Macroscopic Models for Almost Elastic Nonlinear Electron-Phonon Interaction in Semiconductors

Christian Schmeiser[1]

Abstract. A semiclassical transport equation for electrons in a semiconductor crystal is considered. It includes a nonlinear scattering operator modelling electron-phonon interaction. A formal macroscopic limit under the assumption of a small phonon energy is carried out, leading to the so called spherical harmonics expansion (SHE-) model for an energy-dependent distribution function with a scattering operator of Fokker-Planck type. By a further macroscopic limit for electric fields balancing the inelastic scattering operator, a nonlinear, hyperbolic conservation law for the macroscopic density is derived. The flux depends nonlinearly on the electric field. The nonlinear structure of the conservation law and the behaviour for large fields are studied.

Key words: Semiconductors, kinetic equations, phonons, drift-diffusion limit

AMS subject classification: 82A70, 78A35

Acknowledgement: This work has been supported by the Austrian Science Foundation under grant Nr. P11308-MAT, by the TMR-network No. ERB FMBX CT97 0157 on "Asymptotic Methods in Kinetic Theory", and by the program on "Charged Particle Kinetics" of the Erwin-Schrödinger-Institute, Vienna.

[1]Institut für Angewandte und Numerische Mathematik, TU Wien, Wiedner Hauptstraße 8-10, 1040 Wien, Austria. e-mail: cs@bianca.tuwien.ac.at

1 Introduction

The behaviour of charged particles under the action of electric fields and dominantly elastic scattering mechanisms receives increasing attention recently. Two important applications are the transport of light particles undergoing collisions with heavy particles in ionized gases [4], [9], [13] and the transport of charge carriers in semiconductor crystals [3], [5], [1], [12], [14]. In a kinetic description, the dominance of elastic scattering mechanisms causes the distribution function to be almost isotropic in terms of the wave vector (respectively the velocity). Models for approximating distribution functions depending only on the energy have first been derived for particles with rotationally symmetric transport properties by an expansion in terms of spherical harmonics (see, e.g., [15]. Although this procedure can be replaced by an asymptotic approach extendable to nonisotropic situations [5], [1], the resulting models are often called SHE- (spherical harmonics expansion) models.

In general, SHE-models contain scattering terms with a tendency to move the distribution towards equilibrium. Thus, the long time behaviour is described by macroscopic equations for the parameters in the equilibrium distribution. Of recent interest [2] are macroscopic limits for high field situations where the ground state is influenced by an electric field balancing the scattering mechanisms.

The present work is concerned with the transport of electrons in a semiconductor crystal subject to acceleration by a prescribed electric field and to interaction with phonons with constant phonon energy. With the assumptions that a typical energy of the electrons is the thermal energy and that the phonon energy is small compared to that, the electron-phonon interaction is almost elastic and the framework described above applies. The main difference to earlier work [3], [14], is that a nonlinear scattering operator is considered taking into account degeneracy effects for high densities.

In the following section the kinetic model is presented and nondimensionalized according to the above comments. Some properties of the scattering operator are collected in section 3. In section 4 the SHE-model is derived by a Hilbert expansion (following a standard procedure [5], [1], [14]). The scattering operator in the SHE-model is a nonlinear differential operator of Fokker-Planck type. This part of the present work is an extension of [14] to the nonlinear and nonisotropic case.

The comparison to related models is the subject of section 5. Here different scaling assumptions are used, following [1], [3]: The phonon energy is assumed of the order of magnitude of the thermal energy (which is valid for, e.g., optical phonons in silicon), and the average electron energy much larger than that. The macroscopic limit gives a nonlinear extension of the SHE-model derived in [3]. It can be seen as a submodel of the one derived in section 4. The scattering operator is a first order degeneration of the second order Fokker-Planck operator.

Finally, section 6 is concerned with a macroscopic limit for high fields of the SHE-model derived in section 4. This is a nonlinear (and nonisotropic) extension of a result from [2]. A first order continuity equation for the macroscopic density is derived, containing a conductivity matrix with a nonlinear dependence on the density and on the electric field. The asymptotic behaviour for large fields and the nonlinear structure are studied showing that compression shocks are enabled by the nonlinearity.

2 The Kinetic Model

We describe the transport of electrons in a semiconductor crystal by a distribution function $f(x,k,t)$ depending on the position $x \in I\!R^3$, the wave vector $k \in I\!R^3$ and time $t \in I\!R$. The distribution function is a solution of the kinetic equation

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_k \varepsilon_b \cdot \nabla_x f - \frac{q}{\hbar}\mathcal{E} \cdot \nabla_k f = Q_{phon}(f)\,. \tag{2.1}$$

Here $\hbar$ and q denote the reduced Planck constant and the elementary charge, respectively. The (given) electric field $\mathcal{E}(x,t)$ is time and space dependent. The band diagram $\varepsilon_b(k)$, the distribution function (as a function of the wave vector, for fixed x and t) and all other functions of k appearing below are periodic with period $B \subset I\!R^3$, where the Brillouin zone B is a fundamental cell of the dual of the crystal lattice. In the following, reflection symmetry will also be used: The Brillouin zone B is symmetric with respect to the origin and $\varepsilon_b(-k) = \varepsilon_b(k)$ holds. The collision operator

$$\begin{aligned} Q_{phon}(f)(x,k,t) \quad &= \quad \int_B \Phi(x,k,k')\Big[\Big((N_{phon}+1)\delta(\varepsilon_b - \varepsilon_b' + \varepsilon_{phon}) \\ &\qquad + N_{phon}\delta(\varepsilon_b - \varepsilon_b' - \varepsilon_{phon})\Big) f'(1-f) \end{aligned}$$

$$-\Big((N_{phon}+1)\delta(\varepsilon_b'-\varepsilon_b+\varepsilon_{phon})$$
$$+N_{phon}\delta(\varepsilon_b'-\varepsilon_b-\varepsilon_{phon})\Big)f(1-f')\Big]dk' \qquad (2.2)$$

with the phonon occupation number

$$N_{phon}=\left(\exp\left(\frac{\varepsilon_{phon}}{k_BT_L}\right)-1\right)^{-1}$$

is a model for the interaction of the electrons with phonons with constant energy ε_{phon}. The matrix element Φ is a symmetric function of k and k'. In the following it will be assumed to be bounded away from zero: $\Phi(x,k,k')\ge \underline{\Phi}>0$. The Boltzmann constant and the lattice temperature are denoted by k_B and T_L, respectively. In (2.2), the prime is used as a shorthand notation for evaluation at k'. The factors $1-f$ and $1-f'$ account for the Pauli exclusion principle and make the collision operator quadratically nonlinear. In low density approximations they are often left out. The distribution function has to satisfy the inequalities $0\le f\le 1$. We point out that (2.1) is a model equation where other scattering effects (like impurity scattering, electron-electron scattering, band-to-band transitions) are ignored.

As a degenerate example for the band diagram we mention the parabolic band approximation close to a band diagram minumum

$$\varepsilon_b(k)=\frac{\hbar^2|k|^2}{2m_{eff}}\,,\qquad B=\mathbb{R}^3\,, \qquad (2.3)$$

with effective mass m_{eff}. A typical approximation for the matrix element is by a constant:

$$\Phi(x,k,k')=\overline{\Phi}\,.$$

In the following, we shall return to these examples repeatedly.

For a nondimensionalization, we introduce as reference energy the thermal energy $\overline{\varepsilon}=k_BT_L$. Then a reference wave vector length $\overline{k}$ is determined by requiring that the scaled band diagram ε_{bs}, satisfying

$$\varepsilon_b(k)=\overline{\varepsilon}\varepsilon_{bs}\left(\frac{k}{\overline{k}}\right)\,,$$

takes moderate values for moderate values of its argument. For the parabolic band approximation (2.3) we choose

$$\overline{k} = \frac{\sqrt{k_B T_L m_{eff}}}{\hbar}, \qquad \varepsilon_{bs}(k_s) = \frac{|k_s|^2}{2}.$$

The scattering operator is made dimensionless by taking out the typical scattering frequency

$$\overline{Q} = \frac{\overline{\Phi}\,\overline{k}^3 N_{phon}}{\overline{\varepsilon}},$$

where $\overline{\Phi}$ is a typical value of the matrix element. As reference time the relaxation time $\overline{t} = \overline{Q}^{-1}$ is chosen. Balancing the terms on the left hand side of (2.1) then leads to a reference length and a reference field strength:

$$\overline{x} = \frac{\overline{\varepsilon}\,\overline{t}}{\hbar\overline{k}}, \qquad \overline{E} = \frac{\overline{\varepsilon}}{q\overline{x}}.$$

Obviously, $\overline{\varepsilon}/(\hbar\overline{k})$ is a reference velocity, and $\overline{x}$ can be interpreted as a mean free path. Thus, the present scaling is relevant for the observation of microscopic effects. The dimensionless parameter

$$\alpha = \frac{\varepsilon_{phon}}{k_B T_L}$$

is the scaled phonon energy.

When dimensionless quantities are introduced according to

$$\begin{aligned} &x = \overline{x}x_s\,, \qquad k = \overline{k}k_s\,, \qquad t = \overline{t}t_s\,, \qquad B = \overline{k}B_s\,, \\ &\mathcal{E} = \overline{E}\mathcal{E}_s\,, \qquad \varepsilon_b(k) = \overline{\varepsilon}\varepsilon_{bs}\left(\frac{k}{\overline{k}}\right), \qquad \Phi(x,k,k') = \overline{\Phi}\Phi_s\left(\frac{x}{\overline{x}}, \frac{k}{\overline{k}}, \frac{k'}{\overline{k}}\right), \end{aligned}$$

the scaled version of the transport equation becomes

$$\frac{\partial f}{\partial t} + \nabla_k \varepsilon_b \cdot \nabla_x f - \mathcal{E} \cdot \nabla_k f = Q_\alpha(f)\,, \tag{2.4}$$

where the subscripts s have been dropped and the scaled scattering operator is given by

$$\begin{aligned} Q_\alpha(f) \;=\; &\int_B \Phi\Big[\Big(e^\alpha \delta(\varepsilon_b - \varepsilon_b' + \alpha) + \delta(\varepsilon_b - \varepsilon_b' - \alpha)\Big) f'(1-f) \\ &- \Big(e^\alpha \delta(\varepsilon_b' - \varepsilon_b + \alpha) + \delta(\varepsilon_b' - \varepsilon_b - \alpha)\Big) f(1-f')\Big] dk'\,. \end{aligned} \tag{2.5}$$

The scaled parabolic band assumption and constant matrix element become

$$\varepsilon_b(k) = \frac{|k|^2}{2}\,, \qquad \Phi(x,k,k') = 1\,. \tag{2.6}$$

3 The Collision Operator

For further reference we recall a basic identity [11], a consequence of the symmetry of Φ:

$$\int_B Q_\alpha(f) g\,dk = -\frac{1}{2}\int_B\int_B \Phi(1-f)(1-f')\Big(e^{-\varepsilon_b'}\delta(\varepsilon_b' - \varepsilon_b + \alpha)$$
$$+e^{-\varepsilon_b}\delta(\varepsilon_b - \varepsilon_b' + \alpha)\Big)\left(\frac{f'e^{\varepsilon_b'}}{1-f'} - \frac{fe^{\varepsilon_b}}{1-f}\right)(g'-g)dk'dk\,. \tag{3.1}$$

With $g = fe^{\varepsilon_b}/(1-f)$, with the positivity assumption on Φ and for positive α it immediately implies that $Q_\alpha(f) = 0$ iff

$$f(k) = \frac{1}{1+\exp(\varepsilon_b(k) - \mu(\varepsilon_b(k)))}$$

for an arbitrary α-periodic function μ (see [10], [11]). Note that for constant μ this is a Fermi-Dirac distribution with chemical potential μ.

Our aim is to study the situation when α is small. Expansion of (2.5) around $\alpha = 0$ for fixed f gives

$$Q_\alpha(f) = (1+\alpha)Q_0(f) + \alpha^2 Q_2(f) + O(\alpha^3) \tag{3.2}$$

with

$$Q_0(f) \;=\; 2\int_B \Phi\delta(\varepsilon_b - \varepsilon_b')(f'-f)dk'\,, \tag{3.3}$$

a linear, elastic collision operator. The computation of Q_2 is left open at the moment.

For expanding the Delta-distributions in (2.5) and (3.3) the coarea formula [6] is needed:

$$\int_B \psi(k)dk = \int_{-\infty}^{\infty}\int_{\mathcal{S}_\varepsilon} \psi(k)\frac{dS_\varepsilon(k)}{|\nabla_k\varepsilon_b(k)|}d\varepsilon\,,$$

with the manifolds

$$\mathcal{S}_\varepsilon = \{k \in B,\ \varepsilon_b(k) = \varepsilon\}\,, \qquad \varepsilon \in I\!R\,,$$

and the Euclidean surface element $dS_\varepsilon(k)$ on $\mathcal{S}_\varepsilon$. We use the notation $dN_\varepsilon(k) = dS_\varepsilon(k)/|\nabla_k \varepsilon_b(k)|$ and assume that the density of states

$$N(\varepsilon) = \int_{\mathcal{S}_\varepsilon} dN_\varepsilon$$

exists for every $\varepsilon \in I\!R$. Of course it is sufficient to only consider $\varepsilon \in \mathcal{R} = \{\varepsilon_b(k) :\ k \in B\}$, since outside of $\mathcal{R}$, N vanishes and $\mathcal{S}_\varepsilon$ is empty. Note that for physically accurate models with a bounded Brillouin zone B, $\mathcal{R}$ is a bounded interval, whereas for the parabolic band approximation (2.6) $\mathcal{R} = [0, \infty)$ and $N(\varepsilon) = 4\pi\sqrt{2\varepsilon}$ hold.

In the following, some properties of Q_0 will be recalled [1]. From (3.1) with $\alpha = 0$ and $g = f$ we obtain

$$\int_B Q_0(f) f\, dk = -\int_B \int_{\mathcal{S}_{\varepsilon_b}} \Phi(f' - f)^2 dN_{\varepsilon_b}(k') dk\,.$$

An immediate consequence is

$$Q_0(f) = 0 \quad \Longleftrightarrow \quad f(k) = F(\varepsilon_b(k))\,. \tag{3.4}$$

Also, all functions depending on k only through the energy are collision invariants:

$$\int_B Q_0(f) F(\varepsilon_b) dk = 0\,,$$

or, equivalently,

$$\int_{\mathcal{S}_\varepsilon} Q_0(f) dN_\varepsilon = 0 \qquad \forall\, \varepsilon \in \mathcal{R}\,.$$

With the positivity assumption on the matrix element the above can be strengthened [1] to the statement that the condition

$$\int_{\mathcal{S}_\varepsilon} g\, dN_\varepsilon = 0 \qquad \forall\, \varepsilon \in \mathcal{R} \tag{3.5}$$

is sufficient for the unique solvability of

$$Q_0(f) = g\,, \qquad \int_{\mathcal{S}_\varepsilon} f\, dN_\varepsilon = 0\,. \tag{3.6}$$

For the example (2.6) of a parabolic band and constant matrix element, the solution can be given explicitly: $f = -g/(8\pi|k|)$

As a final result of this section we compute some information on the operator Q_2 appearing in (3.2). With $F = F(\varepsilon_b(k))$ and a test function $\psi = \psi(\varepsilon_b(k))$, $\psi \in C_0^1(\mathcal{R})$, straightforward Taylor expansion in (3.1) gives (using (3.4))

$$\int_B Q_2(F)\psi\, dk = -\int_{\mathcal{R}} \Phi_0 (1-F)^2 e^{-\varepsilon} \frac{d}{d\varepsilon}\left(\frac{Fe^\varepsilon}{1-F}\right) \frac{d\psi}{d\varepsilon} d\varepsilon\,.$$

with

$$\Phi_0(x,\varepsilon) = \int_{\mathcal{S}_\varepsilon}\int_{\mathcal{S}_\varepsilon} \Phi(x,k,k') dN_\varepsilon(k') dN_\varepsilon(k)\,.$$

For the parabolic band and constant matrix element (2.6) we obtain $\Phi_0 = 32\pi^2\varepsilon$. With the identity

$$(1-F)^2 e^{-\varepsilon} \frac{d}{d\varepsilon}\left(\frac{Fe^\varepsilon}{1-F}\right) = \frac{dF}{d\varepsilon} + F(1-F)$$

and an integration by parts,

$$\int_B Q_2(F)\psi\, dk = \int_{\mathcal{R}} \frac{d}{d\varepsilon}\left[\Phi_0 \left(\frac{dF}{d\varepsilon} + F(1-F)\right)\right] \psi d\varepsilon$$

follows, implying

$$\int_{\mathcal{S}_\varepsilon} Q_2(F) dN_\varepsilon = S(F) := \frac{d}{d\varepsilon}\left[\Phi_0 \left(\frac{dF}{d\varepsilon} + F(1-F)\right)\right] \tag{3.7}$$

for all $\varepsilon \in \mathcal{R}$.

4 A Macroscopic Limit

In (2.4), we introduce the (macroscopic) diffusion scaling

$$\mathcal{E} \to \alpha\mathcal{E}\,, \qquad x \to \frac{x}{\alpha}\,, \qquad t \to \frac{t}{\alpha^2}\,.$$

In the resulting transport equation

$$\alpha^2 \frac{\partial f}{\partial t} + \alpha \nabla_k \varepsilon_b \cdot \nabla_x f - \alpha \mathcal{E} \cdot \nabla_k f = Q_\alpha(f)\,, \tag{4.1}$$

the limit $\alpha \to 0$ will be carried out in the following by the Hilbert expansion procedure. The ansatz

$$f = f_0 + \alpha f_1 + \alpha^2 f_2 + O(\alpha^3)$$

is substituted in (4.1) and coefficients of equal powers of α are compared (using the expansion (3.2) of the scattering operator):

$$\alpha^0: \qquad 0 = Q_0(f_0)\,, \tag{4.2}$$

$$\alpha^1: \qquad \nabla_k \varepsilon_b \cdot \nabla_x f_0 - \mathcal{E} \cdot \nabla_k f_0 = Q_0(f_1) + Q_0(f_0)\,, \tag{4.3}$$

$$\alpha^2: \qquad \frac{\partial f_0}{\partial t} + \nabla_k \varepsilon_b \cdot \nabla_x f_1 - \mathcal{E} \cdot \nabla_k f_1 = Q_0(f_2) + Q_0(f_1) + Q_2(f_0)\,. \tag{4.4}$$

The first equation, (4.2), and (3.4) imply the existence of a function $F(x, \varepsilon, t)$ such that

$$f_0(x, k, t) = F(x, \varepsilon_b(k), t)\,. \tag{4.5}$$

The higher order equations are needed to specify F. With (4.5), (4.3) becomes

$$\nabla_k \varepsilon_b \cdot \left(\nabla_x F - \mathcal{E} \frac{\partial F}{\partial \varepsilon} \right) = Q_0(f_1)\,,$$

and we can write the general solution as

$$f_1 = -\lambda \cdot \left(\nabla_x F - \mathcal{E} \frac{\partial F}{\partial \varepsilon} \right) + F_1\,, \tag{4.6}$$

where $\lambda(x, k)$ is the solution of (3.6) with $g = -\nabla_k \varepsilon_b$ (satisfying (3.5) by the reflection symmetry) and F_1 (like F) depends on the wave vector only through the energy. Now, for fixed $\varepsilon \in \mathcal{R}$, (4.4) is integrated over $\mathcal{S}_\varepsilon$ after substituting (4.5) and (4.6):

$$N \frac{\partial F}{\partial t} - \left(\nabla_x - \mathcal{E} \frac{\partial}{\partial \varepsilon} \right) \cdot \left[D \left(\nabla_x F - \mathcal{E} \frac{\partial F}{\partial \varepsilon} \right) \right] = S(F)\,, \tag{4.7}$$

where (3.7) has been used for the evaluation of the right hand side, and the diffusion matrix is given by

$$D(x,\varepsilon) = \int_{\mathcal{S}_\varepsilon} \lambda \otimes \nabla_k \varepsilon_b \, dN_\varepsilon \,.$$

Equation (4.7) is a version of the SHE-model (see [1] and the references therein) with a Fokker-Planck type differential operator as scattering operator. It is a generalized version of the equation derived in [14], where the low density assumption and the parabolic band approximation have been used. The domain of the solution of the SHE-equation (4.7) is $x \in I\!R^3$, $\varepsilon \in \mathcal{R}$, $t \in I\!R$. Generically, the diffusion matrix is positive definite except for $\varepsilon \in \partial\mathcal{R}$ where it vanishes [1]. The same holds for the diffusivity Φ_0 in the scattering operator. Therefore, (4.7) is a degenerate parabolic equation in $I\!R^3 \times \mathcal{R}$. As a consequence of the degeneracy, no boundary conditions are needed along the energy boundary except the natural zero flux condition

$$\mathcal{E}^{tr} D \left(-\nabla_x F + \mathcal{E} \frac{\partial F}{\partial \varepsilon} \right) + \Phi_0 \left(\frac{\partial F}{\partial \varepsilon} + F(1-F) \right) = 0 \,, \qquad (x,\varepsilon) \in I\!R^3 \times \partial\mathcal{R} \,. \tag{4.8}$$

This condition will be satisfied whenever F does not have too strong singularities along the energy boundary.

For the parabolic band and the constant matrix element (2.6) the diffusivity is isotropic: $D = \varepsilon/3\,\mathrm{Id}$, $\varepsilon > 0$.

5 An Alternative Scaling

In this section an alternative scaling of the kinetic equation (2.1) is introduced and the corresponding macroscopic limit is carried out. This is motivated by the fact that the assumption of smallness of the phonon energy compared to the thermal energy is not valid for optical phonons. Also, when high electric fields are applied, a reference value for the energy related to the applied potential (instead of the lattice temperature) seems more reasonable. Such a scaling has been introduced in [1] and [5]. The results of this section can be seen as an extension of [3] to a nonlinear scattering model.

We start with the unscaled kinetic model (2.1), (2.2), and introduce a new reference energy (again denoted by) $\overline{\varepsilon}$ different from (actually significantly larger than) $k_B T_L$. Otherwise, the scaling follows the prescription of section 2. Then the scaled problem contains the dimensionless parameters

$$\alpha = \frac{\varepsilon_{phon}}{k_B T_L}, \qquad \gamma^2 = \frac{\varepsilon_{phon}}{\overline{\varepsilon}},$$

where α has already been introduced in section 2 and is assumed to be $O(1)$ now, whereas γ is considered small. The scaled kinetic model has the form (2.4) with the scattering operator replaced by

$$\begin{aligned} Q_{\alpha,\gamma}(f) \;=\; & \int_B \Phi\Big[\Big(e^\alpha \delta(\varepsilon_b - \varepsilon_b' + \gamma^2) + \delta(\varepsilon_b - \varepsilon_b' - \gamma^2)\Big) f'(1-f) \\ & - \Big(e^\alpha \delta(\varepsilon_b' - \varepsilon_b + \gamma^2) + \delta(\varepsilon_b' - \varepsilon_b - \gamma^2)\Big) f(1-f')\Big] dk' \end{aligned} \quad (5.1)$$

Taylor expansion gives

$$Q_{\alpha,\gamma}(f) = Q_{\alpha,0}(f) + \gamma^2 Q_{\alpha,1}(f) + O(\gamma^4),$$

with

$$Q_{\alpha,0}(f) \;=\; (e^\alpha + 1)\int_B \Phi\delta(\varepsilon_b - \varepsilon_b')(f' - f)dk'.$$

Obviously, $Q_{\alpha,0}$ has the same properties as the operator Q_0 discussed in section 3. In particular, its kernel consists of distribution functions depending only on the energy ($f(k) = F(\varepsilon_b(k))$). For such distribution functions we compute

$$\int_{\mathcal{S}_\varepsilon} Q_{\alpha,1}(F)dN_\varepsilon = \tilde{S}(F) := (e^\alpha - 1)\frac{d}{d\varepsilon}[\Phi_0 F(1-f)].$$

Now we proceed as in section 4: After introducing the diffusion scaling

$$\mathcal{E} \to \gamma\mathcal{E}, \qquad x \to \frac{x}{\gamma}, \qquad t \to \frac{t}{\gamma^2},$$

the macroscopic limit is carried out. The result is the SHE-equation (4.7) with the scattering term $S(F)$ replaced by $\tilde{S}(F)$. Since completely different scalings have been used in this and the preceding sections, we compare the resulting equations in their unscaled, dimensional forms. The dimensional version of the SHE-equation (4.7) is given by

$$N\frac{\partial F}{\partial t} - \left(\nabla_x - q\mathcal{E}\frac{\partial}{\partial \varepsilon}\right)\cdot\left[D\left(\nabla_x F - q\mathcal{E}\frac{\partial F}{\partial \varepsilon}\right)\right]$$
$$= \varepsilon_{phon}\frac{\partial}{\partial \varepsilon}\left[\Phi_0\left(k_B T_L\frac{\partial F}{\partial \varepsilon} + F(1-F)\right)\right], \qquad (5.2)$$

where the additional factor $\alpha/(e^\alpha - 1)$ in front of the scattering term has been approximated by 1. If the SHE-model derived in this section is dimensionalized, the same equation results with the only difference that the term $k_B T_L \frac{\partial F}{\partial \varepsilon}$ in the scattering operator disappears.

The equation (5.2) seems to be preferable to its counterpart derived in the present section: It is parabolic whereas dropping the term $k_B T_L \frac{\partial F}{\partial \varepsilon}$ produces an equation of mixed type. Also it contains the correct equilibrium (Fermi-Dirac) distributions as steady state, space homogeneous solutions of the field free equation. Of course, it is inaccurate for smaller energies (of the order of the thermal energy) if α is not small, but this is true for both models.

In [12] a related model has been derived by considering two different scattering mechanisms: Phonon scattering with a constant (not small) phonon energy and a dominating elastic scattering. The macroscopic model is again a SHE-equation with the scattering operator in (5.2) replaced by a difference operator, which can be interpreted as a discretization of the right hand side of (5.2). The grid spacing is the phonon energy. In a numerical approach, the different models could be combined: A discretization of the scattering operator in (5.2) should use the phonon energy as the grid spacing for small energies, whereas larger spacings can be used for energies large compared to the thermal energy. A similar approach is used [7] in models for condensation, where the independent variable is the number of molecules in a droplet instead of the energy.

6 A Further Macroscopic Limit. High Fields

In this section we shall be concerned with a macroscopic limit of the SHE-equation (4.7). As in the beginning of the previous section a rescaling is carried out:

$$x \to \frac{x}{\beta}\,, \qquad t \to \frac{t}{\beta}\,, \tag{6.1}$$

where the small parameter β is a Knudsen number measuring the ratio between the mean free path relevant for the inelastic contribution to the scattering events and a macroscopic length scale. Note that the field is not rescaled. Thus, we allow for field strengths balancing the inelastic collision effects. The rescaled SHE-equation is given by

$$\beta N\frac{\partial F}{\partial t} - \left(\beta\nabla_x - \mathcal{E}\frac{\partial}{\partial\varepsilon}\right)\cdot\left[D\left(\beta\nabla_x F - \mathcal{E}\frac{\partial F}{\partial\varepsilon}\right)\right] = S(F)\,, \tag{6.2}$$

and the rescaled boundary condition (4.8) by

$$\mathcal{E}^{tr}D\left(-\beta\nabla_x F + \mathcal{E}\frac{\partial F}{\partial\varepsilon}\right) + \Phi_0\left(\frac{\partial F}{\partial\varepsilon} + F(1-F)\right) = 0\,, \tag{6.3}$$
$$(x,\varepsilon)\in I\!R^3\times\partial\mathcal{R}\,.$$

Before proceeding, we shortly discuss the corresponding results for the low field scaling $x \to x/\beta$, $\mathcal{E} \to \beta\mathcal{E}$, $t \to t/\beta^2$ (instead of (6.1)). In this case, $S(F)$ is the dominant term in (4.7). The limiting distribution is a Fermi-Dirac distribution with a chemical potential determined by the low field drift-diffusion model [8]. The formulas for the transport coefficients are, however, different from those in [8], since there the drift-diffusion model has been derived directly from a kinetic equation with a different scattering operator and without the detour via the SHE-equation.

In the limit $\beta \to 0$, (6.2) reduces to

$$-\frac{\partial}{\partial\varepsilon}\left(\mathcal{E}^{tr}D\mathcal{E}\frac{\partial F}{\partial\varepsilon}\right) = \frac{\partial}{\partial\varepsilon}\left[\Phi_0\left(\frac{\partial F}{\partial\varepsilon} + F(1-F)\right)\right]\,.$$

The general solution of this equation subject to the limit as $\beta \to 0$ of the boundary condition (6.3) is

$$F(x,\varepsilon,t) = \left(1 + \exp\left(\int_0^\varepsilon \frac{\Phi_0(x,s)ds}{\Phi_0(x,s) + \mathcal{E}(x,t)^{tr}D(x,s)\mathcal{E}(x,t)} - \mu(x,t)\right)\right)^{-1}\,,$$

with arbitrary $\mu(x,t)$. This is compatible with the low field result mentioned above since obviously a Fermi-Dirac distribution with chemical potential μ is obtained for $\mathcal{E}=0$. For the parabolic band approximation and the constant collision cross section (2.6) we get

$$F = \left(1+\exp\left(\frac{\varepsilon}{1+|\mathcal{E}|^2/(96\pi^2)}-\mu\right)\right)^{-1},$$

i.e., a Fermi-Dirac distribution with elevated temperature. In terms of the original dimensional units, the modified temperature is given by

$$T_L\left(1+\left(\frac{|\mathcal{E}|}{E_{ref}}\right)^2\right), \qquad E_{ref}=\sqrt{96}\,\pi\overline{E}\,.$$

An equation for the quasi chemical potential μ is determined by integration of (6.2) with respect to ε, dividing the resulting equation by β and then going to the limit $\beta\to 0$:

$$\frac{\partial\varrho}{\partial t}-\nabla_x\cdot(\Sigma\mathcal{E})=0\,, \tag{6.4}$$

with the macroscopic density ϱ and the (positive definite) conductivity matrix Σ, given by

$$\varrho=\int_{\mathcal{R}} NF\,d\varepsilon\,, \qquad \Sigma=-\int_{\mathcal{R}} D\frac{\partial F}{\partial\varepsilon}d\varepsilon\,.$$

It is easily checked that the relation between ϱ and μ is one-to-one and, thus, (6.4) can be seen as an equation for ϱ with a nonlinear dependence of the conductivity matrix on the density.

Finally, we discuss some qualitative properties of (6.4). In particular, the behaviour for large fields will be analyzed. We have to distinguish between the cases of a bounded Brillouin zone and the parabolic band approximation. For the first case, we set $\mathcal{E}=E\omega$ with $|\omega|=1$ and $E\to\infty$. We easily obtain

$$\varrho\sim\frac{\varrho_{max}}{1+e^{-\mu}}\,, \qquad \text{as } E\to\infty\,, \tag{6.5}$$

where ϱ_{max}, the scaled maximal value of the macroscopic density, is equal to the volume of the scaled Brillouin zone. The asymptotic behaviour of the conductivity matrix is given by

$$\Sigma\sim\frac{e^{-\mu}}{E^2(1+e^{-\mu})^2}M\,, \qquad M=\int_{\mathcal{R}}\frac{\Phi_0 D}{\omega^{tr}D\omega}d\varepsilon\,,$$

and with (6.5) we have

$$\Sigma \sim \frac{1}{E^2}\left(1 - \frac{\varrho}{\varrho_{max}}\right)\frac{\varrho}{\varrho_{max}} M \,.$$

Thus, for a fixed density ϱ, the current density decays like $1/E$ as $E \to \infty$:

$$\Sigma\mathcal{E} \sim \frac{1}{E}\left(1 - \frac{\varrho}{\varrho_{max}}\right)\frac{\varrho}{\varrho_{max}} M\omega \,.$$

Now we turn to the parabolic band model and the constant matrix element (2.6). We compute

$$\begin{aligned} \varrho &= 4\pi\sqrt{2}\,T_E^{3/2}\int_0^\infty \frac{\sqrt{s}\,ds}{1+e^{s-\mu}}\,, \qquad T_E = 1 + \frac{E^2}{96\pi^2}\,, \\ \Sigma &= \sigma\,\mathrm{Id}\,, \qquad \sigma = \frac{T_E}{3}\ln(e^\mu + 1)\,, \end{aligned}$$

and

$$\begin{aligned} \frac{d^2\sigma}{d\varrho^2} &= \left(\frac{d\varrho}{d\mu}\right)^{-3}\left(\frac{d^2\sigma}{d\mu^2}\frac{d\varrho}{d\mu} - \frac{d\sigma}{d\mu}\frac{d^2\varrho}{d\mu^2}\right) \\ &= \left(\frac{d\varrho}{d\mu}\right)^{-3}\frac{2\pi\sqrt{2}\,T_E^{5/2}e^\mu}{3(1+e^\mu)^2}\int_0^\infty \frac{(1-e^s)ds}{\sqrt{s}(1+e^{s-\mu})^2} < 0\,. \end{aligned}$$

This shows genuine nonlinearity of (6.4). Entropy solutions might contain shock waves with the density increasing in the flow direction $-\mathcal{E}$. For large fields,

$$\sigma \sim \frac{2\varrho}{E\sqrt{3\pi}}\,, \qquad \text{as } E \to \infty\,,$$

holds. Thus, asymptotically, the equation (6.4) becomes linear with a velocity saturation effect:

$$\Sigma\mathcal{E} \sim \frac{2\varrho}{\sqrt{3\pi}}\,\omega\,.$$

Velocity saturation has also been observed in the linear model corresponding to (6.4) for parabolic bands and the low density assumption [2].

References

[1] N. Ben Abdallah, P. Degond, On a hierarchy of macroscopic models for semiconductors, *J. Math. Phys.* **37** (1996), pp. 3306–3333.

[2] N. Ben Abdallah, P. Degond, P.A. Markowich, C. Schmeiser, High field approximations of the spherical harmonics expansion model for semiconductors, manuscript, TU Wien, 1998.

[3] E. Bringuier, Kinetic theory of high-field transport in semiconductors, *Phys. Rev. B* **57** (1998), pp. 2280–2285.

[4] P. Degond, B. Lucquin-Desreux, Transport coefficients of plasmas and disparate mass binary gases, *Transp. Th. and Stat. Phys.* **25** (1996), pp. 595–633.

[5] P. Dmitruk, A. Saul, L. Reyna, High electric field approximation to charge transporet in semiconductor devices, *Appl. Math. Letters* **5** (1992), pp. 99–102.

[6] H. Federer, *Geometric measure theory*, Springer, Berlin, 1969.

[7] J.I. Frenkel, *Kinetische Theorie der Flüssigkeiten*, Deutscher Verlag der Wissenschaften, Berlin, 1957.

[8] F. Golse, F. Poupaud, Limite fluide des equations de Boltzmann des semiconducteurs pour une statistique de Fermi-Dirac, *Asymptot. Anal.* **6** (1992), pp. 135–160.

[9] J.L. Lebowitz, A. Rokhlenko, Hydrodynamical equation for electron swarms, preprint, Rutgers University, 1998.

[10] A. Majorana, Equilibrium solutions of the nonlinear Boltzmann equation for an electron gas in a semiconductor, preprint, Universita di Catania, 1994.

[11] P.A. Markowich, F. Poupaud, C. Schmeiser, Diffusion approximation of nonlinear electron-phonon collision mechanisms, *M^2AN* **29** (1995), pp. 857–869.

[12] J. Mohring, *The Spherical Harmonics Expansion Method*, Dissertation, Univ. Kaiserslautern, 1996.

[13] A. Nouri, C. Schmeiser, A diffusion approximation of ionizing collisions in weakly ionized plasmas, manuscript, Univ. de Nice, 1998.

[14] C. Schmeiser, A. Zwirchmayr, Elastic and drift-diffusion limits of electron-phonon interaction in semiconductors, *Math. Models and Meth. in Appl. Sci.* **8** (1998), pp. 37–53.

[15] D. Ventura, A. Gnudi, G. Baccarani, F. Odeh, Multidimensional spherical harmonics expansion of Boltzmann equation for transport in semiconductors, *Appl. Math. Lett.* **5** (1992), pp. 85–90.