Hydrodynamic model for charge carriers involving strong ionization in semiconductors

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Abstract

A set of hydrodynamic equations modeling strong ionization in semiconductors is formally derived from a kinetic framework. To that purpose, a system of Boltzmann transport equations governing the distribution functions of conduction electrons and holes is considered. Apart from impact ionization, the model accounts for phonon, lattice defects, and particle-particle scattering. Also degeneracy effects are included. The band diagram models are approximations close to the extrema of actual band diagrams. Ionization initiated by a charge carrier (and its reverse recombination) is the leading order collisional process. The resulting set of hydrodynamic equations for strong ionization differs from the usual hydrodynamic system for semiconductors, which corresponds to weak ionization. Indeed, it governs the total charge, the crystal momentum and the energy, but the total mass is not a conservation variable. This system is supplemented by an entropy inequality, and proved to be hyperbolic. The particular case of a parabolic band diagram is discussed.

1 Introduction

This study continues the investigation of macroscopic models for semiconductors when impact ionization is a dominant collisional process. The diffusion limit can be found in Ref. [10], and the present paper is devoted to the hydrodynamic limit.

Let us first briefly recall that impact ionization takes place in semiconductors under relatively high electric fields. A charge carrier can then reach a kinetic energy larger than the ionization threshold, and thus generate a conduction electron and a hole while it

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collides with a lattice atom. As this process can occur in transistors and diodes (cf. [10] for further details) and modify the current density, its control is an important challenge. Impact ionization is indeed widely investigated since the last five decades; examples of studies are given in [10].

Hydrodynamic models have been developed to describe semiconductors involving high field phenomena such as heat generation in the bulk device, hot electron effects or impact ionization. These models are derived from the Boltzmann transport equation for conduction electrons. A system of Boltzmann transport equations involving also holes has been likewise investigated assuming a weak coupling between conduction electrons and holes. The set of hydrodynamic conservation equations is obtained retaining at least the first three moments of the Boltzmann transport equations with respect to the momentum variable. The resulting system of conservation laws governs the carrier concentrations, the crystal momentum, the carrier energy or temperature, and eventually higher moments.

A first difficulty arises due to the source terms, since they can hardly be expressed as functions of the conservation variables. To avoid this problem, source terms are often replaced be relaxation time approximations, with relaxation times fitted to experimental data, as in [5].

Moreover, as the number of equations is lower than the number of moments they contain, closure equations are also required. For overcoming this major difficulty, various approaches intended to derive the constitutive relations can be found in the literature. One of the first approaches has been proposed by Bløtekjaer [8]. It assumes that the momentum distribution function is a shifted Maxwellian, see also [26], [13]. The parameters of this Maxwellian are set to coincide with the retained moments. Later on Baccarani and Wordeman [5] have proposed phenomenological closure relations, such as a Fourier law to model the heat flux. Other models are extracted from Monte Carlo simulations [17] or developed to handle nonparabolic effects as in [26] and [27] for example. As underlined in [1], most of these models suffer from theoretical drawbacks concerning both constitutive relations and source terms. The hydrodynamical models proposed more recently by Anile and co-workers do not meet with these drawbacks since they are consistent with the theory of non-equilibrium thermodynamics. The derivation of closure relations, cf. [2]–[4], is based on the maximum entropy principle within the frame of extended thermodynamics.

All these hydrodynamical models can handle the ionization process and its reverse recombination through source terms. But they are seldom applied to the numerical simulation of devices involving this scattering process, cf. [14].

Independently of the treatment of the closure problem, the hydrodynamic models mentioned above share a common property: they are derived from Boltzmann transport equations assuming weak electron-hole coupling. The scattering operators allowing this coupling, such as carrier-carrier interaction or generation-recombination, are assumed to have a lower order of magnitude than the scattering operators governing the system.

Impact ionization takes place under high energy scales (i.e. large applied biases) since the kinetic energy of charge carriers has to reach the ionization threshold. The order of magnitude is above around 1.5 eV cm^{-1} in Silicon or Gallium-Arsenide devices [16], [21]. We shall, thus, consider a typical kinetic energy for charge carriers ε_0 varying from 1 to 5 eV, and a crystal temperature of 300 K. From experiments, the order of magnitude of the phonon collision frequency then is approximately 10^{14} s^{-1} in Si (cf. Refs. [19], [15]) and it lies within the range 10^{12} to 10^{14} s^{-1} in GaAs (cf. Ref. [19]). The order of magnitude of the lattice defect frequency (cf. Ref. [19]) is always much smaller. Referring to [23], [24], we know that the carrier-carrier collision frequency is small for low carrier density and can reach the phonon frequency for very high carrier density. In contrast, the ionization collision frequency does not depend on the carrier density. It is nearly equal to zero as long as the typical kinetic energy of charge carriers is smaller than the ionization energy. Above that value, it increases strongly and reaches values larger than the phonon collision frequency: 10^{16} s^{-1} in Silicon when $\varepsilon_0 \simeq 5$ eV (cf. Refs. [25], [15] and references within). A similar behavior is observed in GalliumArsenide (cf. Ref. [22]).

These results indicate that, when investigating energy scales reaching the ionization threshold, the ionization-recombination operator becomes a leading order term. The purpose of the present paper is thus to derive a system of conservation equations from a system of Boltzmann transport equation with a dominating ionization-recombination operator.

This paper is organized as follows: The scaled system of Boltzmann transport equations for conduction electrons and holes is presented in section 2. It contains models for phonon scattering, lattice defect scattering, particle-particle scattering, as well as impact ionization. It is assumed that, apart from energy, the ionization process also preserves momentum. Since, for a periodic band diagram, the possibility of umklapp processes would destroy macroscopic momentum conservation, we restrict our discussion to approximations of the band diagrams close to the bottom of the conduction band and close to the top of the valence band.

The ionization collision operator is then studied in section 3. The properties it has to satisfy, in order to perform an hydrodynamic approximation, are established. The remaining sections are concerned with the hydrodynamic limit of the system of Boltzmann transport equations. We first consider the case of arbitrary band diagrams in Section 4. The resulting set of conservation equations governs the total charge density, the crystal momentum and the energy of charge carriers. This system is supplemented by an entropy evolution equation and proved to be hyperbolic. The last section corresponds to the particular case of a parabolic band diagram.

2 Scaled system of Boltzmann equations

The detailled presentation of the system of Boltzmann transport equations taking into account impact ionization can be found in [10]. We shall simply give the scaled kinetic system we shall start from, in order to derive an hydrodynamic model for strong ionization in semiconductors.

We shall study the behavior of a coupled system of Boltzmann transport equations governing the distribution functions for conduction electrons $f_n = f_n(x,k,t)$, and holes $f_p = f_p(x,k,t)$. Boundary conditions are not investigated here and the position variable x lies in $\mathbb{R}^3$ as well as the pseudo wave-vector k. Time is denoted by $t \in \mathbb{R}$.

The equations for the distribution functions are scaled in accordance with hot-electron transport in semiconductors. This corresponds to applied biases allowing a typical kinetic energy of charge carriers larger than the ionization threshold. Then, ionization-recombination can be the leading order collision process, as shown in Refs. [25],[15],[22] for instance. The applied biases under consideration are however such that the collision operator dominates the acceleration by the electric field. The collision mechanisms met in this framework are thus: lattice-defects and phonon scatterings, carrier-carrier interactions, ionization and its reverse recombination process.

In dimensionless form, the resulting coupled system of Boltzmann transport equations reads,

$$\begin{aligned}
&\frac{\partial f_n}{\partial t} + \nabla_k \varepsilon_n \cdot \nabla_x f_n + \nabla_x V \cdot \nabla_k f_n \\
&\qquad = \tfrac{1}{\alpha} Q_{n,gr}(f_n, f_p) + Q_{n,ph}(f_n) + Q_{n,ld}(f_n) + Q_{n,c}(f_n, f_p)\ , \\
&\frac{\partial f_p}{\partial t} + \nabla_k \varepsilon_p \cdot \nabla_x f_p - \nabla_x V \cdot \nabla_k f_p \\
&\qquad = \tfrac{1}{\alpha} Q_{p,gr}(f_n, f_p) + Q_{p,ph}(f_p) + Q_{p,ld}(f_p) + Q_{p,c}(f_n, f_p)\ ,
\end{aligned} \tag{1}$$

where α is a small parameter. It reflects the importance, relative to impact ionization, of the other scattering processes. It can also be interpreted as a Knudsen number defined by the ratio of the mean free path of ionizing charge carriers to the macroscopic length scale. The subscripts n and p denote quantities associated with the negative and positive carriers, respectively. The kinetic energies $\varepsilon_n(k), \varepsilon_p(k) \geq 0$, $k \in \mathbb{R}^3$ have to be understood as approximations of the band diagrams close to their extrema. The electric potential $V(x,t)$ will be considered as given.

The dominating collision operator $(Q_{n,gr}, Q_{p,gr})$ models ionization and its reverse recombination process. The generation and recombination of charge carriers requires an additional particle to satisfy the energy conservation. In the present study, this particle is a charge carrier. The carrier transition mechanisms can be schematized by the following reactions:

$$n \quad \longleftrightarrow \quad n\ +\ n\ +\ p\ , \qquad\qquad p \quad \longleftrightarrow \quad p\ +\ p\ +\ n\ , \tag{2}$$

where n represents a conduction electron and p a hole. Let us recall that for high carrier concentrations, the reactions (2) are usually called Auger generation-recombination. For a large current density, the (reverse) recombination reactions get negligible compared with the (direct) generation mechanisms. When reduced to the generation reactions, these processes are generally called impact ionization.

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

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

where the superscripts n and p indicate the additional carrier allowing to satisfy the energetic requirement of the reaction. The operator $Q^n_{n,gr}$, describing the effect of electron triggered ionization events on the electron distribution, can be written as

$$\begin{aligned} Q^n_{n,gr}(f_n, f_p) = 2 \int_{\mathbb{R}^3} \phi_{n,gr} \ \delta_{\varepsilon,n} \ \delta_{k,n} \Big[& \mathcal{F}_0^2 \ f'_n \ (1-\eta f_n)(1-\eta f^*_n)(1-\eta f^+_p) \\ & - f_n \ f^*_n \ f^+_p \ (1-\eta f'_n) \Big] \, dk' \, dk^* \, dk^+ \\ + \int_{\mathbb{R}^3} \phi'_{n,gr} \ \ \delta'_{\varepsilon,n} \ \delta'_{k,n} \Big[& f'_n \ f^*_n \ f^+_p \ (1-\eta f_n) \\ & - \mathcal{F}_0^2 \ f_n \ (1-\eta f'_n)(1-\eta f^*_n)(1-\eta f^+_p) \Big] \, dk' \, dk^* \, dk^+ \ , \end{aligned}$$

where the superscripts $'$, *, and $^+$ denote evaluation at k', k^*, and k^+, respectively. $\phi_{n,gr}$ and $\phi'_{n,gr}$ stand for $\phi_{n,gr}(k, k^*, k^+; k')$, and $\phi_{n,gr}(k', k^*, k^+; k)$, respectively. As a consequence of the principle of detailed balance, the forward and reverse reaction rates are the same up to the constant factor $\mathcal{F}_0^2$. Moreover, the indistinguishability of electrons implies that

$$\phi_{n,gr}(k, k^*, k^+; k') = \phi_{n,gr}(k^*, k, k^+; k') \ . \tag{3}$$

The energy balance in recombination-generation events is reflected by the delta-distributions $\delta_{\varepsilon,n} = \delta(\varepsilon_n + \varepsilon^*_n + \varepsilon^+_p + \Delta - \varepsilon'_n)$ and $\delta'_{\varepsilon,n} = \delta(\varepsilon'_n + \varepsilon^*_n + \varepsilon^+_p + \Delta - \varepsilon_n)$. The ionization energy Δ (i.e., the width of the band gap) is supposed to be constant. The parameter η measures the level of degeneracy of the electron and hole gases. The classical non-degenerate statistics is recovered when η tends to zero.

In the literature, Monte Carlo simulations of impact ionization are reported, neglecting [11] and enforcing [15] momentum conservation. It is the main purpose of this work compared to the previous study [10], to describe the macroscopic effects of including the momentum conservation assumption. For periodic band diagrams microscopic momentum conservation does not imply a macroscopic conservation law because of the possibility of umklapp processes. This is the reason for assuming nonperiodic dispersion relations, which can be interpreted as approximations of the band diagrams close to their extrema. Momentum conservation is expressed by the supports of the delta distributions $\delta_{k,n} = \delta_k(k' - k - k^* - k^+)$ and $\delta'_{k,n} = \delta_k(k - k' - k^* - k^+)$.

The operator $Q^p_{n,gr}$ contains the electron gain and loss terms due to generation initiated by a hole and the corresponding recombination reaction,

$$Q^p_{n,gr}(f_n,f_p) = \int_{\mathbb{R}^3} \phi_{p,gr}\ \delta_{\varepsilon,p}\ \delta_{k,p}\ \Big[\mathcal{F}_0^2\ f'_p\ (1-\eta f_p^+)(1-\eta f_p^*)(1-\eta f_n) \\ -f_p^+\ f_p^*\ f_n\ (1-\eta f'_p)\Big]\ dk'\ dk^*\ dk^+ \ .$$

The properties and definitions of the scattering rate and of the delta distributions are analogous to those in $Q^n_{n,gr}$.

The remaining operators have a lower order of magnitude. $Q_{n,ld}$ models collisions with lattice defects,

$$Q_{n,ld}(f_n) = \int_{\mathbb{R}^3} \phi_{n,ld}\ \delta(\varepsilon'_n - \varepsilon_n)\,(f'_n - f_n)\,dk' \ .$$

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.

The phonon collision operator reads,

$$Q_{n,ph}(f_n) = \int_{\mathbb{R}^3} \phi_{n,ph}\Big\{\Big[(N_{ph}+1)\,\delta(\varepsilon_n - \varepsilon'_n + \varepsilon_{ph}) + N_{ph}\ \delta(\varepsilon_n - \varepsilon'_n - \varepsilon_{ph})\Big] f'_n\ (1-\eta f_n) \\ -\Big[(N_{ph}+1)\,\delta(\varepsilon'_n - \varepsilon_n + \varepsilon_{ph}) + N_{ph}\ \delta(\varepsilon'_n - \varepsilon_n - \varepsilon_{ph})\Big] f_n\ (1-\eta f'_n)\Big\}\ dk' \ ,$$

where ε_{ph} is the phonon energy. The collision cross section satisfies the symmetry property $\phi_{n,ph}(k;k') = \phi_{n,ph}(k';k)$. The phonon occupation number N_{ph} is given by the Bose-Einstein statistics

$$N_{ph} = \frac{1}{\exp\left(\varepsilon_{ph}/T_L\right) - 1} \ ,$$

with the scaled lattice temperature T_L.

The carrier-carrier binary collision integral $Q_{n,c}$ includes a contribution due to electron-electron interactions as well as a coupling term modeling collisions between electrons and holes. Details can be found in [10], but are not needed in the present study.

The collision operators for holes can be immediately obtained from the previous expressions exchanging n and p.

The aim of this paper is to investigate the hydrodynamic limit from the system of Boltzmann transport equations (1). The properties of the collisional operators weighted by the small parameter α are already available in the literature. The lattice defects and elastic phonon collision operators are studied in Ref. [18] for instance. Carrier-carrier collision operators have been investigated in Refs. [6], [7]. Due to the weighting factor, these operators will only lead to source terms in the hydrodynamic limit.

The dominating generation-recombination operator is studied in the following section.

3 Properties of the collision operators

The properties derived below apply to the full system made of electrons and holes, but not to electrons or holes when considered separately. Let us first recall a result obtained in [10], which will be useful in the following.

Lemma 3.1: (H-Theorem)
Let $h(f) = \log\left[f\mathcal{F}_0^{-1}(1-\eta f)^{-1}\right]$. Let $\phi_{n,gr}$, $\phi_{p,gr}$ be nonnegative and satisfy the symmetry relation (3). Then

$$
\begin{aligned}
&\int_{\mathbb{R}^3} Q_{n,gr}(f_n,f_p)h(f_n)dk + \int_{\mathbb{R}^3} Q_{p,gr}(f_n,f_p)h(f_p)dk = \\
&\quad \int_{\mathbb{R}^{12}} \phi_{n,gr}\delta_{\varepsilon,n}\Big[\mathcal{F}_0^2 f_n'(1-\eta f_n)(1-\eta f_n^*)(1-\eta f_p^+) - f_n f_n^* f_p^+(1-\eta f_n')\Big] \\
&\qquad \times\Big[\log\Big(f_n f_n^* f_p^+(1-\eta f_n')\Big) - \log\Big(\mathcal{F}_0^2 f_n'(1-\eta f_n)(1-\eta f_n^*)(1-\eta f_p)\Big)\Big]dk^4 \\
&\quad + \int_{\mathbb{R}^{12}} \phi_{p,gr}\delta_{\varepsilon,p}\Big[\mathcal{F}_0^2 f_p'(1-\eta f_p)(1-\eta f_p^*)(1-\eta f_n^+) - f_p f_p^* f_n^+(1-\eta f_p')\Big] \\
&\qquad \times\Big[\log\Big(f_p f_p^* f_n^+(1-\eta f_p')\Big) - \log\Big(\mathcal{F}_0^2 f_p'(1-\eta f_p)(1-\eta f_p^*)(1-\eta f_n^+)\Big)\Big]dk^4 \le 0\ ,
\end{aligned}
$$

with $dk^4 = dk\ dk'\ dk^*\ dk^+$.

For the determination of the collisional invariants associated with the generation-recombination operator we need a preliminary result.

Lemma 3.2: Let $f : [0,\infty) \to \mathbb{R}$ be continuous at 0 and satisfy $f(x) = f(x+\lambda/x)$ for all $x > 0$ and for a positive constant λ. Then f is a constant function.

Proof: Choose an arbitrary $x_0 > 0$ and define the sequence $\{x_n\}$ recursively by $x_{n+1} = x_n + \lambda/x_n$, $n \ge 0$. Then $x_n \to \infty$ and $f(x_0) = f(x_n)$. However, for $x_n^2 > 4\lambda$, $x_n = y_n + \lambda/y_n$ holds for $y_n = 2\lambda/\left(x_n + \sqrt{x_n^2 - 4\lambda}\right)$, and therefore $f(x_0) = f(y_n) \to f(0)$ as $n \to \infty$. ∎

Theorem 3.1: Assume that $\phi_{n,gr}$ and $\phi_{p,gr}$ are positive and bounded from below. Let the energy bands be parabolic: $\varepsilon_n(k) = |k|^2/(2m_n)$, $\varepsilon_p(k) = |k|^2/(2m_p)$. Then, for continuous ψ_n, ψ_p,

$$
\int_{\mathbb{R}^3} Q_{n,gr}(f_n,f_p)\psi_n dk + \int_{\mathbb{R}^3} Q_{p,gr}(f_n,f_p)\psi_p dk = 0 \quad \forall f_n, f_p \tag{4}
$$

$$
\Longleftrightarrow \quad \exists\ a,c \in \mathbb{R},\ b \in \mathbb{R}^3 : \ \left\{ \begin{aligned} \psi_n(k) &= \ \ a + b\cdot k + c(\varepsilon_n(k) + \Delta/2)\ , \\ \psi_p(k) &= -a + b\cdot k + c(\varepsilon_p(k) + \Delta/2)\ . \end{aligned} \right.
$$

Proof: The $\Leftarrow$-part holds by a simple computation. Assuming (4) and setting $f_n = h^{-1}(\psi_n)$, $f_p = h^{-1}(\psi_p)$, Lemma 3.1 implies that

$$
\psi_n + \psi_n^* + \psi_p^+ = \psi_n'
$$

holds, whenever $k + k^* + k^+ = k'$ and $\varepsilon_n + \varepsilon_n^* + \varepsilon_p^+ + \Delta = \varepsilon_n'$. In terms of the function

$$\phi(\kappa) := \psi_n(\kappa - k^+) + \psi_p(k^+) \,,$$

(where for the moment k^+ is considered as a parameter,) the above becomes

$$\phi(\kappa) + \phi(\kappa^*) = \phi(\kappa + \kappa^*) \,, \tag{5}$$

for all $\kappa, \kappa^* \in \mathbb{R}^3$ satisfying

$$\kappa \cdot \kappa^* = \lambda := m_n \Delta + \left(\frac{m_n}{m_p} + 1 \right) \frac{|k^+|^2}{2} \,. \tag{6}$$

Now for every $\kappa \neq 0$ we introduce the notation $\kappa = z\omega$ with $\omega \in S^2$ and $z > 0$. The vectors $r, s \in S^2$ are chosen such that $\{\omega, r, s\}$ is an orthonormal basis of $\mathbb{R}^3$. Then every κ^* satisfying (6) can be written in the form $\kappa^* = (\lambda/z)\omega + \alpha r + \beta s$ and (5) becomes

$$\phi(z\omega) + \phi\left(\frac{\lambda}{z}\omega + \alpha r + \beta s \right) = \phi\left(\left(z + \frac{\lambda}{z} \right) \omega + \alpha r + \beta s \right) \,, \tag{7}$$

now holding for every $z > 0$; $\alpha, \beta \in \mathbb{R}$; and $\omega \in S^2$ (determining r and s). In the following, the difference operator $D_{t,h} f := f(t = t + h) - f$ will be used (with the subscript t omitted for functions f of one variable). Taking differences with respect to α and β in (7) shows that $f(x) = D_{\alpha,h}\phi(x\omega + \alpha r + \beta s)$ and $f(x) = D_{\beta,h}\phi(x\omega + \alpha r + \beta s)$ satisfy the assumptions of the previous lemma and are therefore both independent of x. With $\omega = e_1$, this implies $\phi(\kappa) = X(\kappa_1) + W(\kappa_2, \kappa_3)$, which, by setting $\omega = e_2$, can be strengthened to $\phi(k) = X(\kappa_1) + Y(\kappa_2) + Z(\kappa_3)$. However, with $\omega = \frac{e_1 - e_2}{\sqrt{2}}$, $\omega = \frac{e_1 + e_2}{\sqrt{2}}$, also $\phi(\kappa) = \overline{X}(\kappa_1 - \kappa_2) + \overline{Y}(\kappa_1 + \kappa_2) + Z(\kappa_3)$ holds. Equating both representations of ϕ and taking differences with respect to κ_1 and κ_2 gives

$$D_h^2 \overline{X}(\kappa_1 - \kappa_2) = D_h^2 \overline{Y}(\kappa_1 + \kappa_2 + h) \,,$$

implying that $\overline{X}$ and $\overline{Y}$ are second order polynomials with the same leading order coefficient. By rotation this argument can be easily extended to show that ϕ is of the form

$$\phi(\kappa) = c \frac{|\kappa|^2}{2m_n} + \tilde{b} \cdot \kappa + \tilde{a} \,.$$

A straightforward computation shows that a ϕ of this form satisfies (7) iff $\tilde{a} = \lambda c / m_n$ holds.

Since so far k^+ has been a parameter, c and $\tilde{b}$ can depend on k^+. Going back to the definition of ϕ, we obtain

$$c \frac{|k|^2}{2m_n} + \left(\tilde{b} + \frac{c}{m_n} k^+ \right) \cdot k + \frac{c}{m_n} \left(\lambda + \frac{|k^+|^2}{2} \right) + \tilde{b} \cdot k^+ = \psi_n(k) + \psi_p(k^+) \,.$$

This implies (e.g., by taking differences with respect to k) that c and $b = \tilde{b} + \frac{c}{m_n} k^+$ are independent of k^+. The above equation can then be written as

$$\psi_n - c(\varepsilon_n + \Delta/2) - b \cdot k = -\psi_p^+ + c(\varepsilon_p^+ + \Delta/2) + b \cdot k^+ .$$

Since the left hand side only depends on k and the right hand side only on k^+, both have to be equal to a constant a, which is equivalent to the statement of the theorem. ■

Note that the proof only used information from the electron triggered events. Thus, a stronger result considering just one of the two types of ionization effects holds.

Corollary 3.3: With the assumptions of Theorem 3.1,

$$Q_{n,gr}(f_n, f_p) = Q_{p,gr}(f_n, f_p) = 0$$

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

$$\begin{aligned} f_n(k) &= \frac{1}{\eta + \mathcal{F}_0^{-1} \exp\left[\left(\varepsilon_n(k) + \Delta/2 - k \cdot u - \mu\right)/T\right]} , \\ f_p(k) &= \frac{1}{\eta + \mathcal{F}_0^{-1} \exp\left[\left(\varepsilon_p(k) + \Delta/2 - k \cdot u + \mu\right)/T\right]} . \end{aligned}$$

Proof: The proof follows directly from Lemma 3.1 and Theorem 3.1. ■

We only have a proof for the case of parabolic bands. In the following, however, the results of Theorem 3.1 and Corollary 3.3 will also be assumed valid for general band diagrams.

The collision invariants $(1, -1)^{tr}$, $(k, k)^{tr}$, and $(\varepsilon_n(k) + \Delta/2, \varepsilon_p(k) + \Delta/2)^{tr}$ correspond to conservation of charge, momentum, and energy, respectively, by the generation-recombination mechanisms. The behaviour of the other scattering mechanisms with respect to these quantities is as follows. Electron and hole densities are conserved individually by lattice defect, phonon, and carrier-carrier scattering. Thus, $(1, -1)^{tr}$ is a collision invariant for all considered processes. The total momentum is only conserved by carrier-carrier scattering. Finally, phonon scattering is the only inelastic process. So $(\varepsilon_n(k) + \Delta/2, \varepsilon_p(k) + \Delta/2)^{tr}$ is a collision invariant for lattice defect and carrier-carrier scattering. H-theorems for the different scattering operators can be found in [6] and [7]. As a consequence we have that

$$\int_{\mathrm{IR}^3} \left[Q_{n,z} \left(h(f_n) + \frac{\varepsilon_n}{T_L} \right) + Q_{p,z} \left(h(f_p) + \frac{\varepsilon_p}{T_L} \right) \right] dk \leq 0 \tag{8}$$

holds for $z = ld, ph, c$.

4 Hydrodynamic model for strong ionization

Motivated by Theorem 3.1, we define the macroscopic quantities conserved by the generation-recombination mechanisms, the total charge density χ, the crystal momentum density $\mathcal{K}$ and the total energy density $\mathcal{E}$:

$$\begin{pmatrix} \chi \\ \mathcal{K} \\ \mathcal{E} \end{pmatrix} = \int_{\mathbb{R}^3} f_n \begin{pmatrix} 1 \\ k \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_{\mathbb{R}^3} f_p \begin{pmatrix} -1 \\ k \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk \ . \tag{9}$$

The balance equations for these quantities are computed by taking the scalar product of (1) with $(1,-1)^{tr}$, $(k,k)^{tr}$, and $(\varepsilon_n+\Delta/2, \varepsilon_p+\Delta/2)^{tr}$, and by integration with respect to the wave vector:

$$\begin{aligned} &\frac{\partial \chi}{\partial t} + \nabla_x \cdot J_\chi = 0 \ , \\ &\frac{\partial \mathcal{K}}{\partial t} + \nabla_x \cdot J_\mathcal{K} = \chi \nabla_x V + R_{ph} + R_{ld} \ , \\ &\frac{\partial \mathcal{E}}{\partial t} + \nabla_x \cdot J_\mathcal{E} = J_\chi \cdot \nabla_x V + W_{ph} \ . \end{aligned} \tag{10}$$

The fluxes are given by

$$\begin{pmatrix} J_\chi \\ J_\mathcal{K} \\ J_\mathcal{E} \end{pmatrix} = \int_{\mathbb{R}^3} f_n \nabla_k \varepsilon_n \begin{pmatrix} 1 \\ \otimes k \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_{\mathbb{R}^3} f_p \nabla_k \varepsilon_p \begin{pmatrix} -1 \\ \otimes k \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk \ . \tag{11}$$

Since particle-particle scattering conserves charge, momentum, and energy, it does not contribute to (10). Phonon scattering, on the other hand, only preserves charge and contributes to the momentum and energy balance by the source terms

$$\begin{pmatrix} R_{ph} \\ W_{ph} \end{pmatrix} = \int_{\mathbb{R}^3} Q_{n,ph}(f_n) \begin{pmatrix} k \\ \varepsilon_n + \Delta/2 \end{pmatrix} dk + \int_{\mathbb{R}^3} Q_{p,ph}(f_p) \begin{pmatrix} k \\ \varepsilon_p + \Delta/2 \end{pmatrix} dk \ . \tag{12}$$

Finally, the interaction with lattice defects is elastic and, therefore, only leads to a source term in the momentum equation:

$$R_{ld} = \int_{\mathbb{R}^3} (Q_{n,ld}(f_n) + Q_{p,ld}(f_p)) k \ dk \ . \tag{13}$$

The definition of a macroscopic entropy density is motivated by Lemma 3.1 and by (8):

$$S[f_n, f_p](x,t) = \int_{\mathbb{R}^3} \tilde{H}(f_n(x,k,t), f_p(x,k,t), x, k, t)\, dk \, ,$$

with the distribution

$$\tilde{H}(f_n, f_p, x, k, t) = H(f_n) + H(f_p) + \frac{\varepsilon_n(k) + \Delta/2 - V(x,t)}{T_L} f_n + \frac{\varepsilon_p(k) + \Delta/2 + V(x,t)}{T_L} f_p \, ,$$

where

$$H(f) = f \ln \frac{f}{\mathcal{F}_0} + \frac{1-\eta f}{\eta} \ln(1-\eta f)$$

is a primitive of $h(f)$. With Lemma 3.1, Theorem 3.1, and (8), a straightforward computation leads to the entropy inequality

$$\frac{\partial S}{\partial t} + \frac{\chi}{T_L}\frac{\partial V}{\partial t} + \nabla_x \cdot J_S \le 0 \tag{14}$$

with the entropy flux

$$J_S = \int_{\mathrm{IR}^3} (H(f_n)\nabla_k \varepsilon_n + H(f_p)\nabla_k \varepsilon_p)dk + \frac{J_{\mathcal{E}} - VJ_\chi}{T_L}.$$

The hydrodynamic model for strong ionization is now derived by the limit $\alpha \to 0$ in (1) and in (10)–(13). By Corollary 3.3, f_n and f_p tend to

$$f_{0n} = \left(\eta + \mathcal{F}_0^{-1} \exp\left[\frac{\varepsilon_n + \Delta/2 - k\cdot u - \mu}{T}\right]\right)^{-1},$$
$$f_{0p} = \left(\eta + \mathcal{F}_0^{-1} \exp\left[\frac{\varepsilon_p + \Delta/2 - k\cdot u + \mu}{T}\right]\right)^{-1},$$

with arbitrary position and time dependent functions μ, T, and u. Note that we assume the validity of Theorem 3.1 (and, thus, Corollary 3.3) also for general bandstructure. If (f_n, f_p) is replaced by (f_{0n}, f_{0p}), in (9), (11)–(13), (10) becomes a closed system for the macroscopic quantities μ, T, and u.

A connection between the densities $(\chi, \mathcal{K}, \mathcal{E})$ of the conserved quantities and (μ, u, T) is provided by the observation that the equilibrium distributions solve the minimization problem for the entropy $S[f_n, f_p]$ with the side condition (9) for given $(\chi, \mathcal{K}, \mathcal{E})$. The vector $(\mu/T - V/T_L, u/T, 1/T_L - 1/T)$ can be interpreted as Lagrange multiplier. By the strict convexity of the entropy (following from the strict convexity of the function H) the minimization problem has a unique solution. This shows the invertibility of the map $(\mu, u, T) \mapsto (\chi, \mathcal{K}, \mathcal{E})$, defined by substituting (f_{0n}, f_{0p}) in (9). Thus, the densities $(\chi, \mathcal{K}, \mathcal{E})$ can be used as the unknowns in (10). In particular, the limiting entropy density can be considered as a function of $(\chi, \mathcal{K}, \mathcal{E})$. Its convexity now follows from a standard argument which we shall outline in the following: Let the vector of densities be denoted by $w = (\chi, \mathcal{K}, \mathcal{E})$ and let $w_1 \neq w_2$ be 2 such vectors, such that $w = \alpha w_1 + (1-\alpha)w_2$ for $0 < \alpha < 1$. Let (g_{1n}, g_{1p}) and (g_{2n}, g_{2p}) denote the minimizing equilibrium distributions corresponding to w_1 and w_2, respectively. Then the pair $(\alpha g_{1n} + (1-\alpha)g_{2n}, \alpha g_{1p} + (1-\alpha)g_{2p})$ realizes w and, therefore $S(w) \le S[\alpha g_{1n} + (1-\alpha)g_{2n}, \alpha g_{1p} + (1-\alpha)g_{2p}]$ holds. By the convexity of S depending on (f_n, f_p) on the other hand,

$$\begin{aligned} &S[\alpha g_{1n} + (1-\alpha)g_{2n}, \alpha g_{1p} + (1-\alpha)g_{2p}] \\ &< \alpha S[g_{1n}, g_{1p}] + (1-\alpha)S[g_{2n}, g_{2p}] = \alpha S(w_1) + (1-\alpha)S(w_2) \end{aligned}$$

holds, proving strict convexity of S as a function of $(\chi, \mathcal{K}, \mathcal{E})$.

For the derivation of the limiting balance equation for the entropy, only the source terms in the limit of (14) have to be computed. This is facilitated by the observation

$$\nabla_{(\chi,\mathcal{K},\mathcal{E})} S = \left(\frac{\mu}{T} - \frac{V}{T_L}, \frac{u}{T}, \frac{1}{T_L} - \frac{1}{T}\right) .$$

As a consequence, for smooth solutions of (10), the entropy density satisfies

$$\frac{\partial S}{\partial t} + \frac{\chi}{T_L}\frac{\partial V}{\partial t} + \nabla_x \cdot J_S = \frac{1}{T}\, u \cdot (R_{ph} + R_{ld}) + \left(\frac{1}{T_L} - \frac{1}{T}\right) W_{ph} \le 0 .$$

Weak solutions are admissible (as limits of the kinetic model) if the equality is replaced by $\le$.

Since (S, Su) is a strictly convex Lax entropy pair, classical arguments (see [12]) imply the following:

Corollary 4.2: The hydrodynamic system for strong ionization (10) is hyperbolic.

5 Low densities and parabolic bands

We specialize the above results to the low density limit $\eta = 0$ and to parabolic bands $\varepsilon_n(k) = |k|^2/(2m_n)$, $\varepsilon_p(k) = |k|^2/(2m_p)$. Then the equilibrium distribution functions become Maxwellians:

$$f_{0n}(k) = \mathcal{F}_0 \exp\left(\frac{\mu + k\cdot u - |k|^2/(2m_n) - \Delta/2}{T}\right) , \tag{15}$$

$$f_{0p}(k) = \mathcal{F}_0 \exp\left(\frac{-\mu + k\cdot u - |k|^2/(2m_p) - \Delta/2}{T}\right) . \tag{16}$$

As a consequence, the macroscopic electron and hole densities

$$\rho_n = \int_{\mathbb{R}^3} f_{0n}\, dk , \qquad \rho_p = \int_{\mathbb{R}^3} f_{0p}\, dk ,$$

satisfy the generalized Saha law

$$\rho_n \rho_p = n_i(u,T)^2 \quad \text{with} \quad n_i(u,T) = \mathcal{F}_0 (2\pi T\sqrt{m_n m_p})^{3/2} \exp\left(\frac{(m_n + m_p)|u|^2 - 2\Delta}{4T}\right) .$$

The quantities in the hydrodynamic system can be written in terms of the unknowns χ, u, and T. In particular, for the macroscopic densities, we have

$$\rho_n = \frac{1}{2}\left(\chi + \sqrt{\chi^2 + 4n_i(u,T)^2}\right) , \qquad \rho_p = \frac{1}{2}\left(-\chi + \sqrt{\chi^2 + 4n_i(u,T)^2}\right) .$$

The hydrodynamic system for strong ionization (10) can be written as

$$
\begin{aligned}
\frac{\partial \chi}{\partial t} + \nabla_x \cdot (\chi u) &= 0\,, \\
\frac{\partial \mathcal{K}}{\partial t} + \nabla_x \cdot (\mathcal{K} \otimes u) + \nabla_x p &= \chi \nabla_x V + R_{ph} + R_{ld}\,, \\
\frac{\partial \mathcal{E}}{\partial t} + \nabla_x \cdot [(\mathcal{E} + p) u] &= \chi u \cdot \nabla_x V + W_{ph}\,,
\end{aligned}
\tag{17}
$$

with

$$
\mathcal{K} = (m_n \rho_n + m_p \rho_p) u\,, \qquad p = (\rho_n + \rho_p) T\,,
$$
$$
\mathcal{E} = (m_n \rho_n + m_p \rho_p) \frac{|u|^2}{2} + (\rho_n + \rho_p) \frac{3T + \Delta}{2}\,.
$$

The source terms in the momentum and energy equations have to be determined from (12) and (13). For the derivation of typical examples, we make several approximations. First we assume small mean velocities and replace the equilibrium distributions (15), (16) by their quadratic Taylor polynomials about $u = 0$. For the matrix element for scattering of electrons with lattice defects we assume that $\phi_{n,ld}$ is proportional to $\varepsilon_n^{\alpha_n}$, and analogously for the scattering of holes with lattice defects. Then the momentum source term due to scattering with lattice defects has the form

$$
R_{ld} = -\sqrt{T}\,(c_n T^{\alpha_n} \rho_n + c_p T^{\alpha_p} \rho_p)\, u\,. \tag{18}
$$

The phonon collision operators can be written as the sum of an elastic operator of the form of the collisions with lattice defects and an inelastic part. For simplicity, we make the assumption that the phonon energy is small compared to the thermal energy of the lattice, i.e., $\varepsilon_{ph}/T_L \ll 1$. If we also assume that the scattering matrix element only depends on the kinetic energy, the inelastic part of the electron-phonon collision operator can be approximated by a term of the form (see [20])

$$
Q_{n,ph,inelastic}(f_n) = \frac{\partial}{\partial \varepsilon} \left[\sqrt{\varepsilon} \phi_{n,ph}(\varepsilon) \left(\frac{\partial \langle f_n \rangle}{\partial \varepsilon} + \frac{\langle f_n \rangle}{T_L} \right) \right]\,, \tag{19}
$$

where $\langle f_n \rangle$ denotes the mean value of f_n over the sphere corresponding to kinetic energy ε. The elastic parts of the phonon collision operators contribute to the momentum source term R_{ph} (an additional term of the form (18)), but not to the energy source term W_{ph}. On the other hand, the inelastic parts do not contribute to R_{ph}. With the final assumption that $\phi_{n,ph}(\varepsilon)$ is proportional to ε^{β_n}, (19) produces the energy source term

$$
W_{n,ph} = d_n T^{\beta_n - 1/2} \rho_n \left(3T\Gamma(2 + \beta_n) + \frac{\Delta}{2} \Gamma(1 + \beta_n) \right) \left(\frac{1}{T} - \frac{1}{T_L} - \frac{|u|^2}{T^2} \right)\,.
$$

A second term of the same form originates from hole-phonon interaction.

Finally, we outline the computation of the characteristic speeds of the left hand side of (17) for the spatially one-dimensional case. More details can be found in [9]. The Jacobian F' of the flux vector $F = (\chi u, \mathcal{K}u + p, (\mathcal{E} + p)u)^{tr}$ with respect to the conserved quantities $(\chi, \mathcal{K}, \mathcal{E})$ can be written as

$$\begin{aligned} F' &= u\,\mathrm{Id} + (\chi, \mathcal{K}, \mathcal{E} + p) \otimes \nabla u + (0, 1, u) \otimes \nabla p \\ &= u\,\mathrm{Id} + a_1 \otimes b_1 + a_2 \otimes b_2\,, \end{aligned} \tag{20}$$

where the gradients are with respect to the conserved quantities. It is easily seen that u is an eigenvalue of this matrix. The other eigenvalues are of the form $u + \lambda$ where λ is an eigenvalue of

$$\begin{pmatrix} a_1 \cdot b_1 & a_2 \cdot b_1 \\ a_1 \cdot b_2 & a_2 \cdot b_2 \end{pmatrix}.$$

Thus, for the strict hyperbolicity of (17) it would be necessary that a_1 and a_2 as well as b_1 and b_2 are linearly independent. However, for $\chi = 0$ and $(m_n + m_p)u^2 = 2(5T + \Delta)$, the vectors $(\chi, \mathcal{K}, \mathcal{E} + p)$ and $(0, 1, u)$ are linearly dependent, and u is a double eigenvalue of F'.

In strictly hyperbolic situations, the form (20) of the Jacobian shows that the eigenvectors corresponding to the eigenvalue u are orthogonal to ∇u and ∇p. Therefore, the field corresponding to the eigenvalue u is linearly degenerate, and the pressure p is constant across a contact discontinuity.

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