilon_p, \varepsilon^*_p, \varepsilon'_p \in [0,\overline{\varepsilon}_p]$. For electron energies this implies $\varepsilon_n, \varepsilon^*_n \le \overline{\varepsilon}_n - \Delta$ and $\varepsilon'_n \ge \Delta$ in (14), and $\varepsilon_n \le \overline{\varepsilon}_p - \Delta$ in (15).

Replacing ε_n by $\varepsilon_n + h$ in (14) and taking the difference with (14) gives

$$
\psi_n(\varepsilon_n + h) - \psi_n(\varepsilon_n) = \psi_n(\varepsilon'_n + h) - \psi_n(\varepsilon'_n)\,.
$$

Further differencing with respect to ε_n keeping ε_n' fixed, and vice versa, gives

$$\psi_n(\varepsilon_n + h) - 2\psi_n(\varepsilon_n) + \psi_n(\varepsilon_n - h) = 0\,, \tag{16}$$
$$\psi_n(\varepsilon_n' + h) - 2\psi_n(\varepsilon_n') + \psi_n(\varepsilon_n' - h) = 0\,. \tag{17}$$

Noting that h can be made arbitrarily small and the above restrictions on ε_n and ε_n', this shows that ψ_n is an affine function in the intervals $(0, \overline{\varepsilon}_n - \Delta)$ and $(\Delta, \overline{\varepsilon}_n)$. Analogously, by taking a second difference of (15), it can be shown that ψ_n is affine in $(0, \overline{\varepsilon}_p - \Delta)$. By the assumption (12) these three intervals cover the whole electron energy interval $(0, \overline{\varepsilon}_n)$ showing that ψ_n is of the form $\psi_n = a_n + c_n\varepsilon_n$. In the same way $\psi_p = a_p + c_p\varepsilon_p$ can be proven. Substitution in (14) shows $c_n = c_p = c$ and $a_n - c\Delta/2 = -a_p + c\Delta/2 = a$. ∎

Corollary 4.5: With the assumptions of the previous lemma and the notation $f = (f_n, f_p)$, $Q^0(f) = (Q_n^0(f_n), Q_p^0(f_p))$, $Q_{gr}(f) = (Q_{n,gr}(f_n, f_p), Q_{p,gr}(f_n, f_p))$,

$$Q^0(f) + Q_{gr}(f) = 0\ ,$$

holds iff there exist $\mu \in I\!R$ and $T > 0$ such that

$$f_n(k) = (F_n)_{\mu,T} = \frac{1}{\eta + \mathcal{F}_0^{-1}\exp\left[\left(\varepsilon_n(k) + \Delta/2 - \mu\right)/T\right]}\ ,$$
$$f_p(k) = (F_p)_{\mu,T} = \frac{1}{\eta + \mathcal{F}_0^{-1}\exp\left[\left(\varepsilon_p(k) + \Delta/2 + \mu\right)/T\right]}\ .$$

Proof: The proof follows directly from lemma 4.1 (ii), corollary 4.3 and lemma 4.4. ∎

In the nondegenerate limit $\eta \to 0$, the equilibrium Fermi-Dirac distributions reduce to the Maxwellians

$$F_n = \mathcal{F}_0 \exp\left(\frac{\mu - \Delta/2 - \varepsilon_n}{T}\right)\ , \qquad F_p = \mathcal{F}_0 \exp\left(\frac{-\mu - \Delta/2 - \varepsilon_p}{T}\right)\ .$$

The macroscopic densities

$$\rho_n = \int_B F_n\, dk\ , \qquad \rho_p = \int_B F_p\, dk\ ,$$

then satisfy the equilibrium condition

$$\rho_n\rho_p = n_i^2\ , \qquad \text{with } n_i(T)^2 = \mathcal{F}_0^2 e^{-\Delta/T}\int_B e^{-\varepsilon_n(k)/T}dk \int_B e^{-\varepsilon_p(k)/T}dk\ ,$$

known as the Saha law in plasma physics, where the temperature dependent intrinsic density is denoted by n_i.

For later reference we compute the linearization of the generation-recombination operator.

Lemma 4.6: Let $DQ_{gr} = (DQ_{n,gr}, DQ_{p,gr})$ denote the linearization of the generation-recombination operator at an equilibrium distribution $F = (F_n, F_p)$ (as defined in corollary 4.5). Then,

$$\begin{aligned} DQ_{n,gr}(f_n, f_p) = & \int_{B^3} 2A_{n,gr} \left[\varphi_n' - \varphi_n - \varphi_n^* - \varphi_p^+\right] dk' dk^* dk^+ \\ & - \int_{B^3} A_{n,gr}' \left[\varphi_n - \varphi_n' - \varphi_n^* - \varphi_p^+\right] dk' dk^* dk^+ \\ & + \int_{B^3} A_{p,gr} \left[\varphi_p' - \varphi_p^+ - \varphi_p^* - \varphi_n\right] dk' dk^* dk^+ , \end{aligned}$$

with the notations $A'_{n,gr} = A_{n,gr}(k', k^*, k^+; k)$,

$$\begin{aligned} A_{n,gr} &= \tfrac{1}{2}\, \phi^r_{n,gr}\, \delta^{gr}_{\varepsilon_n}\, F_n\, F_n^*\, F_p^+\, (1 - \eta F_n') , \\ A_{p,gr} &= \tfrac{1}{2}\, \phi^r_{p,gr}\, \delta^{gr}_{\varepsilon_p}\, F_p^+\, F_p^*\, F_n\, (1 - \eta F_p') . \end{aligned}$$

and

$$\varphi_n = \frac{f_n}{F_n(1-\eta F_n)} , \qquad \varphi_p = \frac{f_p}{F_p(1-\eta F_p)} .$$

The linearization $DQ_{p,gr}$ can be deduced from $DQ_{n,gr}$ by exchanging n and p.

Let us introduce the following scalar product of $f = (f_n, f_p)$ and $g = (g_n, g_p)$:

$$\langle f, g\rangle_F = \int_B f_n\, g_n\, \frac{dk}{F_n(1-\eta F_n)} + \int_B f_p\, g_p\, \frac{dk}{F_p(1-\eta F_p)} ,$$

and the associated norm $\|\ \|_F$. Let H_F be the Hilbert space induced by this norm. F_n and F_p denote equilibrium distribution functions as defined in corollary 4.5. We analyze the linearization of the equilibrium equation.

Lemma 4.7 : Let $g = (g_n, g_p) \in H_F$ be given. Then, the system of equations $Q^0(f) + DQ_{gr}(f) = g$ is solvable iff

$$\int_B g_n \begin{pmatrix} 1 \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_B g_p \begin{pmatrix} -1 \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk = 0 .$$

The solution $f = (f_n, f_p)$ is unique under the side condition

$$\int_B f_n \begin{pmatrix} 1 \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_B f_p \begin{pmatrix} -1 \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk = 0 .$$

Proof: With $g = (g_n, g_p) = (F_n(1-\eta F_n)\psi_n, F_p(1-\eta F_p)\psi_p)$, the computation

$$\begin{aligned} \langle DQ_{gr}(f), g\rangle_F = & - \int_{B^4} A_{n,gr}(\varphi_n + \varphi_n^* + \varphi_p^+ - \varphi_n')(\psi_n + \psi_n^* + \psi_p^+ - \psi_n') dk^4 \\ & - \int_{B^4} A_{p,gr}(\varphi_p + \varphi_p^* + \varphi_n^+ - \varphi_p')(\psi_p + \psi_p^* + \psi_n^+ - \psi_p') dk^4 , \end{aligned} \tag{18}$$

where dk^4 is given in lemma 4.2, shows that DQ_{gr} is symmetric with respect to $\langle .,. \rangle_F$ and non-positive. It is well known [31], [34] that the same holds for the elastic operator Q^0. Boundedness of $Q^0 + DQ_{gr}$ is a consequence of the boundedness of the coefficient functions. $Q^0 + DQ_{gr}$ is thus a bounded, self-adjoint, non-positive operator on H_F. It can be written in the form $Q^0(f) + DQ_{gr}(f) = -\mathcal{V} f + \mathcal{C}(f)$, with a positive definite diagonal matrix $\mathcal{V}$ and a compact integral operator $\mathcal{C}$.

The nonpositivity of $Q^0 + DQ_{gr}$ implies $spectrum(Q^0 + DQ_{gr}) \subseteq (-\infty, 0]$. From (18) with $f = \psi$ and from lemma 4.4 we deduce

$$\begin{aligned} Ker(Q^0 + DQ_{gr}) = span\Big\{ &\big(F_n(1-\eta F_n), -F_p(1-\eta F_p)\big), \\ &\big(F_n(1-\eta F_n)(\varepsilon_n + \Delta/2), F_p(1-\eta F_p)(\varepsilon_p + \Delta/2)\big) \Big\} \ . \end{aligned}$$

$Q^0 + DQ_{gr}$, thus, has a zero eigenvalue of multiplicity 2. Weyl's theorem [39] then implies that $spectrum(Q^0 + DQ_{gr}) \subseteq \{0\} \cup (-\infty, -\sigma]$ with $\sigma > 0$. An application of the Fredhlom alternative completes the proof. ■

5 ET model for strong generation-recombination

We set $\alpha_c = \alpha$ and $\alpha_{gr} = 1$ to derive the ET model associated with strong generation-recombination and weak carrier-carrier scattering, i.e., with the leading operator $Q^0 + Q_{gr}$ studied in the preceding section. To that purpose, we introduce the diffusion scaling $t \to t/\alpha^2$, $x \to x/\alpha$, in the system of Boltzmann equations (14):

$$\begin{aligned} &\frac{\partial f_n}{\partial t} + \alpha^{-1} \Big[\nabla_k \varepsilon_n \cdot \nabla_x f_n + \nabla_x V \cdot \nabla_k f_n \Big] = \\ &\qquad \alpha^{-2}\ Q_n^0(f_n) + \alpha^{-2}\ Q_{n,gr}(f_n, f_p) + Q_{n,c}(f_n, f_p) + Q_n^1(f_n) \ , \\ &\frac{\partial f_p}{\partial t} + \alpha^{-1} \Big[\nabla_k \varepsilon_p \cdot \nabla_x f_p - \nabla_x V \cdot \nabla_k f_p \Big] = \\ &\qquad \alpha^{-2}\ Q_p^0(f_p) + \alpha^{-2}\ Q_{p,gr}(f_n, f_p) + Q_{p,c}(f_n, f_p) + Q_p^1(f_p) \ . \end{aligned} \tag{19}$$

We expand the solution in powers of α:

$$\begin{pmatrix} f_n \\ f_p \end{pmatrix} = \begin{pmatrix} f_{0n} \\ f_{0p} \end{pmatrix} + \alpha \begin{pmatrix} f_{1n} \\ f_{1p} \end{pmatrix} + \alpha^2 \begin{pmatrix} f_{2n} \\ f_{2p} \end{pmatrix} + \mathcal{O}(\alpha^3) \ .$$

We insert the expansion in the system (19) and compare coefficients of equal powers of α. This leads to systems of equations to be successively solved:

Order α^{-2}:

$$\begin{aligned} Q_n^0(f_{0n}) + Q_{n,gr}(f_{0n}, f_{0p}) = 0 \ , \\ Q_p^0(f_{0p}) + Q_{p,gr}(f_{0n}, f_{0p}) = 0 \ , \end{aligned} \tag{20}$$

Order α^{-1}:

$$\begin{aligned} Q_n^0(f_{1n}) + DQ_{n,gr}(f_{1n}, f_{1p}) &= \nabla_k \varepsilon_n \cdot \nabla_x f_{0n} + \nabla_x V \cdot \nabla_k f_{0n} \ , \\ Q_p^0(f_{1p}) + DQ_{p,gr}(f_{1n}, f_{1p}) &= \nabla_k \varepsilon_p \cdot \nabla_x f_{0p} - \nabla_x V \cdot \nabla_k f_{0p} \ , \end{aligned} \tag{21}$$

Order α^0:

$$\begin{aligned} & Q_n^0(f_{2n}) + DQ_{n,gr}(f_{2n}, f_{2p}) \\ & \quad = \frac{\partial f_{0n}}{\partial t} + \nabla_k \varepsilon_n \cdot \nabla_x f_{1n} + \nabla_x V \cdot \nabla_k f_{1n} - Q_n^1(f_{0n}) \ , \\ & Q_p^0(f_{2p}) + DQ_{p,gr}(f_{2n}, f_{2p}) \\ & \quad = \frac{\partial f_{0p}}{\partial t} + \nabla_k \varepsilon_p \cdot \nabla_x f_{1p} - \nabla_x V \cdot \nabla_k f_{1p} - Q_p^1(f_{0p}) \ . \end{aligned} \tag{22}$$

¿From (20) and lemma 4.5, we conclude that there exist $\mu \in I\!R$ and $T > 0$ such that

$$\begin{aligned} f_{0n} &= \left[\eta + \mathcal{F}_0^{-1} \exp\left(\frac{\varepsilon_n + \Delta/2 - \mu}{T} \right) \right]^{-1} \ , \\ f_{0p} &= \left[\eta + \mathcal{F}_0^{-1} \exp\left(\frac{\varepsilon_p + \Delta/2 + \mu}{T} \right) \right]^{-1} \ , \end{aligned} \tag{23}$$

where $\mu = \mu(x,t)$ and $T = T(x,t)$ are functions of x and t which are still to be determined.

Next, a simple computation shows that the right hand side of (21) satisfies the solvabiblity condition of lemma 4.7. The solution can be written in the form

$$f_{1q} = \left[\nabla_x \left(\frac{\mu}{T} \right) - \frac{\nabla_x V}{T} \right] \cdot \psi_{1q} + \nabla_x \left(-\frac{1}{T} \right) \cdot \psi_{2q} + F_{1q} \ , \quad q = n, p,$$

where $\psi_1 = (\psi_{1n}, \psi_{1p})$, $\psi_2 = (\psi_{2n}, \psi_{2p})$ are the unique solutions (as described in lemma 4.7) of

$$\Big(Q^0 + DQ_{gr} \Big)(\psi_i) = g_i \ , \qquad i = 1, 2,$$

with

$$g_1 = \Big(f_{0n}(1 - \eta f_{0n}) \nabla_k \varepsilon_n, -f_{0p}(1 - \eta f_{0p}) \nabla_k \varepsilon_p \Big) \, , \tag{24}$$

$$g_2 = \Big(f_{0n}(1 - \eta f_{0n})(\varepsilon_n + \Delta/2) \nabla_k \varepsilon_n, f_{0p}(1 - \eta f_{0p})(\varepsilon_p + \Delta/2) \nabla_k \varepsilon_p \Big) \, . \tag{25}$$

(F_{1n}, F_{1p}) is an arbitrary element of $Ker(Q^0 + DQ_{gr})$.

We introduce the charge density $\chi = \chi(\mu, T)$ and the total energy density $\mathcal{E} = \mathcal{E}(\mu, T)$ by

$$\begin{pmatrix} \chi \\ \mathcal{E} \end{pmatrix} = \int_B f_{0n} \begin{pmatrix} 1 \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_B f_{0p} \begin{pmatrix} -1 \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk \ . \tag{26}$$

The ET model is now obtained as the solvability condition for (22). To that purpose, cf. lemma 4.7, we compute the balance equations for the charge and total energy densities by integrating the scalar products of (22) with $(1,-1)^\top$ and with $(\varepsilon_n+\Delta/2,\ \varepsilon_p+\Delta/2)^\top$, over B. The obtained ET system governs the evolution of χ and $\mathcal{E}$ in terms of the associated charge and energy fluxes, $J_\chi = J_\chi(\mu,T)$ and $J_\mathcal{E} = J_\mathcal{E}(\mu,T)$, as follows:

$$\begin{aligned} &\frac{\partial \chi}{\partial t} + div\, J_\chi = 0\ , \\ &\frac{\partial \mathcal{E}}{\partial t} + div\, J_\mathcal{E} - \nabla_x V \cdot J_\chi = W_{ph}\ , \end{aligned} \tag{27}$$

where

$$\begin{aligned} \begin{pmatrix} J_\chi \\ J_\mathcal{E} \end{pmatrix} &= \int_B f_{1n} \begin{pmatrix} 1 \\ \varepsilon_n + \Delta/2 \end{pmatrix} \nabla_k \varepsilon_n\, dk \\ &+ \int_B f_{1p} \begin{pmatrix} -1 \\ \varepsilon_p + \Delta/2 \end{pmatrix} \nabla_k \varepsilon_p\, dk = -D \begin{pmatrix} \nabla_x \left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T} \\ \nabla_x \left(\frac{-1}{T}\right) \end{pmatrix} . \end{aligned} \tag{28}$$

The diffusion matrix D is defined by

$$D = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}\ , \tag{29-a}$$

where the components of the matrices D_{ij} can be conveniently written using the scalar product introduced in the previous section:

$$D_{ij}^{lm} = \langle g_i^l, \psi_j^m \rangle\ , \qquad i,j = 1,2, \quad l,m = 1,2,3. \tag{29-b}$$

The energy source term is

$$W_{ph} = \int_B Q_n^1(f_{0n})\varepsilon_n\, dk + \int_B Q_p^1(f_{0p})\varepsilon_p\, dk\ . \tag{30}$$

Qualitative results on the diffusion matrix and the energy source term can be proven analogously to [34]:

Lemma 5.1:
(i) Assume that the vector functions $(\partial_{k_i}\varepsilon_n, -\partial_{k_i}\varepsilon_p)$, $((\varepsilon_n+\Delta/2)\partial_{k_i}\varepsilon_n, (\varepsilon_p+\Delta/2)\partial_{k_i}\varepsilon_p)$, $i = 1,2,3$, are linearly independent. Then, the matrix $D(\mu,T)$ is symmetric (satisfying the Onsager relation $D_{ij}^{tr} = D_{ji}$) and positive-definite for any $\mu \in I\!R$ and $T > 0$.
(ii) The source term W_{ph} is a relaxation term towards the lattice temperature,

$$W_{ph}(T - T_L) \le 0\ .$$

Remark 5.2: The ET system (27) can be rewritten as a modified hydrodynamic system where some transport terms in the momentum equation are neglected:

$$\begin{aligned} &\frac{\partial \chi}{\partial t} + div(\chi u) = 0 \ , \\ &\nabla_x p = \chi \nabla_x V - T\chi^2 D_{11}^{-1} u + \left(p + \mathcal{E} - \chi D_{11}^{-1} D_{12}\right) \frac{\nabla_x T}{T} \ , \\ &\frac{\partial \mathcal{E}}{\partial t} + div\left(D_{21} D_{11}^{-1} \chi u + q\right) = \chi u \cdot \nabla_x V + W_{ph} \ , \end{aligned} \tag{31}$$

where the velocity is determined from $J_\chi = \chi u$ and the pressure is defined by

$$p = -\frac{T}{\eta}\left[\int_B \log(1-\eta f_{0n})dk + \int_B \log(1-\eta f_{0p})dk\right] . \tag{32}$$

The above momentum equation corresponds to the zero mass limit, as in Ref. [34] and [26]. The terms on the right hand side correspond to the Coulomb force, to a force due to elastic collisions with the crystal, and to the so-called thermal force (also appearing in plasma models), respectively.

The heat flux is given by

$$q = -\kappa \nabla_x T \ , \qquad \text{with } \kappa = \frac{1}{T^2}(D_{22} - D_{21} D_{11}^{-1} D_{12}) \ ,$$

where the heat conductivity tensor κ is positive-definite by the positive-definiteness of the diffusion matrix D.

Remark 5.3: A macroscopic entropy density S for the ET-model can be deduced from the kinetic entropy of corollary 4.3 at equilibrium:

$$S(\chi, \mathcal{E}) = \int_B \int H(f_{0n}) df_{0n} \ dk + \int_B \int H(f_{0p}) df_{0p} \ dk \ .$$

Straightforward computations show that S is convex and

$$\frac{\partial S}{\partial \chi} = \frac{\mu}{T} \ , \qquad \frac{\partial S}{\partial \mathcal{E}} = -\frac{1}{T} \ .$$

So, although the variables of the present problem as well as the definition of H are not standard, we recover the usual entropic variables. The evolution of the entropy is governed by

$$\frac{\partial S}{\partial t} + div(G) = -\mathcal{Y}^\top D \mathcal{Y} - \frac{1}{T} W_{ph} \ , \tag{33}$$

with the entropy flux $G = (\mu J_\chi - J_\mathcal{E})/T$ and with $\mathcal{Y}^\top = (\nabla_x(\mu/T) - (\nabla_x V)/T, \nabla_x(-1/T))$. In a closed system, the entropy decays except, possibly, for the effects of phonon scattering.

Remark 5.4: When the generation-recombination and carrier-carrier frequencies have the same order of magnitude, $\alpha_{gr} = \alpha_c = 1$, we recover the previous results up to the definition of ψ_1 and ψ_2. These functions now solve

$$\Big(Q^0 + DQ_{gr} + DQ_c\Big)(\psi_i) = g_i \,, \qquad i = 1, 2,$$

with the linearization DQ_c of the collision operator $(Q_{n,c}, Q_{p,c})$ at equilibrium. In the ET model (27)-(30) only the definition of the diffusion matrix is modified. Its properties stated in lemma 5.1 remain the same.

Remark 5.5: The results obtained in this section can be extended to generation-recombination collisions dominating all the other collisional processes, including elastic phonons. The key point of this extension is to show that the equilibrium distribution function of Q_{gr} is also the equilibrium distribution function (f_{0n}, f_{0p}) of $Q^0 + Q_{gr}$. The proof is given in Ref. [40]. Then, as in the previous remark, the only difference compared to the ET model (27)-(30) lies in the definition of the functions ψ_1 and ψ_2.

6 ET model derived through a SHE model

The ET model for strong generation-recombination proposed in this section is still derived from the system of BTE (14), but using now the multiple scaling approach presented in [31]. The derivation passes through an intermediate level: the SHE model. The resulting macroscopic model is close to the previous one, introduced in Sec. 5, since we recover the system (27). The main difference lies in the definition of the diffusion matrix, which turns out to be simpler. Consequently, the diffusion matrix can be computed explicitly in particular cases.

In (14), we set $\alpha_c = \alpha_{gr} = \alpha$ and introduce, as in the preceding section, the diffusion scaling $t \to t/\alpha^2$, $x \to x/\alpha$:

$$\begin{aligned}
&\frac{\partial f_n}{\partial t} + \alpha^{-1} \Big[\nabla_k \varepsilon_n \cdot \nabla_x f_n + \nabla_x V \cdot \nabla_k f_n\Big] = \\
&\qquad \alpha^{-2}\, Q_n^0(f_n) + Q_{n,gr}(f_n, f_p) + Q_{n,c}(f_n, f_p) + Q_n^1(f_n) \;, \\
&\frac{\partial f_p}{\partial t} + \alpha^{-1} \Big[\nabla_k \varepsilon_p \cdot \nabla_x f_p - \nabla_x V \cdot \nabla_k f_p\Big] = \\
&\qquad \alpha^{-2}\, Q_p^0(f_p) + Q_{p,gr}(f_n, f_p) + Q_{p,c}(f_n, f_p) + Q_p^1(f_p) \;.
\end{aligned} \tag{34}$$

Since the leading order operator Q^0 is decoupled, the analysis of the limit $\alpha \to 0$ is analogous to the case of a scalar equation discussed in [31] and will only be outlined here.

The main steps are similar to the preceding section. The relevant properties of the elastic collision operator for electrons Q_n^0 are the following: The kernel of Q_n^0 consists of all functions depending on the wave vector k only through the kinetic energy $\varepsilon_n(k)$. The solvability condition for equations of the form $Q_n^0(f) = g$ is

$$\int_{S_n(\varepsilon)} g \; d\mathcal{N}_\varepsilon(k) = 0 \qquad \text{for all } \varepsilon \,,$$

where the coarea formula has been used as in [31] to rewrite integrals over the Brillouin zone as iterated integrals over the range $\varepsilon_n(B)$ of the band diagram and over surfaces $S_n(\varepsilon) = \{k \in B : \ \varepsilon_n(k) = \varepsilon\}$ of constant kinetic energy:

$$\int_B f\, dk = \int_{\varepsilon_n(B)} \int_{S_n(\varepsilon)} f\, d\mathcal{N}_\varepsilon(k)\, d\varepsilon\ .$$

The electron density of states is defined as

$$N_n(\varepsilon) = \int_{S_n(\varepsilon)} d\mathcal{N}_\varepsilon(k)\, .$$

The preceding discussion also applies to holes (by replacing the subscript n by p).

In a Hilbert expansion for the solution of (34)

$$f_n = f_{0n} + \alpha f_{1n} + \alpha^2 f_{2n} + \mathcal{O}(\alpha^3)\, , \qquad f_p = f_{0p} + \alpha f_{1p} + \alpha^2 f_{2p} + \mathcal{O}(\alpha^3)\, ,$$

the leading order terms have to be in the kernel of Q^0: $f_{0n}(x,k,t) = \mathcal{F}_n(x, \varepsilon_n(k), t)$ and $f_{0p}(x,k,t) = \mathcal{F}_p(x, \varepsilon_p(k), t)$. The solvability condition for the system of order α^{-1} is satisfied. Its solution is given by

$$f_{1n} = -\Phi_n \cdot \left(\nabla_x \mathcal{F}_n + \nabla_x V \frac{\partial \mathcal{F}_n}{\partial \varepsilon} \right) + \mathcal{G}_n\ , \qquad f_{1p} = -\Phi_p \cdot \left(\nabla_x \mathcal{F}_p + \nabla_x V \frac{\partial \mathcal{F}_p}{\partial \varepsilon} \right) + \mathcal{G}_p\ ,$$

with a solution Φ_n of $-Q_n^0(\Phi_n) = \nabla_k \varepsilon_n$, Φ_p defined analogously, and an arbitrary element $(\mathcal{G}_n, \mathcal{G}_p)$ of the kernel of Q^0.

The last step, leading to the following SHE model, is writing down the solvability condition for the system of order α^0:

$$\begin{aligned} N_n \frac{\partial \mathcal{F}_n}{\partial t} + div\, \mathcal{J}_n + \nabla_x V \cdot \frac{\partial \mathcal{J}_n}{\partial \varepsilon} &= \mathcal{Q}_n(\mathcal{F}_n, \mathcal{F}_p)\ , \\ N_p \frac{\partial \mathcal{F}_p}{\partial t} + div\, \mathcal{J}_p - \nabla_x V \cdot \frac{\partial \mathcal{J}_p}{\partial \varepsilon} &= \mathcal{Q}_p(\mathcal{F}_n, \mathcal{F}_p)\ . \end{aligned} \tag{35}$$

The fluxes of electrons and holes are expressed by

$$\mathcal{J}_n = -\mathcal{D}_n \left(\nabla_x \mathcal{F}_n + \nabla_x V \frac{\partial \mathcal{F}_n}{\partial \varepsilon} \right)\ , \qquad \mathcal{J}_p = -\mathcal{D}_p \left(\nabla_x \mathcal{F}_p - \nabla_x V \frac{\partial \mathcal{F}_p}{\partial \varepsilon} \right)\ , \tag{36-a}$$

with the 3×3 diffusion matrices

$$\mathcal{D}_n(\varepsilon) = \int_{S_n(\varepsilon)} \nabla_k \varepsilon_n \otimes \Phi_n\, d\mathcal{N}_\varepsilon(k)\ , \qquad \mathcal{D}_p(\varepsilon) = \int_{S_p(\varepsilon)} \nabla_k \varepsilon_p \otimes \Phi_p\, d\mathcal{N}_\varepsilon(k)\ . \tag{36-b}$$

We know from proposition 3.6 in Ref. [31] that $\mathcal{D}_n$ and $\mathcal{D}_p$ are symmetric and positive-definite, and satisfy the inequality:

$$\mathcal{D}_n \geq \frac{C_n}{N_n} \int_{S_n(\varepsilon)} \nabla_k \varepsilon_n \otimes \nabla_k \varepsilon_n\, d\mathcal{N}_\varepsilon(k) \quad \text{with} \quad C_n > 0\ , \tag{36-c}$$

with an analogous estimate for $\mathcal{D}_p$. As in [31] the collision terms

$$
\begin{aligned}
\mathcal{Q}_n(\mathcal{F}_n,\mathcal{F}_p) &= \mathcal{Q}_n^1(\mathcal{F}_n) + \mathcal{Q}_{n,c}(\mathcal{F}_n,\mathcal{F}_p) + \mathcal{Q}_{n,gr}(\mathcal{F}_n,\mathcal{F}_p)\ , \\
\mathcal{Q}_p(\mathcal{F}_n,\mathcal{F}_p) &= \mathcal{Q}_p^1(\mathcal{F}_p) + \mathcal{Q}_{p,c}(\mathcal{F}_n,\mathcal{F}_p) + \mathcal{Q}_{p,gr}(\mathcal{F}_n,\mathcal{F}_p)\ ,
\end{aligned}
\tag{37}
$$

are obtained by evaluating their counterparts on the kinetic level at $(\mathcal{F}_n,\mathcal{F}_p)$ and by integrating over $S_{n,p}(\varepsilon_{n,p})$.

Now we assume that generation-recombination effects dominate in (35), i.e., the scattering rates for carrier-carrier interaction and for the inelastic phonon scattering are much smaller than that for generation-recombination. Therefore, we take a second small parameter β^2 out of the former scattering rates and introduce the further time-position rescaling $t \to t/\beta^2$, $x \to x/\beta$:

$$
\begin{aligned}
N_n\frac{\partial \mathcal{F}_n}{\partial t} + div\,\mathcal{J}_n + \nabla_x V\cdot\frac{\partial \mathcal{J}_n}{\partial\varepsilon} &= \mathcal{Q}_n^1 + \mathcal{Q}_{n,c} + \tfrac{1}{\beta^2}\mathcal{Q}_{n,gr}\ , \\
N_p\frac{\partial \mathcal{F}_p}{\partial t} + div\,\mathcal{J}_p - \nabla_x V\cdot\frac{\partial \mathcal{J}_p}{\partial\varepsilon} &= \mathcal{Q}_p^1 + \mathcal{Q}_{p,c} + \tfrac{1}{\beta^2}\mathcal{Q}_{p,gr}\ .
\end{aligned}
\tag{38}
$$

The ET model is derived by the limit $\beta \to 0$ in (38). Applying the coarea formula, we can easily extend to $\mathcal{Q}_{gr} = (\mathcal{Q}_{n,gr},\mathcal{Q}_{p,gr})$ the properties stated in Sec. 4 for Q_{gr}. Denoting the limit as $\beta \to 0$ of $(\mathcal{F}_n,\mathcal{F}_p)$ by $(\mathcal{F}_{0n},\mathcal{F}_{0p})$ and the limit of the fluxes $(\mathcal{J}_n,\mathcal{J}_p)$ by $(\mathcal{J}_{0n},\mathcal{J}_{0p})$, identifying the terms of leading order in (38) and applying lemma 4.5, we obtain the form (23) for $(\mathcal{F}_{0n},\mathcal{F}_{0p})$. The limiting fluxes then become

$$
\begin{aligned}
\mathcal{J}_{0n} &= -\mathcal{D}_n\mathcal{F}_{0n}(1-\eta\mathcal{F}_{0n})\left[\nabla_x\left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T} + (\varepsilon+\Delta/2)\,\nabla_x\left(-\frac{1}{T}\right)\right], \\
\mathcal{J}_{0p} &= -\mathcal{D}_p\mathcal{F}_{0p}(1-\eta\mathcal{F}_{0p})\left[-\nabla_x\left(\frac{\mu}{T}\right) + \frac{\nabla_x V}{T} + (\varepsilon+\Delta/2)\,\nabla_x\left(-\frac{1}{T}\right)\right].
\end{aligned}
$$

The charge density $\chi = \chi(\mu,T)$ and the total energy $\mathcal{E} = \mathcal{E}(\mu,T)$ are now written as

$$
\begin{pmatrix}\chi\\ \mathcal{E}\end{pmatrix} = \int_{\varepsilon_n(B)}\mathcal{F}_{0n}\begin{pmatrix}1\\ \varepsilon+\Delta/2\end{pmatrix}N_n d\varepsilon + \int_{\varepsilon_p(B)}\mathcal{F}_{0p}\begin{pmatrix}-1\\ \varepsilon+\Delta/2\end{pmatrix}N_p d\varepsilon\ .
$$

Finally, we derive the ET system computing the balance equations for the charge and the total energy densities. Going to the limit $\beta \to 0$, we recover the evolution equations previously obtained in (27) and (28)-(29-a). The difference compared with the ET model of the preceding section lies in the definition of the diffusion matrix D:

$$
\begin{aligned}
D &= \int_{\varepsilon_n(B)}\mathcal{D}_n\mathcal{F}_{0n}(1-\eta\mathcal{F}_{0n})\begin{pmatrix}1 & \varepsilon+\Delta/2\\ \varepsilon+\Delta/2 & (\varepsilon+\Delta/2)^2\end{pmatrix}d\varepsilon \\
&\quad + \int_{\varepsilon_p(B)}\mathcal{D}_p\mathcal{F}_{0p}(1-\eta\mathcal{F}_{0p})\begin{pmatrix}1 & -\varepsilon-\Delta/2\\ -\varepsilon-\Delta/2 & (\varepsilon+\Delta/2)^2\end{pmatrix}d\varepsilon\ .
\end{aligned}
\tag{39}
$$

Besides, the energy source term is now computed by

$$W_{ph} = \int_{\varepsilon_n(B)} \mathcal{Q}_n^1(\mathcal{F}_{0n})\varepsilon \ d\varepsilon + \int_{\varepsilon_p(B)} \mathcal{Q}_p^1(\mathcal{F}_{0p})\varepsilon \ d\varepsilon \ .$$

Using (36-c) and the corresponding estimate for $\mathcal{D}_p$, we have

$$\begin{aligned} D \ \geq \ & C_n \int_B \frac{1}{N_n} \mathcal{F}_{0n}(1-\eta\mathcal{F}_{0n}) r_n \otimes r_n \ dk \\ & + C_p \int_B \frac{1}{N_p} \mathcal{F}_{0p}(1-\eta\mathcal{F}_{0p}) r_p \otimes r_p \ dk \ , \end{aligned} \tag{40}$$

with the 6-vectors $r_n = (\nabla_k \varepsilon_n, (\varepsilon_n + \Delta/2)\nabla_k \varepsilon_n)$, $r_p = (\nabla_k \varepsilon_p, -(\varepsilon_p + \Delta/2)\nabla_k \varepsilon_p)$. This shows that Lemma 5.1 (i) remains true for the ET model derived here. The statement of Lemma 5.1 (ii) for the present model is derived from Lemma 5.1 (ii) applying the coarea formula.

A particular case, allowing to compute the diffusion matrix explicitly, is now discussed.

Remark 6.2: We consider a device with a phonon population mainly made of acoustical and non polar optical phonons (such as a Si device at room temperature). We can thus assume that the cross sections ϕ_n^0 and ϕ_p^0 for elastic collisions do not depend on the pseudo wave-vector. Moreover, we consider a parabolic band model and a non-degenerate gas, i.e., the limit $\eta \to 0$. Then, referring to [31], we have:

$$\mathcal{D}_n(x,\varepsilon) = \frac{2\gamma\varepsilon}{3\phi_n^0} Id \quad \text{and} \quad \mathcal{D}_p(x,\varepsilon) = \frac{2\varepsilon}{3\gamma\phi_p^0} Id \ ,$$

where Id is the 3×3 identity matrix. Consequently, the diffusion matrix can also be computed explicitly:

$$D = \frac{\sqrt{T}}{(2\pi)^{3/2}} \begin{pmatrix} \mathcal{C}\ Id & (2T+\Delta/2)\mathcal{S}\ Id \\ (2T+\Delta/2)\mathcal{S}\ Id & (6T^2 + 2T\Delta + \Delta^2/4)\mathcal{C}\ Id \end{pmatrix} ,$$

with

$$\begin{aligned} &\mathcal{C} = D_n\rho_n + D_p\rho_p \ , && \mathcal{S} = D_n\rho_n - D_p\rho_p \ , \\ &\rho_n = n_i(T)\gamma^{-3/2} e^{\mu/T} \ , && D_n = \frac{2\gamma^{5/2}}{3\phi_n^0} \ , \\ &\rho_p = n_i(T)\gamma^{3/2} e^{-\mu/T} \ , && D_p = \frac{2}{3\gamma^{5/2}\phi_p^0} \ , \end{aligned}$$

In the following two remarks, we stay within the frame of the previous remark in order to investigate two limiting problems: a flow strongly dominated by one charge carrier, and a flow satisfying local electro-neutrality.

Remark 6.3: We consider the case $\mu/T >> 1$. The carrier population is thus dominated by conduction electrons: $\rho_n >> \rho_p$ holds for the electron and, respectively, hole densities, leading to $\chi \simeq \rho_n$. Moreover we assume that $\mathcal{C}_n$ is of the order of $\mathcal{C}_p$. The charge transport equation of (27) then reduces to a transport equation that rules the density ρ_n of conduction electrons. With the notation $\mathcal{E} = \mathcal{E}_n + \rho_n\Delta/2$, we obtain:

$$\begin{aligned}
&\frac{\partial \rho_n}{\partial t} + \nabla_x J_{\rho_n} = 0 \ , \\
&\frac{\partial \mathcal{E}_n}{\partial t} + \nabla_x J_{\mathcal{E}_n} - \nabla_x V \cdot J_{\rho_n} = W_{ph} \ .
\end{aligned}$$

The fluxes are given by

$$\begin{pmatrix} J_{\rho_n} \\ J_{\mathcal{E}_n} \end{pmatrix} = -\frac{D_n \mathcal{F}_0 T^2}{\gamma^{3/2}} e^{\mu_n/T} \begin{pmatrix} Id & 2T\,Id \\ 2T\,Id & 6T^2 Id \end{pmatrix} \begin{pmatrix} \nabla_x \left(\frac{\mu_n}{T}\right) - \frac{\nabla_x V}{T} \\ \nabla_x \left(\frac{-1}{T}\right) \end{pmatrix},$$

with the chemical potential $\mu_n = \mu - \Delta/2$. Consequently, in the limit of charge carriers dominated by conduction electrons, the ET system for strong generation-recombination reduces to the usual ET system governing the density ρ_n and the energy density $\mathcal{E}_n$ of conduction electrons, cf. [31] for instance.

Remark 6.4: We investigate an undoped semiconductor with the charge neutrality assumption $\chi = 0$. The Saha equilibrium condition then implies $\rho_n = \rho_p = n_i$. We look for special solutions of the resulting problem where the potential is chosen such that $J_\chi = 0$ holds. The resulting relation,

$$\nabla_x \left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T} = -(2T + \Delta/2)\frac{D_n - D_p}{D_n + D_p} \nabla_x \left(-\frac{1}{T}\right) \ ,$$

allows to rewrite the flux of the energy $\mathcal{E} = (\rho_n + \rho_p)(3T + \Delta)/2$ as a diffusive flux $J_{\mathcal{E}} = -D_{\mathcal{E}} \nabla_x \mathcal{E}$ with

$$D_{\mathcal{E}} = \frac{\sqrt{T}[2T^2(D_n^2 + D_p^2 + 10 D_n D_p) + \Delta(8T + \Delta) D_n D_p]}{(2\pi)^{3/2}(D_n + D_p)(3T^2 + (3T + \Delta)^2/2)} \ .$$

Thus, the energy density solves a reaction diffusion equation with nonlinear diffusion.

In the limit $T \ll \Delta$, corresponding to weak ionization, the diffusivity reduces to

$$D_{\mathcal{E}} = \frac{\sqrt{T}}{(2\pi)^{3/2}} \frac{2 D_n D_p}{D_n + D_p} \ .$$

In the opposite limit $\Delta \ll T$, associated with strong ionization,

$$D_{\mathcal{E}} = \frac{8\sqrt{T}}{5(2\pi)^{3/2}} \frac{D_n^2 + D_p^2 + 10 D_n D_p}{6(D_n + D_p)} \ ,$$

the diffusion coefficient is bigger.

Acknowledgments

This work has been supported by the TMR network on Asymptotic Methods in Kinetic Theory Ref. ERB FMRX CT97 0157.

References

[1] S. Selberherr, "Analysis and simulation of semicondictor devices," Springer-Verlag, Wien (1984).

[2] L. Reggiani, "Hot-electron transport in semiconductors," Springer-Verlag, Berlin (1985).

[3] P. L. Landsberg, "Recombination in semiconductors," Cambridge University Press, Cambridge (1991).

[4] D. C. Herbert, *"Ionization in GaAs multilayers,"* Semiconductors Science and Technology, Vol. 10, p. 405 (1995).

[5] S. Tagaki and A. Torium, *"Observation of anisotropic impact ionization in Si MOSFET,"* Semiconductor Science and Technology, Vol. 7, No. 3B, pp. 601-603 (1992).

[6] M. Tanizawa, M. Ikeda, N. Kotani, K. Tsukamoto and K. Horie, *"A complete substrate current model including band-to-band tunneling current in circuit simulation,"* IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, Vol. 12, N0. 11, pp. 1749-1757 (1993).

[7] C. Fiegna and E. Sangiorgi, *"Modeling oh high-energy electrons in MOS devices at the microscopic level,"* IEEE Transactions on Electron Devices, Vol. 40, No. 3, p. 619 (1993).

[8] H. Shichijo, K. Hess and G. E. Stillman, *"Simulation of high-field transport in GaAs using Monte Carlo method and pseudopotential band structures,"* Applied Physics Letters, Vol. 38, No. 2, p. 89 (1981).

[9] H. Shichijo and K. Hess, *"Band-structure-dependent transport and impact ionization in GaAs,"* Physical Review B, Vol. 23, No. 8, pp. 4197-4207 (1981).

[10] C. A. Lee, R. A. Logan, R. L. Batdorf, J. J. Kleimack and W. Wiegmann, *"Ionization rates of holes and electrons in silicon,"* Physical Review, Vol. 134, p. A 761 (1964).

[11] T. P. Pearsall, F. Capasso, R. E. Nahory, M. A. Pollack and J. R. Chelikowsky, *"The band-structure-dependence of impact ionization by hot carriers in semiconductors: GaAs,"* Solid State Electron., Vol. 21, p. 297 (1978).

[12] R. Raghunathan and B. J. Baliga, "*Temperature dependence of hole impact ionization coefficients in 4H and 6H-SiC,*" Solid-State Electron., Vol. 43 p.199 (1999).

[13] P. A. Wolff, Physcal Review, Vol. 95, p. 1415 (1954).

[14] W. Shockley, "*Problems related to p-n junctions in silicon,*" Solid State Electron., Vol. 2, p. 35 (1961).

[15] G. A. Baraff, "*Distribution functions and ionization rates for hot electrons in semiconductors ,*" Phys. Rev., Vol. 128, p. 2507 (1962).

[16] L. V. Keldysh, "*Kinetic theory of impact ionization in semiconductors,*" Sov. Phys. JETP, Vol. 37, p. 509 (1959).

[17] M. V. Fischetti and S. E. Laux, "*DAMOCLES Theoretical Manual,*" IBM, Yorktown Heights, 1994.

[18] K. Kim, K. Kahen, J. P. Leburton and K. Hess, "*Band structure dependence of impact ionization rate in GaAs,*" Journal of Applied Physics, Vol. 59, p. 2595 (1986).

[19] N. Sano, T. Aoki, M. Tomizawa and A. Yoshii, "*Electron transport and impact ionization in Si,*" Physical Review B, Vol. 41, No. 17, pp. 12122-12128 (1990).

[20] T. Thoma, H. Peifer, W. Engl, W. Quade, R. Brunetti and C. Jacoboni, "*A generalized impact-ionization model for high-energy electron transport in Si with Monte Carlo simulation,*" Journal of Applied Physics, Vol. 69, p. 2300 (1991).

[21] T. Kunikiyo, M. Takenaka, Y. Kamakura, M. Yamaji, H. Mizuno, M. Morifuji, K. Taniguchi and C. Hamaguchi, "*A Monte Carlo simulation of anisotropic electron transport in Silicon including full band structure and anisotropic impact-ionization model,*" Journal of Applied Physics, Vol. 75, No. 1, pp. 297-312 (1994).

[22] W. V. van Roosbroeck, "*Theory of flow of electrons and holes in Germanium and other semiconductors,*" Bell Syst. Techn. J, Vol. 29, p. 560 (1950).

[23] F. Poupaud, "*Diffusion approximation of the linear semiconductor equation: analysis of boundary layers,*" Asymptotic Analysis, Vol. 4, p. 293 (1991).

[24] F. Golse and F. Poupaud, "*Limite fluide des équations de Boltzmann des semiconducteurs pour une statistique de Fermi-Dirac,*" Asymptotic Analysis, Vol. 6, p. 135 (1992).

[25] P. A. Markowich, "The stationary semiconductor device equation," Springer, Wien (1986).

[26] P. Degond, *"Mathematical modeling of microelectronics semiconductor devices,"* Rapport Interne 99-03, MIP, Universite Paul Sabatier, (1999).

[27] S. P. Wilson and A. B. Walker, *"Mechanism of impact ionization enhancement in GaAs p-i-n diodes under high illumination conditions,"* Semiconductors Science and Technology, Vol. 13, p. 190 (1998).

[28] N. Goldsman, L. Henrickson and J. Frey, *"A physics based analytical numerical solution of the Boltzmann transport equation for use in device simulation,"* Solid-State Electronics, Vol. 34, p. 389 (1991).

[29] A. Gnudi, D. Ventura, G. Baccarani and F. Odeh, *"Two-dimensional MOSFET simulation by means of a multidimensional spherical harmonic expansion of the Boltzmann transport equation,"* Solid-State Electronics, Vol. 36, p. 575 (1993).

[30] P. Dmitruk, A. Saul and L. Reyna, *"High electric field approximation in semiconductor devices,"* Appl. Math. Letters, Vol. 5, p. 99 (1992).

[31] N. Ben Abdallah, P. Degond, *"On a hierarchy of macroscopic models for semiconductors,"* J. Maths. Phys., Vol. 37, p. 3306 (1996).

[32] A. Gnudi, D. Ventura and G. Baccarani *"Modelling impact ionization in a BJT by means of spherical harmonics expansion of the Boltzmann transport equation,"* IEEE Trans. on Computer-Aided Design of Integrated Circuits and Systems, Vol. 12, p. 1706 (1993).

[33] R. Stratton, *"Diffusion of hot and cold electrons in semiconductor barriers,"* Phys. Rev., Vol. 126, p. 2002 (1962).

[34] N. Ben Abdallah, P. Degond and S. Genieys, *"An energy-transport model for semiconductors derived from the Boltzmann equation,"* J. Stat. Phys., Vol. 84, p. 205 (1996).

[35] C. Schmeiser, *"Stability of thermal equilibrium for a semiconductor model including traps,"* Proc. ECMI 7, A. Fasano and M. Primicerio Eds., Teubner, Stuttgart, (1994).

[36] R. Stratton, *"Semiconductor current flow equations (diffusion and degeneracy),"* IEEE Transactions on Electron Devices ED-19, pp-650-656 (1986).

[37] J. Tang and K. Hess, *"Impact ionization of hot electrons in silicon (staedy state),"* Journal of Applied Physics, Vol. 54, pp. 5139-5145, (1983).

[38] P. A. Markowich, C. Ringhofer, C. Schmeiser, "Semiconductor equations," Springer-Verlag, Wien, (1990).

[39] T. Kato, "Perturbation theory for linear operators," Springer-Verlag, (1976).

[40] I. Choquet, P. Degond, C. Schmeiser, "Hydrodynamic models for charge carriers involving impact ionization in semiconductors", in preparation.

[41] G. Albinus, "Convex analysis of the energy model of semiconductor devices," preprint No. 285, Weierstraß-Institut, Berlin (Berlin).

[42] P. Degond, S. Génieys, A. Jüngel, "Symmetrization and entropy inequality for general diffusion equations," preprint (?).

[43] P. Degond, S. Génieys, A. Jüngel, "A steady-state system in nonequilibrium thermodynamics including thermal and electrical effects," preprint (?).

[44] N. A. Krall, A. W. Trivelpiece, "Principles of plasma physics," San Francisco Press, 19??.