Kinetic Boundary Layers and Fluid-Kinetic Coupling in Semiconductors

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Abstract. The semiconductor Boltzmann equation with elastic collisions as the dominating scattering effects is considered. For the corresponding fluid limit, the spherical harmonics expansion model, kinetic boundary layers are analyzed and higher order accurate boundary conditions are constructed. In a further step, boundary value problems for the energy transport model and the drift-diffusion model are derived. As an application, interface conditions for the fluid-kinetic coupling in a domain decomposition approach are presented.

Key words: Semiconductor Boltzmann equation, spherical harmonics expansion model, energy transport model, drift-diffusion model, domain decomposition, Milne problem.

AMS subject classification: 35Q20, 76P05, 82A70, 78A35

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1 Introduction

For many applications, a semiclassical Boltzmann equation is a sufficiently accurate model for charge transport in semiconductor crystals. However, its complexity makes its use in numerical simulations very expensive. Macroscopic models, on the other hand, are by their comparable simplicity well suited for numerical computations. The classical drift-diffusion model belongs to this category. It has been used extensively for simulation purposes despite its shortcomings regarding physical accuracy.

The derivation of macroscopic models intermediate to the Boltzmann equation and the drift-diffusion model has been the subject of a large amount of work. These attempts have been given a mathematical basis by introducing the classical Hilbert expansion method in a variant used for neutron transport models [1] to the field of semiconductor modelling [12]. It amounts to asymptotic expansions of the distribution function in terms of the Knudsen number, i.e., the scaled mean free path of the electrons. For an overview on the connection between different models by asymptotic methods see [2].

Frequently, kinetic effects cannot be neglected in the whole simulation domain. They can play an important role near boundaries and material interfaces as well as in bulk material when the electric field is large. In the first case, the accuracy of a macroscopic model can be improved by using modified boundary conditions based on higher order asymptotic expansions. For the standard drift-diffusion model, this has been carried out in [17]. The formulation of the higher order boundary conditions involves the computation of the extrapolation length [5] from the solution of a half space problem for a simplified, stationary kinetic equation [12]. In this work, we extend the results of [17] to other macroscopic models. The derivation of higher order transmission conditions for heterojunctions is the subject of [6].

For situations where kinetic effects are important in parts of the bulk material, domain decomposition strategies are natural, where the Boltzmann equation is solved in regions with strong kinetic effects and a macroscopic model is used whereever it is accurate enough. Then the two models need to be coupled at the kinetic-fluid interface. Coupling conditions connecting the Boltzmann equation and the standard drift-diffusion model have been derived in [10]. An extension of these results to other macroscopic models is carried out in this work.

The basic assumption in the following is that elastic scattering of electrons with lattice defects is the dominating effect in macroscopic regions. This means that the energy gained or lost by an electron in a scattering event is small compared to the mean energy of the electrons. The macroscopic model related to this assumption is the so called spherical harmonics expansion (SHE-) model [2], [7], [14], [16]. Its name is related to one way it can be derived [16]. Calling it a macroscopic model is not quite justified since it contains the electron energy as an independent variable. In other words, the shape of the distribution function is only specified to be isotropic. The SHE-model was referred to by one of its fathers F. Odeh as "poor man's Boltzmann".

From the SHE-model other macroscopic models can be derived by successively assuming the dominance of other scattering mechanisms. If electron-electron interaction is considered as the dominant effect, the distribution function is relaxed to a Fermi-Dirac distribution with arbitrary chemical potential and temperature. The corresponding fluid model is the energy transport (ET-) model [2], [3], [15], consisting of balance equations for charge and electron energy. By a direct derivation of the ET-model from the Boltzmann equation [3], compared to the derivation via the SHE-model [2], different transport coefficients are obtained. In the latter case, their evaluation is much easier since it is based on the linear elastic collision operator.

In the ET-model, the inelastic contributions of the scattering with lattice defects are contained in an energy relaxation term. For sufficiently large time scales and length scales, this term drives the temperature towards the temperature of the crystal lattice. Then the ET-model is reduced to the charge conservation equation, which can be interpreted as a generalized drift-diffusion (DD-) model for Fermi-Dirac statistics. In the nondegenerate limit it reduces to the standard drift-diffusion model.

In section 2 we consider a scaled Boltzmann equation and recall the derivation of the corresponding SHE-model. We also show that the leading order equation is actually accurate up to the order of the square of the Knudsen number.

This motivates the construction of boundary conditions in section 3, which are also second order accurate. We consider the case of general, nonequilibrium inflow data. The half space problems to be solved involve the elastic scattering operator. Simplifying physical assumptions lead to partially explicit solutions.

In section 4 we are concerned with the ET-model and the DD-model.

A heuristic derivation of the bulk equations from the SHE-model is given which can be based on formal asymptotic methods [2]. Then, by the same heuristic approach boundary conditions are constructed. The main argument for this procedure is the simplicity of the involved computations. The data in the boundary conditions can be derived from those for the SHE-model by integrations.

Interface conditions for fluid-kinetic coupling are presented in section 5, where the fluid model can be the SHE-model, the ET-model or the DD-model. This is a straightforward application of the boundary layer analysis and an adaption of the ideas in [10]. The formulation of the coupling conditions again requires the solution of certain half space problems which can be efficiently carried out by a recently developped iteration method [8]. The method is outlined in section 6, and the resulting approximations are given.

2 The Hilbert Expansion

To make this work self contained, a short formal derivation of the SHE-model is given in this section. More details can be found in [2] (see also [7], [14]). Our starting point is the following scaled Boltzmann equation for electrons in the conduction band of a semiconductor:

$$\frac{\partial f}{\partial t} + \frac{1}{\alpha} v \cdot \nabla_x f + \frac{1}{\alpha} \nabla_x V \cdot \nabla_k f = \frac{1}{\alpha^2} Q_0(f) + Q_1(f) \tag{2.1}$$

This is an equation for the distribution function $f(x, k, t)$, depending on position $x \in \Omega \subset I\!R^3$, wave vector $k \in B \subset I\!R^3$ and time t. Here Ω denotes the region occupied by the semiconductor crystal, and B denotes the Brillouin zone, i.e. the elementary cell of the dual L^* of the crystal lattice. The Brillouin zone has to be understood as a representation of the torus $I\!R^3/L^*$. Therefore any function of k will be considered as L^*-periodic, i.e. satisfying periodic boundary conditions on ∂B.

The velocity $v(k) = \nabla_k \varepsilon(k)$ is given in terms of the prescribed energy band diagram $\varepsilon(k)$. We assume ε to be an even function of k which can be interpreted as a reflection symmetry of the crystal.

The right hand side of (2.1) describes scattering effects such as scattering of electrons with lattice defects and short range electron-electron interaction. The operator Q_0 is obtained by neglecting the energies gained or lost by an electron during collisions with lattice defects. The necessary corrections and electron-electron scattering are contained in Q_1. The elastic scattering operator Q_0 is given by

$$Q_0(f)(k) = \int_B \Phi(x,k,k')\delta(\varepsilon' - \varepsilon)(f' - f)dk' \,, \tag{2.2}$$

where the prime denotes evaluation at k', δ is the one-dimensional delta measure and $\Phi(x,k,k')$ is the sum of the scattering cross sections for all lattice defects taken into account. As in [2] we write integrals over the Brillouin zone as

$$\int_B \psi(k)dk = \int_{-\infty}^{\infty} \left(\int_{S_\varepsilon} \psi(k) dN_\varepsilon(k) \right) d\varepsilon \,,$$

with $S_\varepsilon = \{k \in B : \ \varepsilon(k) = \varepsilon\}$ and $dN_\varepsilon(k) = dS_\varepsilon(k)/|\nabla\varepsilon(k)|$, where $dS_\varepsilon(k)$ denotes the Euclidean surface element on S_ε. The density of states is then given by

$$N(\varepsilon) = \int_{S_\varepsilon} dN_\varepsilon(k) \,.$$

With this notation the scattering operator (2.2) gets the form

$$Q_0(f) = \int_{S_\varepsilon} \Phi(x,k,k')(f' - f)dN_\varepsilon(k') \,. \tag{2.3}$$

In the appendix we shall show that computations become considerably simpler, when the relaxation time model $\Phi(x,k,k') = \frac{1}{\tau(x,\varepsilon)N(\varepsilon)}$ is used:

$$Q_0(f) = \frac{1}{\tau}\left(\frac{1}{N} \int_{S_\varepsilon} f' dN_\varepsilon(k') - f \right) \,. \tag{2.4}$$

For silicon the assumption $\Phi(x,k,k') = \Phi_0$ and, thus, $\tau = (\Phi_0 N)^{-1}$ is reasonably justified.

The splitting of the collision operators in an elastic part and an inelastic correction has also been used in [7] and [2]. The precise form of Q_1 will not be important for the following and therefore no explicit expression will be given.

The dimensionless parameter $\alpha > 0$ measures the relative strength of the inelastic corrections and the electron-electron scattering compared to the elastic approximation. Our main assumption is smallness of α. For a discussion of the validity of this assumption see [2]. The scaled Boltzmann equation (2.1) then gets its form by choosing appropriate scales for time, length and energy.

In this section we shall be concerned with an asymptotic expansion in powers of α of the solution of (2.1) away from boundaries. The limiting equation for the time dependent, multi-dimensional case can be found in [2]. A rigorous justification is given in [14]. Here we are interested in carrying the expansion one step further in order to achieve $O(\alpha^2)$-accuracy.

For the following we shall need some assumptions on the collision operators. Let the scattering cross section Φ satisfy

$$0 < \underline{\Phi} \leq \Phi(x,k,k') \leq \overline{\Phi} < \infty \,,$$
$$\Phi(x,k,k') = \Phi(x,k',k) = \Phi(x,-k,-k') \,, \qquad (2.5)$$

for all k, k' such that $\varepsilon(k) = \varepsilon(k')$. Note that for the relaxation time model (2.4) these assumptions reduce to a positivity and boundedness assumption on the relaxation time τ.

The last condition in (2.5) implies that the sets of even and of odd functions of k are, respectively, invariant under the action of Q_0. This last property we also assume for Q_1. Further important properties of Q_0 can be shown. For a proof of the following lemma see [2].

Lemma 2.1 *Assume (2.5) holds. Then*

(i) $-Q_0$ *is a bounded, symmetric, nonnegative operator on* $L^2(B;\, w(\varepsilon(k))dk)$ *for every positive weight function* w. $Q_0(\psi f) = \psi Q_0(f)$ *for every* $\psi = \psi(\varepsilon(k))$.

(ii) $Ker\, Q_0 = \{f : \ \exists g \ \text{with} \ f(k) = g(\varepsilon(k))\}$.

(iii) $Pf = \frac{1}{N(\varepsilon)} \int_{S_\varepsilon} f dN_\varepsilon(k)$ *defines the orthogonal projection onto* $Ker\, Q_0$.

(iv) $R(Q_0) = (Ker\, Q_0)^\perp = \{f : \ Pf = 0\}$.

(v) *For every* $g \in R(Q_0)$ *the equation* $Q_0(f) = g$ *has a unique solution* $f \in (Ker\, Q_0)^\perp$. *If* g *is even (odd) then* f *is even (odd).*

(vi) $-Q_0$ *is coercive on* $R(Q_0)$*:*

$$-\int_{S_\varepsilon} Q_0(f) f dN_\varepsilon \geq \underline{\Phi} N \int_{S_\varepsilon} (f - Pf)^2 dN_\varepsilon \,.$$

Now we can carry out the Hilbert expansion. The ansatz

$$f = f_0 + \alpha f_1 + \alpha^2 f_2 + \ldots$$

and comparison of coefficients of α^{-2} in (2.1) gives

$$Q_0(f_0) = 0 \qquad \Longrightarrow \qquad f_0(x,k,t) = F_0(x, \varepsilon(k), t)$$

with an arbitrary function F_0 by Lemma 2.1, (ii). At the order of α^{-1} we get

$$v \cdot \widetilde{\nabla}_x F_0 = Q_0(f_1) \qquad \text{with } \widetilde{\nabla}_x F = \nabla_x F + \nabla_x V \frac{\partial F}{\partial \varepsilon} \,. \tag{2.6}$$

We claim that this equation can be solved for f_1. In fact the inhomogeneity is an odd function of k since $\widetilde{\nabla}_x F_0$ is even depending on k only through $\varepsilon(k)$, and the components of $v(k)$ are odd as derivatives of an even function. By Lemma 2.1, (iv) we have $v \cdot \widetilde{\nabla}_x F_0 \in R(Q_0)$. The solution of (2.6) can be written as

$$f_1(x,k) = -\lambda(x,k) \cdot \widetilde{\nabla}_x F_0(x, \varepsilon(k)) + F_1(x, \varepsilon(k)) \,, \tag{2.7}$$

with an arbitrary function F_1 and the unique solution $\lambda \in (Ker\, Q_0)^\perp$ of $Q_0(\lambda) = -v$ (This equation has to be understood componentwise). Note that by Lemma 2.1, (v), the components of $\lambda(x,k)$ are odd functions of k. For the relaxation time model (2.4), $\lambda = \tau v$ holds.

The coefficients of α^0 in (2.1) give

$$\begin{aligned} &\frac{\partial F_0}{\partial t} - \nabla_x \cdot (v \otimes \lambda \widetilde{\nabla}_x F_0) - \nabla_x V \cdot \nabla_k (\lambda \cdot \widetilde{\nabla}_x F_0) + v \cdot \widetilde{\nabla}_x F_1 \\ &= Q_0(f_2) + Q_1(F_0) \,. \end{aligned} \tag{2.8}$$

The solvability condition for this equation for f_2 is an equation for F_0. We integrate (2.8) over surfaces of equal energy and obtain

$$N \frac{\partial F_0}{\partial t} - \widetilde{\nabla}_x \cdot (D \widetilde{\nabla}_x F_0) = \overline{Q_1}(F_0) \,, \tag{2.9}$$

with $\overline{Q_1}(F_0) = \int_{S_\varepsilon} Q_1(F_0) dN_\varepsilon(k)$ and the diffusivity matrix $D(x,\varepsilon) = \int_{S_\varepsilon} \lambda \otimes v \, dN_\varepsilon(k)$ whose positive definitness has been proven in [2]. For the relaxation time model this result is easy to obtain since the diffusivity matrix is then given by $D = \tau \int_{S_\varepsilon} v \otimes v \, dN_\varepsilon(k)$. An explicit formula is obtained when a constant elastic collision cross section $\Phi = \Phi_0$ and the parabolic band assumption $\varepsilon = |k|^2/2$ is used: Then the diffusivity matrix can be replaced by the scalar diffusivity $D = 2\varepsilon/(3\Phi_0)$.

The computations leading to (2.9) are straightforward except the integration of $\nabla_k(\lambda \cdot \widetilde{\nabla}_x F_0)$ where the following argument is used: For an arbitrary $\psi = \psi(\varepsilon)$ we have

$$\int_{-\infty}^{\infty} \psi \int_{S_\varepsilon} \nabla_k(\lambda \cdot \widetilde{\nabla}_x F_0) dN_\varepsilon(k) d\varepsilon = - \int_B \frac{d\psi}{d\varepsilon} v(\lambda \cdot \widetilde{\nabla}_x F_0) dk$$
$$= - \int_{-\infty}^{\infty} \frac{d\psi}{d\varepsilon} D \widetilde{\nabla}_x F_0 d\varepsilon = \int_{-\infty}^{\infty} \psi \frac{\partial}{\partial \varepsilon} (D \widetilde{\nabla}_x F_0) d\varepsilon \,,$$

and, thus, $\int_{S_\varepsilon} \nabla_k(\lambda \cdot \widetilde{\nabla}_x F_0) dN_\varepsilon(k) = \frac{\partial}{\partial \varepsilon}(D\widetilde{\nabla}_x F_0)$. The SHE-equation (2.9) can be seen as the limiting equation for (2.1) as $\alpha \to 0$ [2].

So far our computations have been only a specialization of earlier work. Now we want to improve the accuracy by computing f_1, which means that we need an equation for F_1. This is achieved by comparing coefficients of α^1 in (2.1):

$$\frac{\partial f_1}{\partial t} + v \cdot \nabla_x f_2 + \nabla_x V \cdot \nabla_k f_2 = Q_0(f_3) + L_1[F_0](f_1) \,, \qquad (2.10)$$

where $L_1[F_0]$ is the Frechet derivative of Q_1 at F_0. For the following it is important that $L_1[F_0]$ inherits from Q_1 the property that it maps the set of even (odd) functions into itself. Returning to the equation (2.8) for f_2 we note that all the inhomogeneities except $v \cdot \widetilde{\nabla}_x F_1$ (which is odd) are even functions of k. Therefore f_2 can be written as $f_2 = f_{2,even} - \lambda \cdot \widetilde{\nabla}_x F_1$ where $f_{2,even}$ is even. Using this and the representation (2.7) for f_1, the solvability condition for (2.10) becomes

$$N \frac{\partial F_1}{\partial t} - \widetilde{\nabla}_x \cdot (D \widetilde{\nabla}_x F_1) = \overline{L_1}[F_0](F_1) \,, \qquad (2.11)$$

where $\overline{L_1}[F_0]$ is the linearization of $\overline{Q_1}$. Since (2.11) is the linearization of (2.9) the function $F_0 + \alpha F_1$ satisfies (2.9) up to an $O(\alpha^2)$-error. An interpretation of this fact is that no accuracy is gained by using the additional equation (2.11). An approximation

$$f_{as} = F_{as} - \alpha\lambda \cdot \widetilde{\nabla}_x F_{as} \tag{2.12}$$

can be accurate up to $O(\alpha^2)$ if F_{as} solves (2.9) and satisfies appropriate boundary conditions.

3 Analysis of Boundary Layers

Now we shall analyse the situation when inflow boundary conditions are prescribed along $\partial\Omega$:

$$f = f_B\,, \quad \text{for } x \in \partial\Omega,\ v\cdot\nu > 0\,,$$

where ν denotes the inward unit normal along $\partial\Omega$. Obviously, an approximation for f of the form (2.12) cannot satisfy these conditions in general. Even for $f_B = f_B(\varepsilon(k))$ the boundary conditions could only be satisfied up to $O(\alpha)$ by (2.12). Therefore boundary layer corrections are necessary. We introduce local coordinates y in a neighbourhood of $\partial\Omega$ by $x = x_B(y') + y_1\nu(y')$, where x_B is a parametrization of the boundary with parameters $y' = (y_2, y_3)$. The rescaled distance from the boundary $\xi = y_1/\alpha$ is a boundary layer variable. We make the ansatz

$$f_{as} = F_0 + \hat{f}_0 - F_0(y_1 = 0) + \alpha(F_1 - \lambda\cdot\widetilde{\nabla}_x F_0 + \hat{f}_1 - F_1(y_1 = 0))\,, \tag{3.1}$$

with $F_i = F_i(x, \varepsilon(k), t)$ as in the preceding section, $\hat{f}_i = \hat{f}_i(\xi, y', k, t)$ and $\hat{f}_i(\xi = \infty) = F_i(y_1 = 0)$. Equating coefficients of α^{-2} in the Boltzmann equation (2.1) and coefficients of α^0 in the boundary conditions, we obtain the Milne problem

$$\begin{aligned} v\cdot\nu\frac{\partial \hat{f}_0}{\partial\xi} &= Q_0(\hat{f}_0)\,, \quad \xi > 0\,,\\ \hat{f}_0(\xi = 0, v\cdot\nu > 0) &= f_B\,. \end{aligned} \tag{3.2}$$

We assume (as can be proven by extending the methods of [1]) that (3.2) has a unique bounded solution and that, as $\xi \to \infty$, $\hat{f}_0$ tends to an element of $Ker\,Q_0$ depending on the inflow data:

$$F_0(y_1 = 0) = \hat{f}_0(\xi = \infty) = \Lambda[f_B]\,. \tag{3.3}$$

This is the leading order boundary condition for the solution of (2.9). A standard result for Milne problems and a straightforward consequence of the above assumption is vanishing flux:

$$\int_{S_\varepsilon} v \cdot \nu \hat{f}_0 dN_\varepsilon = 0\,. \tag{3.4}$$

The problem for the $O(\alpha)$-boundary layer term is

$$v \cdot \nu \frac{\partial \hat{f}_1}{\partial \xi} + \left[v \cdot \left(\frac{\partial y'}{\partial x}(y_1 = 0) \nabla_{y'} \hat{f}_0 \right) + \nabla_x V(y_1 = 0) \cdot \nabla_k \hat{f}_0 \right]_\infty^\xi = Q_0(\hat{f}_1)\,,$$
$$\hat{f}_1(\xi = 0, v \cdot \nu > 0) = \lambda(y_1 = 0) \cdot \widetilde{\nabla}_x F_0(y_1 = 0)\,, \tag{3.5}$$

where we again assume existence and uniqueness of a bounded solution. Here and in the following we use the abbreviation $g_\infty^\xi = g(\xi) - g(\infty)$ for functions of ξ. The solution of (3.5) can be split in the form

$$\hat{f}_1 = \chi \cdot \widetilde{\nabla}_x F_0(y_1 = 0) + \tilde{\chi} \tag{3.6}$$

where χ solves a problem of the form (3.2) with f_B replaced by $\lambda(y_1 = 0)$ and $\tilde{\chi}$ solves (3.5) with vanishing inflow data. We finally obtain

$$F_1(y_1 = 0) = \hat{f}_1(\xi = \infty) = \Lambda[\lambda] \cdot \widetilde{\nabla}_x F_0(x = 0) + \tilde{\chi}_\infty\,, \tag{3.7}$$

with $\tilde{\chi}_\infty = \tilde{\chi}(\xi = \infty)$. This is the boundary condition for (2.11).

Now we return to the comments at the end of the preceding section. An $O(\alpha^2)$-approximation F_{as} of $F_0 + \alpha F_1$ satisfies the boundary condition

$$F_{as} - \alpha \Lambda[\lambda] \cdot \widetilde{\nabla}_x F_{as} = \Lambda[f_B] + \alpha \tilde{\chi}_\infty\,, \tag{3.8}$$

at $y_1 = 0$. If this boundary condition is used together with the SHE-model (2.9), then an $O(\alpha^2)$-approximation of the distribution function away from boundary layers is given by (2.12).

For inflow data $f_B = f_B(\varepsilon) \in Ker\, Q_0$, $\hat{f}_0 = f_B$ holds and therefore $\Lambda[f_B] = f_B$. Thus, the inhomogeneity in the problem for $\tilde{\chi}$ vanishes implying $\tilde{\chi} = 0$. Then we still need the solution of a Milne problem for the formulation of the above boundary condition. The vector $\Lambda[\lambda](\varepsilon)$ is a generalization of the extrapolation length [1].

We conclude this section with a few remarks about the solution of the Milne problems (3.2) and (3.5). The first observation is that there is no coupling between different values of the energy. Thus, the Milne problem can be solved by considering one surface of constant energy at a time. In other words, the values of $\Lambda[f_B]$, $\Lambda[\lambda]$ and $\tilde{\chi}(\xi=\infty)$ at different ε can be computed independently from each other.

The computation of the extrapolation length vector becomes particularly simple, when the relaxation time model (2.4) and a spherically symmetric band diagram $\varepsilon = \varepsilon(|k|^2/2)$ are used. We assume $\varepsilon(0) = 0$ and $\varepsilon' > 0$. This allows us to invert: $|k| = |k|(\varepsilon)$. Typically, a model of this kind is used as an approximation of the band diagram close to a minimum. To be consistent, we replace the Brillouin zone B by $I\!R^3$ in this case. Typical models have the form $\varepsilon(1+\varepsilon/\varepsilon_{ref}) = |k|^2/2$, including the parabolic band approximation for $\varepsilon_{ref} = \infty$.

With the notation

$$\begin{aligned} k &= |k| s\nu + k^\perp\,, \qquad s = \frac{k\cdot\nu}{|k|} \in [-1,1] \\ K(\varepsilon) &= |k|\tau\varepsilon'\,, \end{aligned}$$

the Milne problem for the determination of the extrapolation length can be written as

$$\begin{aligned} Ks\frac{\partial\chi}{\partial\xi} &= \frac{1}{N}\int_{S_\varepsilon} \chi dN_\varepsilon(k) - \chi\,, \quad \xi > 0\,, \\ \chi(\xi=0) &= K\frac{k}{|k|}\,, \quad s > 0\,. \end{aligned}$$

When the solution is split into its component parallel to ν and an orthogonal part: $\chi = \chi_\nu \nu + \chi^\perp$, it is easily checked that

$$\chi^\perp = \begin{cases} K\frac{k^\perp}{|k|}\exp\left(-\frac{\xi}{Ks}\right)\,, & s > 0\,, \\ 0\,, & s < 0\,, \end{cases}$$

holds and that $\hat{\chi} = \chi_\nu/K$ only depends on $\eta = \xi/K$ and s and solves the generic problem

$$\begin{aligned} s\frac{\partial\hat{\chi}}{\partial\eta} &= \frac{1}{2}\int_{-1}^{1}\hat{\chi}ds - \hat{\chi}\,, \quad \eta > 0\,, \\ \hat{\chi}(\eta=0) &= s\,, \quad s > 0\,. \end{aligned}$$

This is a classical problem from radiative transfer [5]. Results about existence and uniqueness of the solution and its convergence as $\eta \to \infty$ can be found in [1]. Numerical computations [5] give

$$\hat{\chi}(\eta = \infty) = \Lambda_c \approx 0.7104 \,. \tag{3.9}$$

The extrapolation length vector in the boundary conditions (3.8) is, thus, parallel to ν and given by

$$\Lambda[\lambda] = \chi(\xi = \infty) = K(\varepsilon)\Lambda_c \nu \,.$$

This means that for equilibrium inflow data $f_B = f_B(\varepsilon)$ all the terms in the high order boundary conditions for the SHE-model are given explicitely.

Since $\Lambda[\lambda]$ is a positive multiple of ν, (3.8) is a Robin boundary condition and well posedness of the boundary value problem for the SHE-model can be expected. In the general case, a necessary condition for wellposedness is that $\Lambda[\lambda]$ points into Ω. This is proved in the following.

Lemma 3.1 *Assume problem (3.2) with f_B replaced by λ has a continuous solution χ converging to an element of the kernel of Q_0 as $\xi \to \infty$. Then $\Lambda[\lambda] \cdot \nu = \chi(\xi = \infty) \cdot \nu > 0$ holds.*

Comment: The assumptions of the lemma can be proved to hold by a straightforward extension of the methods of [1].

Proof: $\chi_\nu = \chi \cdot \nu$ solves the scalar Milne problem

$$v \cdot \nu \frac{\partial \chi_\nu}{\partial \xi} = Q_0(\chi_\nu) \,, \tag{3.10}$$

$$\chi_\nu(\xi = 0, v \cdot \nu > 0) = \lambda \cdot \nu \,. \tag{3.11}$$

Integration of (3.10) over surfaces of constant energy and using the boundedness of χ_ν gives the zero flux property

$$\int_{S_\varepsilon} (v \cdot \nu)\chi_\nu dN_\varepsilon = 0 \,.$$

Now we multiply (3.10) by $\lambda \cdot \nu$ and integrate again:

$$\frac{\partial}{\partial \xi} \int_{S_\varepsilon} (\lambda \cdot \nu)(v \cdot \nu)\chi_\nu dN_\varepsilon = \int_{S_\varepsilon} (\lambda \cdot \nu) Q_0(\chi_\nu) dN_\varepsilon = \int_{S_\varepsilon} (v \cdot \nu)\chi_\nu dN_\varepsilon = 0 \,.$$

Integration with respect to ξ gives

$$\Lambda[\lambda] \cdot \nu(\nu^{tr} D\nu) = \int_{S_\varepsilon} (\lambda \cdot \nu)(v \cdot \nu)\chi_\nu(\xi = 0) dN_\varepsilon \,. \tag{3.12}$$

By the positive definiteness of the diffusion matrix D it remains to prove that the right hand side of the above equation is positive.

Multiplication of (3.10) by χ_ν and integration gives

$$\int_{S_\varepsilon^-} (-v \cdot \nu)\chi_\nu(\xi = 0)^2 dN_\varepsilon = A - 2B \tag{3.13}$$

with

$$A = \int_{S_\varepsilon^+} (v \cdot \nu)(\lambda \cdot \nu)^2 dN_\varepsilon \,, \qquad B = -\int_0^\infty \int_{S_\varepsilon} Q_0(\chi_\nu)\chi_\nu dN_\varepsilon d\xi \,,$$

where the surface S_ε has been split into two parts $S_\varepsilon^+ = \{k \in B : \varepsilon(k) = \varepsilon,\ v(k) \cdot \nu > 0\}$ and $S_\varepsilon^- = \{k \in B : \varepsilon(k) = \varepsilon,\ v(k) \cdot \nu < 0\}$.

Now this splitting is carried out in the right hand side of (3.12) and the integral over S_ε^- estimated by the Cauchy-Schwarz inequality:

$$\int_{S_\varepsilon} (\lambda \cdot \nu)(v \cdot \nu)\chi_\nu(\xi = 0) dN_\varepsilon$$
$$\geq A - \left(\int_{S_\varepsilon^-} (-v \cdot \nu)(\lambda \cdot \nu)^2 dN_\varepsilon \int_{S_\varepsilon^-} (-v \cdot \nu)\chi_\nu(\xi = 0)^2 dN_\varepsilon \right)^{1/2} .$$

The first term under the square root is equal to A because of the oddness of v and λ (Lemma 2.1 (v)) and the symmetry of the Brillouin zone. For the second term under the square root we use (3.13):

$$\int_{S_\varepsilon} (\lambda \cdot \nu)(v \cdot \nu)\chi_\nu(\xi = 0) dN_\varepsilon \geq A - \sqrt{A(A - 2B)} \geq B > 0 \,,$$

where the last inequality follows from the coercivity of Q_0 (Lemma 2.1 (vi)) and the observation that the boundary condition (3.11) prevents χ_ν from being an element of the kernel of Q_0. $\blacksquare$

4 Application to the Energy Transport and the Drift-Diffusion Model

If other scattering mechanisms besides elastic scattering dominate in the Boltzmann equation, the complexity of the transport model (2.9) can be reduced further. We shall consider two examples: First, electron-electron interaction will be assumed to be the dominant part of the collision term $\overline{Q_1}(F_0)$. Then, the case of a dominating role of the inelastic corrections according to lattice defect scattering will be treated. Without giving full details of the derivation (which can be found in [2]), we just follow a simple recipe: All we need to know is the null set and the collision invariants of the dominating scattering terms. Then the general element of the null set is used for an ansatz for the distribution function, and the free parameters are determined from the conservation laws corresponding to the collision invariants. Here this procedure is applied to the SHE-model. A direct derivation from the Boltzmann equation (resulting in different transport coefficients) is also possible (see [3], [9]). The advantage of passing through the SHE-model will become apparent below: When the relaxation time model for the elastic collision operator is used, then explicit formulas for the transport coefficients will be obtained.

The elements of the null set of the electron-electron collision operator also lying in $Ker\, Q_0$ have the form

$$\mathcal{F}_{\mu,T}(\varepsilon) = \frac{1}{\eta + e^{(\varepsilon-\mu)/T}} \,,$$

with arbitrary $\mu, T \in I\!R$. This is the Fermi-Dirac distribution with chemical potential μ and temperature T. The dimensionless parameter η results from scaling [2] and measures the degeneracy of the electron gas. In the nondegenerate limit $\eta \to 0$, the Fermi-Dirac distribution tends to the Maxwellian $e^{(\mu-\varepsilon)/T}$. The collision invariants corresponding to the two degrees of freedom are 1 and ε.

Now we apply the procedure described above. We make the ansatz

$$F_{as}(x,\varepsilon,t) = \mathcal{F}_{\mu(x,t),T(x,t)}(\varepsilon) \,,$$

define the macroscopic density and energy by

$$n(\mu,T) = \int_{-\infty}^{\infty} \mathcal{F}_{\mu,T}(\varepsilon) N(\varepsilon) d\varepsilon \,, \qquad n\mathcal{E}(\mu,T) = \int_{-\infty}^{\infty} \mathcal{F}_{\mu,T}(\varepsilon)\varepsilon N(\varepsilon) d\varepsilon \,,$$

multiply (2.9) by 1 and, respectively, ε and integrate with respect to ε. A preliminary step in this computation is

$$\widetilde{\nabla}_x \mathcal{F}_{\mu,T} = \mathcal{F}_{\mu,T}(1-\eta\mathcal{F}_{\mu,T}) \left[\nabla_x \left(\frac{\mu}{T}\right) - \frac{1}{T}\nabla_x V - \varepsilon \nabla_x \left(\frac{1}{T}\right)\right] .$$

The resulting relations are the charge conservation and energy conservation equations

$$\begin{aligned}
&\frac{\partial n}{\partial t} - \nabla_x \cdot \left[D_{11}\left(\nabla_x\left(\frac{\mu}{T}\right) - \frac{1}{T}\nabla_x V\right) - D_{12}\nabla_x\left(\frac{1}{T}\right)\right] = 0\,,\\
&\frac{\partial n\mathcal{E}}{\partial t} - \nabla_x \cdot \left[D_{21}\left(\nabla_x\left(\frac{\mu}{T}\right) - \frac{1}{T}\nabla_x V\right) - D_{22}\nabla_x\left(\frac{1}{T}\right)\right]\\
&\qquad +\nabla_x V \left[D_{11}\left(\nabla_x\left(\frac{\mu}{T}\right) - \frac{1}{T}\nabla_x V\right) - D_{12}\nabla_x\left(\frac{1}{T}\right)\right] = Q_{n\mathcal{E}}\,, \qquad (4.1)
\end{aligned}$$

with

$$\begin{aligned}
D_{ij}(\mu,T) &= \int_{-\infty}^{\infty} \varepsilon^{i+j-2} D\mathcal{F}_{\mu,T}(1-\eta\mathcal{F}_{\mu,T})d\varepsilon\,, \qquad (4.2)\\
Q_{n\mathcal{E}}(\mu,T) &= \int_{-\infty}^{\infty} \varepsilon\overline{Q_1}(\mathcal{F}_{\mu,T})d\varepsilon\,.
\end{aligned}$$

Here we have assumed charge conservation, i.e. the integral of $\overline{Q_1}$ with respect to ε vanishes. This means that we do not consider interactions with other energy bands or other valleys of the same energy band.

Equations (4.1) are a version of the ET-model which is well established in the literature. An account of different approaches to the computation of the transport coefficients can be found in [3].

$Q_{n\mathcal{E}}$ can be interpreted as an energy relaxation term [2]. The diffusion matrix (D_{ij}) is symmetric and positive definite [2]. If the relaxation time model (2.4) is used, then the diffusion matrix is given by

$$D_{ij}(\mu,T) = \int_B \tau\varepsilon^{i+j-2} v\otimes v\mathcal{F}_{\mu,T}(1-\eta\mathcal{F}_{\mu,T})dk\,.$$

This explicit formula is the main motivation to derive the ET-model via the SHE-model. It simplifies even further when the assumptions of a constant elastic scattering cross section $\Phi = \Phi_0$, of a parabolic band diagram $\varepsilon =$

$|k|^2/2$ and nondegeneracy $\eta \to 0$ are used [2]. By isotropy the submatrices D_{ij} can be reduced to scalars and we have:

$$(D_{ij}) = \begin{pmatrix} 1 & 2T \\ 2T & 6T^2 \end{pmatrix} \sqrt{\frac{T}{2}} \frac{n}{3\pi^{3/2}\Phi_0} \,. \tag{4.3}$$

The term $Q_{n\mathcal{E}}$ results from the inelastic corrections corresponding to the interaction of electrons with lattice defects. As mentioned above it is an energy relaxation term with the tendency to drive the electron temperature T towards the (given, constant) lattice temperature T_L. For sufficiently long time scales and length scales, $Q_{n\mathcal{E}}$ is the dominating term in (4.1). In this case a further simplification amounts to replacing the energy balance equation in (4.1) by the relation $T = T_L$. Then the model reduces to the charge conservation equation

$$\frac{\partial n(\mu, T_L)}{\partial t} - \nabla_x \cdot \left[\frac{D_{11}(\mu, T_L)}{T_L} \nabla_x (\mu - V) \right] = 0 \tag{4.4}$$

for the determination of μ. Models of this form have been derived from the Boltzmann equation in [9] and [13] using simplified collision models driving the distribution function towards a Fermi-Dirac distribution with $T = T_L$. In [13] an explicit formula for the diffusivity has been derived. It differs from (4.2) which can be easily explained by the differences in the collision model. We conclude our discussion of transport models by the observation that in the nondegenerate limit $\eta \to 0$ equation (4.4) reduces to the classical drift-diffusion model for semiconductors (see, e.g., [11]), and (4.4) can be considered as a generalized drift-diffusion (DD-) model including degeneracy effects.

The derivation of the transport models (4.1) and (4.4) for bulk material from the SHE-model (2.9) can be based on formal asymptotic expansions which in turn can be rigorously justified. For the derivation of the corresponding boundary conditions from (3.8) we shall follow a more heuristic approach based on mimicking the procedure used in the bulk. For the ET-model we look for boundary conditions for the density and the energy. These can be obtained from (3.8) by substituting the Fermi-Dirac distribution for F_{as}, multiplying by N and, respectively, by εN and integrating with respect to ε:

$$n - \alpha\Lambda_{11} \cdot \left(\nabla_x \left(\frac{\mu}{T} \right) - \frac{1}{T} \nabla_x V \right) + \alpha\Lambda_{12} \cdot \nabla_x \left(\frac{1}{T} \right)$$

$$= \Lambda_0[f_B] + \alpha\tilde{\chi}_{\infty 0}\,,$$

$$n\mathcal{E} - \alpha\Lambda_{21}\cdot\left(\nabla_x\left(\frac{\mu}{T}\right) - \frac{1}{T}\nabla_x V\right) + \alpha\Lambda_{22}\cdot\nabla_x\left(\frac{1}{T}\right)$$

$$= \Lambda_1[f_B] + \alpha\tilde{\chi}_{\infty 1}\,, \tag{4.5}$$

for $x = 0$, with

$$\begin{aligned} \Lambda_j[f_B] &= \int_{-\infty}^{\infty} \Lambda[f_B](\varepsilon)\varepsilon^j N(\varepsilon)d\varepsilon\,, \\ \tilde{\chi}_{\infty j} &= \int_{-\infty}^{\infty} \tilde{\chi}_\infty(\varepsilon)\varepsilon^j N(\varepsilon)d\varepsilon\,, \end{aligned}$$

and the matrix of extrapolation length vectors

$$\Lambda_{ij}(\mu,T) = \int_{-\infty}^{\infty} \varepsilon^{i+j-2}\Lambda[\lambda]\mathcal{F}_{\mu,T}(1-\eta\mathcal{F}_{\mu,T})N(\varepsilon)d\varepsilon\,.$$

When the ET-model is used together with the boundary conditions (4.5), it can be expected that certain kinetic effects near the boundaries are taken into account.

The reduction to the DD-model is again simple. The first equation in (4.5) with $T = T_L$ is a boundary condition for (4.4). It has already been derived for the nondegenerate case in [17] directly from the Boltzmann equation. The extrapolation length derived there differs from ours, since it is determined from the solution of a Milne problem for a different collision operator.

Finally, we keep track of the simplifications which can be obtained by using the relaxation time model and a spherically symmetric band diagram. In this case $N(\varepsilon) = 4\pi|k|/\varepsilon'$ holds, and we recall the result $\Lambda[\lambda] = \tau|k|\varepsilon'\Lambda_c\nu$ from the preceding section. The extrapolation matrix is therefore given by

$$\Lambda_{ij}(\mu,T) = 4\pi\Lambda_c\nu\int_0^{\infty}\tau|k|^2\varepsilon^{i+j-2}\mathcal{F}_{\mu,T}(1-\eta\mathcal{F}_{\mu,T})d\varepsilon\,.$$

With the parabolic band assumption $\varepsilon = |k|^2/2$, the nondegenerate limit $\eta \to 0$ and a constant elastic scattering cross section $\Phi = \Phi_0$, the extrapolation matrix becomes

$$(\Lambda_{ij}) = \begin{pmatrix} 1 & 3T/2 \\ 3T/2 & 15T^2/4 \end{pmatrix}\frac{\Lambda_c n}{4\pi\Phi_0}\nu\,.$$

A comparison with the matrix of diffusivities (4.3) shows that the two matrices are in general not multiples of each other, meaning that it is not the electron flux and the energy flux appearing in the boundary conditions (4.5).

5 Fluid-Kinetic Coupling

In applications it occurs frequently that regions, where a macroscopic model is a sufficiently accurate description of the flow, coexist with regions where kinetic effects are important. In these cases, a domain decomposition approach to the numerical simulation of the flow seems natural. A macroscopic model can be used whereever it is accurate enough, and a kinetic model is used only in the regions with significant kinetic effects. This raises the question of finding appropriate coupling conditions at the fluid-kinetic interfaces. For coupling between the nondegenerate drift-diffusion model and the Boltzmann equation, a strategy based on a boundary layer analysis has been developped recently by Klar [10]. In this section, his ideas are adapted to the SHE-model (2.9), the ET-model (4.1), and the DD-model (4.4).

When the solution of the kinetic problem is close enough to equilibrium at the interface, then the coupling problem is not very critical and can be handled by standard approaches such as a straightforward adaption of the Marshak conditions used in radiative transfer (see, e.g., [4]). For a nonequilibrium situation at the interface, however, it has been pointed out in [10] and shown by numerical experiments that a more refined approach is necessary. The boundary layer analysis of the preceding section can be used.

We consider a situation where the Boltzmann equation is solved in the complement of $\Omega \subset I\!R^3$ and the SHE-model, the ET-model, or the DD-model for $x \in \Omega$. For given outflow data $f_{out} = f(x \in \partial\Omega, v \cdot \nu > 0)$ from the kinetic region, the two preceding sections tell us how to compute boundary conditions for the macroscopic models. After solving the problem for $x \in \Omega$, one step of an iteration procedure (called Schwarz iteration in the domain decomposition literature) is completed by solving the Boltzmann equation outside of Ω. Therefore we need to discuss the construction of inflow data $f_{in} = f(x \in \partial\Omega, v \cdot \nu < 0)$ from the outflow data and from the macroscopic solution in Ω.

We start by rewriting some results of section 3. With the notation $F_{as} = F_0 + \alpha F_1$, the representation (3.1) shows that the approximation

$$f_{as} = F_{as} - F_{as}(x \in \partial\Omega) - \alpha\lambda \cdot \widetilde{\nabla}_x F_{as} + \hat{f}_0 + \alpha \hat{f}_1$$

of the distribution function in the boundary layer is accurate up to $O(\alpha^2)$. Also, the first order boundary layer term can be decomposed as in (3.6)

$$\hat{f}_1 = \chi \cdot \widetilde{\nabla}_x F_{as} + \tilde{\chi}\,,$$

where χ solves a Milne problem with inflow data λ, and $\tilde{\chi}$ solves a Milne problem with homogeneous inflow data and an inhomogeneous transport equation where the inhomogeneity depends on $\hat{f}_0$. In the resulting formula for f_{as}, the terms $\hat{f}_0$ and $\tilde{\chi}$ depend on the boundary data f_B, and the remaining terms are given in terms of F_{as}. Now the inflow data for the kinetic region are determined by replacing f_B by the outflow data and evaluating $f_{as}(x \in \partial\Omega, v \cdot \nu < 0)$. We obtain

$$f_{in} = \mathcal{A}[f_{out}] + \alpha(\mathcal{A}[\lambda] - \lambda) \cdot \widetilde{\nabla}_x F_{as} + \alpha\tilde{\chi}(\xi = 0, v \cdot \nu < 0)\,, \tag{5.1}$$

where $\mathcal{A}$ is the Albedo operator for the Milne problem, mapping the incoming part of the distribution function to the outgoing part. A peculiarity of this boundary condition for the kinetic problem becomes apparent when the flux into the boundary from the kinetic region is computed:

$$\begin{aligned}
\nu \cdot \int_B v f\, dk \;\; &= \;\; \int_0^\infty \left[\int_{S_\varepsilon^+} (v \cdot \nu) f_{out} dN_\varepsilon + \int_{S_\varepsilon^-} (v \cdot \nu)\mathcal{A}[f_{out}] dN_\varepsilon\right] d\varepsilon \\
&\quad + \alpha \int_0^\infty \left[\int_{S_\varepsilon^-} (v \cdot \nu)(\mathcal{A}[\lambda] - \lambda) dN_\varepsilon\right] \cdot \widetilde{\nabla}_x F_{as} d\varepsilon \\
&\quad + \alpha \int_0^\infty \int_{S_\varepsilon^-} (v \cdot \nu)\tilde{\chi}(\xi = 0) dN_\varepsilon d\varepsilon\,.
\end{aligned}$$

With the property

$$\int_{S_\varepsilon^+} (v \cdot \nu) f_B dN_\varepsilon + \int_{S_\varepsilon^-} (v \cdot \nu)\mathcal{A}[f_B] dN_\varepsilon = 0$$

of the Albedo operator, the right hand side can be written as

$$-\alpha\nu \cdot \int_0^\infty D\widetilde{\nabla}_x F_{as} d\varepsilon + \alpha \int_0^\infty \int_{S_\varepsilon^-} (v \cdot \nu)\tilde{\chi}(\xi = 0) dN_\varepsilon d\varepsilon\,.$$

The first term is the flux out of the boundary into the macroscopic region. The second term does not vanish in general. This means that the condition (5.1) violates local flux conservation. The integral of this term along the boundary $\partial\Omega$, however, vanishes. Globally, charge is conserved. A physical interpretation is by electrons entering Ω, then remaining within the boundary layer before leaving Ω again through a different point on the boundary. To prove our claim that charge is conserved globally, we derive the identity

$$\int_{S_\varepsilon^-} (v \cdot \nu)\tilde{\chi}(\xi = 0) dN_\varepsilon = \int_0^\infty \frac{\partial y'_j}{\partial x_i}(y_1 = 0)\frac{\partial J_i}{\partial y'_j} d\xi\,, \tag{5.2}$$

where the summation convention and the abbreviation

$$J = \int_{S_\varepsilon} v \hat{f}_0 dN_\varepsilon$$

are used. Equation (5.2) is obtained by integrating the differential equation (3.5) for $\tilde{\chi}$ over S_ε and with respect to ξ from 0 to ∞, and by using the fact that $\tilde{\chi}$ satisfies a homogeneous inflow condition at $\xi = 0$.

Let $R \subset I\!R^2$ denote the parameter region for the parametrization of $\partial\Omega = x_B(R)$. Recall the local coordinate transformation $x = x_B(y') + y_1 \nu(y')$ with $y' = (y_2, y_3)$. With the notation

$$\mathcal{D} = \left| \det \frac{\partial x}{\partial y} \right| ,$$

we have $ds = \mathcal{D}(y_1 = 0) dy'$ for the Euclidean surface element ds on $\partial\Omega$. The total flux through the boundary of particles with energy ε due to $\tilde{\chi}$ can therefore be written as

$$\begin{aligned} F &= \int_{\partial\Omega} \int_{S_\varepsilon^-} (v \cdot \nu) \tilde{\chi}(\xi = 0) dN_\varepsilon ds \\ &= \int_R \int_0^\infty \frac{\partial y_j'}{\partial x_i}(y_1 = 0) \mathcal{D}(y_1 = 0) \frac{\partial J_i}{\partial y_j'} d\xi dy' . \end{aligned} \tag{5.3}$$

In the following we shall use the identity

$$\nabla_y \cdot \left(\frac{\partial y}{\partial x_i} \mathcal{D} \right) = 0 , \qquad i = 1, 2, 3,$$

valid for every smooth coordinate transformation. It implies

$$\begin{aligned} \frac{\partial y_j'}{\partial x_i}(y_1 = 0) \mathcal{D}(y_1 = 0) \frac{\partial J_i}{\partial y_j'} &= \nabla_{y'} \cdot \left(\frac{\partial y'}{\partial x_i}(y_1 = 0) \mathcal{D}(y_1 = 0) J_i \right) \\ &\quad + J_i \frac{\partial}{\partial y_1} \left(\frac{\partial y_1}{\partial x_i} \mathcal{D} \right) (y_1 = 0) . \end{aligned}$$

The second term vanishes since by $\frac{\partial y_1}{\partial x} = \nu$ this term is independent of y_1, and $J \cdot \nu = 0$ by (3.4). Finally, the divergence theorem is applied to the integral over R in (5.3), implying $F = 0$, which proves our claim.

The equation (5.1) can be used for all the macroscopic models we consider here: The difference is only that for the SHE-model F_{as} is a general function of the energy, while for the ET-model and the DD-model it is a Fermi-Dirac distribution (with $T = T_L$ for the DD-model).

Of course, for an implementation of the boundary conditions (3.8) or (4.5) for the kinetic-to-fluid coupling and (5.1) for the fluid-to-kinetic coupling, it is necessary to solve Milne problems very efficiently. An iterative procedure, based on a Chapman-Enskog type expansion has been developped in [8]. It has been implemented in [10] for kinetic-drift-diffusion coupling and it proved to be very efficient. We suggest to use the Milne problem for the elastic collision operator for two reasons: First, it is linear and the iterative method of [8] can be applied (Explicit results are given in the following section.) Second, it has a physical justification since in many applications the elastic part of the scattering operator dominates. A numerical implementation is the subject of future work.

6 Approximate Solution of Milne Problems

In this section approximations for the solutions of Milne problems are computed. The resulting formulas are needed for an implementation of the boundary conditions (3.8) or (4.5) for macroscopic models and for the fluid-to-kinetic coupling conditions (5.1). The iteration procedure of [8] is adapted to the present situation. Explicit computations are possible for the relaxtion time model for Q_0, and with the assumption of an isotropic band diagram: $\varepsilon = \varepsilon(|k|^2/2)$, $B = I\!R^3$ with $\varepsilon(0) = 0$ and $\varepsilon' > 0$.

We first consider the Milne problem (3.2). We introduce normalized vectors t_1 and t_2 tangential to $\partial\Omega$ such that $\{\nu, t_1, t_2\}$ becomes an orthonormal basis of $I\!R^3$. Then the variable transformation from $k \in I\!R^3$ to $(\varepsilon, s, \varphi) \in [0, \infty) \times [-1, 1] \times [0, 2\pi)$ is determined by

$$k = |k|(\varepsilon)(s\nu + \sqrt{1-s^2}\,\cos\varphi\, t_1 + \sqrt{1-s^2}\,\sin\varphi\, t_2)\,.$$

With $\xi = K\eta$ (as in section 3), (3.2) can be written as

$$s\frac{\partial \hat{f}_0}{\partial \eta} = \frac{1}{4\pi}\int_{-1}^{1}\int_0^{2\pi} \hat{f}_0' d\varphi' ds' - \hat{f}_0\,,$$
$$\hat{f}_0(\eta = 0, s > 0) = f_B\,.$$

For the averages with respect to φ,

$$\overline{f}_0 = \frac{1}{2\pi}\int_0^{2\pi} \hat{f}_0 d\varphi\,, \qquad \overline{f}_B = \frac{1}{2\pi}\int_0^{2\pi} f_B d\varphi\,,$$

we have

$$\hat{f}_0 = \overline{f}_0 + \begin{cases} e^{-\eta/s}(f_B - \overline{f}_B)\,, & s > 0\,, \\ 0\,, & s < 0\,, \end{cases} \tag{6.1}$$

and

$$\begin{aligned} s\frac{\partial \overline{f}_0}{\partial \eta} &= \frac{1}{2}\int_{-1}^{1} \overline{f}_0' ds' - \overline{f}_0\,, \\ \overline{f}_0(\eta = 0, s > 0) &= \overline{f}_B\,. \end{aligned} \tag{6.2}$$

Formula (6.1) shows that both the asymptotic state $\Lambda[f_B]$ and the Albedo operator $\mathcal{A}[f_B]$ can be computed from the solution of the φ-independent Milne problem (6.2). For this problem the iteration procedure of Golse and Klar [8] is applied. One iteration step consists of the following substeps:

1. Obtain the mass balance equation by integrating the transport equation,

   $$\frac{\partial}{\partial \eta}\int_{-1}^{1} s\overline{f}_0 ds = 0\,,$$

   and compute the flux by taking into account the situation at $\eta = \infty$:

   $$\int_{-1}^{1} s\overline{f}_0 ds = 0\,. \tag{6.3}$$

2. Compute a second macroscopic equation by multiplying the transport equation by s and integrating again. Use the result of step 1:

   $$\frac{\partial}{\partial \eta}\int_{-1}^{1} s^2\overline{f}_0 ds = -\int_{-1}^{1} s\overline{f}_0 ds = 0\,. \tag{6.4}$$

3. Replace the solution of the Milne problem by an element c_1 of the kernel of the collision operator (i.e., c_1 independent of s) in (6.4) and in the

gain term of the transport equation. Solve the resulting problem,

$$\frac{2}{3}\frac{\partial c_1}{\partial \eta} = 0\,,$$
$$s\frac{\partial \overline{f}_{01}}{\partial \eta} = c_1 - \overline{f}_{01}\,, \qquad \overline{f}_{01}(\eta = 0, s > 0) = \overline{f}_B\,,$$

explicitly:

$$c_1 \text{ independent of } \eta,$$
$$\overline{f}_{01} = c_1 + \begin{cases} e^{-\eta/s}(\overline{f}_B - c_1)\,, & s > 0\,, \\ 0\,, & s < 0\,. \end{cases}$$

4. Compute the free constant in c_1 by enforcing the flux equation (6.3) at $\eta = 0$:

$$\int_{-1}^{1} s\overline{f}_{01}(\eta = 0)ds = 0 \qquad \Longrightarrow \qquad c_1 = 2\int_0^1 s\overline{f}_B ds\,.$$

Now the procedure is iterated by applying the above steps to the Milne problem satisfied by $\overline{f}_0 - \overline{f}_{01}$. The computations are straightforward but lengthy and, therefore, omitted here. The result are the following approximations for the asymptotic state and for the Albedo operator:

$$\Lambda[f_B] \approx \int_0^1 \left[(1-3s^2)s\left(s\ln\frac{s+1}{s} - 1\right) + 2s(1-A)\right]\overline{f}_B ds\,,$$
$$\mathcal{A}[f_B] \approx \Lambda[f_B] + \int_0^1 \left[s'\left(3s^2 + \frac{3}{2}s - s(1-3s^2)\ln\frac{s-1}{s}\right)\right.$$
$$\left. + \frac{1}{2}(1-3s'^2)\frac{s'}{s'-s}\right]\overline{f}'_B ds'\,,$$

with

$$A = \int_0^1 (1-3s^2)s\left(s\ln\frac{s+1}{s} - 1\right)ds = \frac{13 - 16\ln 2}{30} \approx 6.365 \times 10^{-2}\,.$$

An approximation for the constant Λ_c (see (3.9)) is obtained by setting $f_B = s$:

$$\Lambda_c \approx \frac{3}{4} - \frac{2}{3}A \approx 0.7076\,.$$

Compared to the value given in (3.9), the approximation has a relative error of roughly 0.4%. This accuracy motivates us, not to carry the iteration further. For the fluid-to-kinetic coupling we also need

$$\mathcal{A}[\lambda] \approx K\nu\left[\Lambda_c + s\left(\frac{s}{2}-\frac{1}{3}\right)\ln\frac{s-1}{s} - \frac{1}{8} + \frac{1}{2}s + \frac{1}{4}s^2 - \frac{3}{2}s^3\right].$$

Finally, the asymptotic state and the outgoing distribution for the Milne problem

$$\begin{aligned} &v\cdot\nu\frac{\partial\tilde\chi}{\partial\xi} + \left[v\cdot\left(\frac{\partial y'}{\partial x}\nabla_{y'}\hat f_0\right) + \nabla_x V(y_1=0)\cdot\nabla_k \hat f_0\right]_\infty^\xi = Q_0(\tilde\chi)\,,\\ &\tilde\chi(\xi=0, v\cdot\nu>0) = 0\,, \end{aligned} \tag{6.5}$$

have to be computed. Unfortunately, the application of the approximation procedure to this problem leads to very involved computations and the resulting formulas are too complicated to be practically useful. Also we recall from the preceding section that the terms involving $\tilde\chi$ in the fluid-to-kinetic coupling violate local flux conservation. Therefore we suggest to replace (6.5) by a problem where only one-dimensional effects in the direction orthogonal to the boundary are included. Thus, in the inhomogeneity we omit the derivatives with respect to y' (i.e., along the boundary) and the tangential components of the electric field. Also we use the same variable transformations as above:

$$\begin{aligned} &s\frac{\partial\tilde\chi}{\partial\eta} - E_\nu\left[Ks\frac{\partial\hat f_0}{\partial\varepsilon} + \frac{\tau}{|k|}(1-s^2)\frac{\partial\hat f_0}{\partial s}\right]_\infty^\eta = \frac{1}{4\pi}\int_{-1}^1\int_0^{2\pi}\tilde\chi' d\varphi' ds' - \tilde\chi\,,\\ &\tilde\chi(\eta=0, s>0) = 0\,, \end{aligned}$$

with

$$E_\nu = -\nabla_x V(y_1=0)\cdot\nu\,.$$

A similar argument as above shows that it suffices to solve the φ-averaged problem. As approximation for $\overline{f}_0$ we use $\overline{f}_{01}$:

$$\begin{aligned} &s\frac{\partial\overline\chi}{\partial\eta} - E_\nu\left[Ks\frac{\partial\overline f_{01}}{\partial\varepsilon} + \frac{\tau}{|k|}(1-s^2)\frac{\partial\overline f_{01}}{\partial s}\right]_\infty^\eta = \frac{1}{2}\int_{-1}^1\overline\chi' ds' - \overline\chi\,,\\ &\overline\chi(\eta=0, s>0) = 0\,. \end{aligned}$$

We carry out one step of the approximation procedure. The result is

$$
\begin{aligned}
\tilde{\chi}(\xi=\infty) &\approx -3E_\nu \frac{\tau}{|k|}\int_0^1 \left(s^2-\frac{s}{4}-s^3\ln\frac{s+1}{s}\right)\overline{f}_B\, ds\,,\\
\tilde{\chi}(\xi=0,s<0) &\approx \tilde{\chi}(\xi=\infty)\\
&- \frac{3}{2}E_\nu\frac{\tau}{|k|}\int_0^1\left[\frac{s'^2}{s-s'}+s'\left(1+2s+2s^2\ln\frac{s-1}{s}\right)\right]\overline{f}'_B\, ds'\,.
\end{aligned}
$$

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