THE DRIFT-DIFFUSION LIMIT FOR ELECTRON-PHONON INTERACTION IN SEMICONDUCTORS

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A scattering operator modelling the interaction of electrons with phonons of given constant energy in semiconductors is analyzed by means of an expansion in terms of spherical harmonics. An application is the derivation of the drift-diffusion limit of the corresponding Boltzmann equation for the transport of electrons in a semiconductor crystal.

Keywords: Semiconductors, Boltzmann equation, drift-diffusion limit
AMS subject classification: 82A70, 78A35

1. Introduction

We consider a situation where the transport of electrons in a semiconductor crystal is dominated by the interaction of electrons with phonons of a given constant energy. In particular, we deal with a scaled version of the semiconductor Boltzmann equation:

$$\alpha^2 \frac{\partial F}{\partial t} + \alpha \left(v \cdot \nabla_x F + \frac{1}{2} \nabla_x \Phi \cdot \nabla_v F \right) = Q(F) \,, \tag{1.1}$$

where $\Phi = \Phi(x,t)$ is the (given, scaled) electric potential, α, the scaled mean free path, a dimensionless parameter, and Q the (scaled) scattering operator. Details of the scaling can be found in [6].

The scattering operator modeling electron-phonon interaction is given by (see, e.g., [1])

$$Q(F)(x,v,t) \quad = \quad \int_{\mathbb{R}^3} [aW(v,v') + W(v',v)] F(x,v',t)\, dv'$$

$$-F(x,v,t)\int_{\mathbb{R}^3}[aW(v',v)+W(v,v')]\,dv'$$

with a dimensionless parameter $a>1$ and $W(v,v')=K(v,v')\delta\left(|v'|^2-|v|^2-1\right)$. Here, '1' in the argument of the Delta-function is the scaled version of the phonon energy. The overlap factor K is assumed to be $O(3)$-invariant, i.e.,

$$K(Sv,Sv')=K(v,v') \qquad \text{for every orthogonal matrix } S.$$

As a consequence, K can be written in the form

$$K(v,v')=k\left(|v|^2,|v'|^2,\frac{v}{|v|}\cdot\frac{v'}{|v'|}\right).$$

In this work we carry out the limit $\alpha\to 0$ in initial value problems for the transport equation (1.1). As a necessary basis, Majorana's analysis [2] of the scattering operator Q is extended in Section 2. In particular, conditions for the solvability of equations of the form

$$Q(F)=G \tag{1.2}$$

are given. The main mathematical difficulties are related to the noncompactness of Q caused by the fact that the scattering rate W is a measure. The case of regular scattering rates is well understood by now [8]. In the present situation, Q is a combination of an integral operator in the angular directions and a difference operator in the radial direction. Our main tool is an expansion of Q in terms of spherical harmonics reducing (1.2) to a sequence of difference equations.

In Section 3 the limit $\alpha\to 0$ is carried out formally by a Hilbert expansion procedure. The limit of the distribution function F lies in the kernel of the collision operator Q consisting of products of Maxwellian distributions with periodic functions of the energy, where the period is the energy of a phonon. The periodic factor in the limiting distribution is determined by a drift-diffusion equation where drift and diffusion in position-energy space occur in the direction of constant total energy $|v|^2-\Phi$. The drift-diffusion limits for a relaxation time approximation of the scattering operator considered here and for a nonlinear scattering operator including degeneracy effects have been obtained in [6] and [4], respectively.

Finally, in Section 4 the drift-diffusion limit is rigorously justified. We prove weak convergence of the distribution function to the element of the kernel of the collision operator determined by the drift-diffusion equation.

2. The Collision Operator

We rewrite the collision operator Q by introducing the variable transformation

$$v=\sqrt{u}\,\omega,\quad v'=\sqrt{u'}\,\omega',\qquad u,u'\geq 0,\quad \omega,\omega'\in S^2.$$

Carrying out the u'-integration gives

$$\begin{aligned} Q(F)(\sqrt{u}\,\omega) &= a\frac{\sqrt{u+1}}{2}\int_{S^2} k(u,u+1,\omega\cdot\omega')F(\sqrt{u+1}\,\omega')d\omega' \\ &\quad +\frac{\sqrt{(u-1)_+}}{2}\int_{S^2} k(u,(u-1)_+,\omega\cdot\omega')F(\sqrt{(u-1)_+}\,\omega')d\omega' \\ &\quad -r(u)F(\sqrt{u}\,\omega) \end{aligned}$$

(the subscript '+' denotes the positive part of a function). The scattering frequency r is given by

$$r(u) = p(u) + aq(u)$$

with

$$\begin{aligned} p(u) &= \frac{\sqrt{u+1}}{2}\int_{S^2} k(u,u+1,\omega\cdot\omega')d\omega', \\ q(u) &= \frac{\sqrt{(u-1)_+}}{2}\int_{S^2} k(u,(u-1)_+,\omega\cdot\omega')d\omega'. \end{aligned}$$

Note that r is independent of the angular variable ω because of the rotational invariance of the overlap factor.

As physically reasonable we shall assume that the overlap factor is continuous for $v \neq v'$, positive and symmetric in the first two arguments:

$$k(u,u',s) = k(u',u,s) > 0. \tag{2.1}$$

The constant a is strictly larger than 1.

We start with stating basic properties of the collision operator Q.

Theorem 2.1 *Let the overlap factor $k \in C([0,\infty)^2 \times [-1,1] \setminus \{(u,u,1) \mid u \geq 0\})$ satisfy (2.1) and let $r \in L^\infty(\mathbb{R}^+)$. Then Q has the following properties:*

1. *$Q:\ L^1(\mathbb{R}^3_v) \to L^1(\mathbb{R}^3_v)$ is bounded.*
2. *$Q(F) = 0$ iff $F(v) = a^{-|v|^2}P(|v|^2)$, where $P = P(u)$ is 1-periodic, i.e. $P(u+1) = P(u)$ a.e. in $(0,\infty)$.*
3. *$Q(F)P = Q(FP)$ for all functions $P = P(|v|^2)$, where P is 1-periodic in $(0,\infty)$.*
4. *(H-Theorem) Let $\kappa = \kappa(r)$ be increasing on $\mathbb{R}$. Then for all $F = F(v)$*

   $$\int_{\mathbb{R}^3_v} Q(F)\kappa\left(a^{|v|^2}F\right)dv \leq 0\,.$$

   If κ is strictly increasing then equality holds iff $F(v) = a^{-|v|^2}P(|v|^2)$, where $P = P(u)$ is 1-periodic on $(0,\infty)$.

The proofs of (1) and (3) are straightforward calculations. (2) and (4) are proven in [2].

Note that $a^{-|v|^2}$ is the scaled Maxwellian and that (3) implies that all functions $P = P(|v|^2)$, where $P = P(u)$ is 1-periodic and bounded in $(0, \infty)$, are collision invariants since the mass-conservation property

$$\int_{\mathbb{R}_v^3} Q(F)dv = 0$$

holds for all $F \in L^1(\mathbb{R}_v^3)$.

Obviously, (3) implies that all eigenspaces of Q are infinite dimensional. Also, the gain part $Q^+ = Q + rI$ of Q is not compact (in v) and the Fredholm alternative cannot be employed to solve inhomogeneous equations of the form

$$Q(F) = G\,, \tag{2.2}$$

as it was done in the case of regular scattering rates [7]. The measure valued scattering rates describing phonon interaction introduce a defect of compactness, which necessitates a different approach to solve equations of the form (2.2). The approach to be presented now is based on an explicit diagonalization of Q in terms of spherical harmonics, which relies on the fact that Q^+ is compact in the angular variable $\omega = v/|v|$ and of recursion form in the energy variable $u = |v|^2$. In order to explain the expansion procedure, which has already — to some extent — been employed to solve the semiconductor Boltzmann equation numerically [11], [10], we consider the operator

$$(Kf)(\omega) = \int_{S^2} k(\omega \cdot \omega')f(\omega')d\omega'\,, \qquad k:\ L^2(S^2) \to L^2(S^2), \tag{2.3}$$

with the kernel function $k \in L^2(-1,1)$. Denoting by P_l the Legendre polynomial of degree l:

$$P_l(s) = \frac{1}{2^l l!}\frac{d^l}{ds^l}(s^2-1)^l\,,$$

we set up the Fourier expansion

$$k(s) = \sum_{l=0}^{\infty} k_l P_l(s)\,, \qquad k_l = \frac{2l+1}{2}\int_{-1}^{1} k(s)P_l(s)ds\,.$$

Also, let Y_{lm} be the spherical harmonic

$$Y_{lm}(\omega) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\vartheta)e^{im\varphi}\,, \qquad -l \le m \le l,$$

where $\omega = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$ and the associated Legendre functions are defined by

$$P_l^m(s) = \frac{1}{2^l l!}(1-s^2)^{m/2}\frac{d^{l+m}}{ds^{l+m}}(s^2-1)^l\,.$$

The well known summation formula

$$P_l(\omega\cdot\omega') = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\omega)\overline{Y_{lm}(\omega')}\,, \qquad \omega,\omega'\in S^2,$$

(the bar denotes complex conjugation) then gives the 'bilinear' expansion of the kernel k:

$$k(\omega\cdot\omega') = 4\pi\sum_{l=0}^{\infty}\frac{k_l}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\omega)\overline{Y_{lm}(\omega')}\,.$$

Thus, by the Hilbert-Schmidt theory, the eigenvalues μ_l of K are given by

$$\mu_l = \frac{4\pi k_l}{2l+1}\,, \qquad l=0,1,\ldots,$$

and the eigenspace corresponding to μ_l is spanned by $\{Y_{lm}(\omega)\}_{m=-l}^{l}$.

By expanding the function $f\in L^2(S^2)$ into a Fourier series with respect to the spherical harmonics,

$$f(\omega) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}Y_{lm}(\omega)\,,$$

we obtain the expansion of $(Kf)(\omega)$:

$$(Kf)(\omega) = 4\pi\sum_{l=0}^{\infty}\frac{k_l}{2l+1}\sum_{m=-l}^{l} f_{lm}Y_{lm}(\omega)\,, \qquad \omega\in S^2.$$

This procedure can be applied to the collision operator Q by considering the variable u as a parameter since Q^+ is the sum of two operators of the form (2.3) with different kernel functions. These operators have different eigenvalues but identical eigenspaces.

Setting

$$F(\sqrt{u}\,\omega) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} F_{lm}(u)Y_{lm}(\omega)\,, \qquad F_{lm}(u) = \int_{S^2} F(\sqrt{u}\,\omega)\overline{Y_{lm}(\omega)}d\omega\,,$$

and

$$\begin{aligned} k(u,u+1,s) &= \sum_{l=0}^{\infty} k_l(u)P_l(s)\,,\\ k_l(u) &= \frac{2l+1}{2}\int_{-1}^{1} k(u,u+1,s)P_l(s)ds\,, \end{aligned}$$

we obtain the expansion of $Q(F)$:

$$Q(F)(\sqrt{u}\,\omega) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Q_{lm}(F)(u)Y_{lm}(\omega)\,, \tag{2.4}$$

with the coefficients

$$Q_{lm}(F)(u) = ap(u)\lambda_l(u)F_{lm}(u+1) + q(u)\lambda_l((u-1)_+)F_{lm}((u-1)_+) \quad (2.5)$$
$$-r(u)F_{lm}(u)\,, \quad (2.6)$$

where we set

$$\lambda_l(u) = \frac{k_l(u)}{(2l+1)k_0(u)}\,.$$

Note that $q(u) = 0$ for $u \in (0,1)$.

With the function $G = G(v)$ given by

$$G(\sqrt{u}\,\omega) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} G_{lm}(u)Y_{lm}(\omega)\,, \qquad G_{lm}(u) = \int_{S^2} G(\sqrt{u}\,\omega)\overline{Y_{lm}(\omega)}d\omega\,,$$

the equation (2.2) takes the form

$$ap(u)\lambda_l(u)F_{lm}(u+1) + q(u)\lambda_l((u-1)_+)F_{lm}((u-1)_+) - r(u)F_{lm}(u)$$
$$= G_{lm}(u)\,, \qquad u > 0, \quad l = 0,1,\ldots, \quad m = -l,\ldots,l. \quad (2.7)$$

Before we start with the analysis of the recursions (2.7) we analyze the properties of the Legendre coefficients.

Lemma 2.1 *For $u \in [0,\infty)$ and $l \in \mathbb{N}$ fixed let $0 < k(u,u+1,\cdot) \in C^l([-1,1])$ and*

$$\frac{\partial^k}{\partial s^k}k(u,u+1,s) \ge 0\,, \qquad s \in [-1,1], \quad k = 1,\ldots,l.$$

Then

$$0 \le \lambda_l(u) \le 1 - \frac{k(u,u+1,-1)}{k_0(u)}\,.$$

Proof. We have

$$k_l(u) = \frac{2l+1}{2^{l+1}l!}\int_{-1}^{1} k(u,u+1,s)\frac{d^l}{ds^l}(s^2-1)^l ds\,.$$

$k_l(u) \ge 0$ follows by performing l integrations by part:

$$k_l(u) = \frac{2l+1}{2^{l+1}l!}\int_{-1}^{1} \frac{\partial^l}{\partial s^l}k(u,u+1,s)(1-s^2)^l ds\,.$$

To prove the upper bound we estimate $(1-s^2) = (1+s)(1-s) \le 2(1-s)$ and obtain

$$\begin{aligned} k_l(u) &\le \frac{2l+1}{2l!}\int_{-1}^{1}\frac{\partial^l}{\partial s^l}k(u,u+1,s)(1-s)^l ds \\ &= (2l+1)\left(k_0(u) - \sum_{j=1}^{l}\frac{2^{j-1}}{j!}\frac{\partial^{j-1}}{\partial s^{j-1}}k(u,u+1,-1)\right) \\ &\le (2l+1)\big(k_0(u) - k(u,u+1,-1)\big)\,. \quad \square \end{aligned}$$

The commonly used models for the overlap factor k are of the form

$$k\left(|v|^2, |v'|^2, \frac{v}{|v|}\cdot\frac{v'}{|v'|}\right) = (|v-v'|^2+\beta)^{-n}, \qquad \beta \geq 0, \quad n \geq \frac{1}{2}, \tag{2.8}$$

(see, e.g., [2]). We then have

$$\begin{aligned}\frac{\partial^l}{\partial s^l}k(u,u+1,s) &= \left(2\sqrt{u(u+1)}\right)^l \prod_{j=0}^{l-1}(n+j) \\ &\quad \times\left(2u+1-2s\sqrt{u(u+1)}+\beta\right)^{-n-l} > 0\end{aligned}$$

for $l \in \mathbb{N}_0$ (as usual we set $\prod_{j=0}^{-1} a_j = 1$). By a simple but lengthy asymptotic analysis it can be shown that

$$\lim_{u\to\infty} \lambda_l(u) \begin{cases} = 1, & n \geq 1, \\ < 1, & \frac{1}{2} \leq n < 1. \end{cases}$$

We begin the analysis of (2.7) with the case $l > 0$:

Lemma 2.2 *Let $l > 0$ and $k_0, k_l \in C([0,\infty))$. Also assume that (2.1) holds and that*

$$0 \leq \lambda_l(u) < 1 - a^{-\delta u} H(u-U), \qquad u \geq 0, \tag{2.9}$$

for some $0 < \delta < 1$, $U > 0$, where H denotes the Heavyside function. If $G_{lm} \in L^2\left((0,\infty);\ \frac{\sqrt{u}}{r(u)} a^{(1+\delta)u} du\right)$ then the recursion (2.7) has a unique solution $F_{lm} \in L^2\left((0,\infty);\ \sqrt{u}\, r(u) a^{(1-\delta)u} du\right)$ and the estimate

$$\int_0^\infty \sqrt{u}\, r(u) a^{(1-\delta)u} |F_{lm}(u)|^2 du \leq C \int_0^\infty \frac{\sqrt{u}}{r(u)} a^{(1+\delta)u} |G_{lm}(u)|^2 du$$

holds with a constant $C > 0$ independent of G_{lm}. Also $F_{lm} \geq 0$ if $G_{lm} \leq 0$.

Proof. In order to simplify the notation we set $f = F_{lm}$, $g = G_{lm}$, $\lambda = \lambda_l$. Then (2.7) reads

$$ap(u)\lambda(u)f(u+1) + q(u)\lambda(u-1)f(u-1) - r(u)f(u) = g(u), \qquad u \geq 0, \tag{2.10}$$

where we extended f and λ to the interval $(-1,0)$ (note that $q(u) = 0$ for $u \in (0,1)$). Multiplication by $\sqrt{u}\, a^u \overline{\varphi(u)}$, where φ is a test function on $[0,\infty)$ and integration gives after some manipulations

$$\begin{aligned}&\int_0^\infty \left([1-\lambda(u)]\frac{p(u)}{r(u)} + a[1-\lambda(u-1)]\frac{q(u)}{r(u)}\right)\sqrt{u}\, r(u) a^u f(u)\overline{\varphi(u)}\, du \\ &+ \int_0^\infty \lambda(u)\sqrt{u} p(u) a^u \left(f(u) - af(u+1)\right)\left(\overline{\varphi(u)} - a\overline{\varphi(u+1)}\right) du \\ &= -\int_0^\infty \sqrt{u}\, a^u g(u)\overline{\varphi(u)}\, du\,.\end{aligned}$$

Writing this equation in variational form

$$a_\lambda(f,\varphi) = G(\varphi)\,,$$

it is easy to see that the assumption $0 \le \lambda \le 1$ is sufficient to guarantee that a_λ is a bounded bilinear form on $L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^u\,du\big)$. Also G is a bounded linear functional on $L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^u\,du\big)$ if $g \in L^2\big((0,\infty);\ \frac{\sqrt{u}}{r(u)}a^u\,du\big)$. If

$$0 \le \lambda(u) \le \overline{\lambda} < 1\,, \qquad u > 0, \tag{2.11}$$

holds, then a_λ is coercive on $L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^u\,du\big)$ and the existence of a unique solution f satisfying

$$\int_0^\infty \sqrt{u}\,r(u)a^u|f(u)|^2du \le \frac{1}{(1-\overline{\lambda})^2}\int_0^\infty \frac{\sqrt{u}}{r(u)}a^u|g(u)|^2du$$

follows from the Lax-Milgram lemma.

Now let $\lambda \in C\big([0,\infty)\big)$ satisfy (2.9) instead of (2.11). We introduce the cut-off

$$\lambda_n(u) = \begin{cases} \lambda(u), & -1 < u \le n, \\ 0, & u > n, \end{cases}$$

for $n \in \mathbb{N}$. Then the existence of a sequence of solutions $f_n \in L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^u\,du\big)$ follows. We estimate using (2.9):

$$\begin{aligned} a_{\lambda_n}(f_n,f_n) \;\ge\; & \sigma(U)\int_0^{U+1} \sqrt{u}\,r(u)a^u|f_n(u)|^2du \\ & + \int_{U+1}^\infty \sqrt{u}\,r(u)a^{(1-\delta)u}|f_n(u)|^2du\,, \end{aligned}$$

where $\sigma(U)$ is chosen such that $\lambda(u) \le 1-\sigma(U)$ for $u \in [0,U+1]$. Then we obtain

$$a_{\lambda_n}(f_n,f_n) \ge D\int_0^\infty \sqrt{u}\,r(u)a^{(1-\delta)u}|f_n(u)|^2du\,.$$

Since

$$\begin{aligned} |G(f_n)| \;\le\; & \left(\int_0^\infty \sqrt{u}\,r(u)a^{(1-\delta)u}|f_n(u)|^2du\right)^{1/2} \\ & \times\left(\int_0^\infty \frac{\sqrt{u}}{r(u)}a^{(1+\delta)u}|g(u)|^2du\right)^{1/2}, \end{aligned}$$

we have the uniform estimate

$$\int_0^\infty \sqrt{u}\,r(u)a^{(1-\delta)u}|f_n(u)|^2du \le \frac{1}{D^2}\int_0^\infty \frac{\sqrt{u}}{r(u)}a^{(1+\delta)u}|g(u)|^2du\,. \tag{2.12}$$

Thus, there exists a subsequence n_k and a function f satisfying (2.12) such that

$$f_{n_k}\overset{k\to\infty}{\longrightarrow} f \qquad \text{in } L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^{(1-\delta)u}du\big) \text{ weakly.}$$

It is clear that f satisfies (2.10). Uniqueness is immediate since the estimate (2.12) can be obtained a priorily for any solution of (2.10).

Now let $g(u) \le 0$ for $u > 0$. Since $\lambda_n(u) = 0$ for $u > n$ we have

$$f_n(u) = -\frac{g(u)}{r(u)} \ge 0\,, \qquad u > n+1.$$

Setting $f_n(u) = a^{-u}\tilde{f}_n(u)$ in (2.10) with $\lambda = \lambda_n$ gives

$$\begin{aligned}
r(u)\tilde{f}_n(u) - p(u)\lambda(u)\tilde{f}_n(u+1) &= -a^u g(u), \qquad 0 < u < 1,\\
-aq(u)\lambda(u-1)\tilde{f}_n(u-1) + r(u)\tilde{f}_n(u) - p(u)\lambda(u)\tilde{f}_n(u+1) &= -a^u g(u),\\
&\qquad\qquad 1 < u < n,\\
-aq(u)\lambda(u-1)\tilde{f}_n(u-1) + r(u)\tilde{f}_n(u) &= -a^u g(u), \qquad n < u < n+1.
\end{aligned}$$

Defining $\tilde{f}_{n,i}(w) := \tilde{f}_n(w+i)$, $w \in (0,1)$, $i = 0, \dots, n$, this problem can be written in matrix form

$$A_n(w)\tilde{F}_n(w) = -\tilde{G}_n(w)\,,$$

where $A_n(w)$ is an M-matrix. Thus $g(u) \le 0$ implies $f_n \ge 0$ and $f \ge 0$ follows since f is the weak limit of f_n. $\square$

Theorem 2.1 implies that the equation (2.2) with $G \in L^1(\mathbb{R}^3_v)$ can only have an $L^1(\mathbb{R}^3_v)$-solution F if

$$\int_{\mathbb{R}^3_v} G(v)P(|v|^2)dv = 0 \qquad\qquad \forall\, P \in L^\infty(0,\infty)$$
$$\text{with } P(u+1) = P(u) \text{ a.e. in } (0,\infty). \tag{2.13}$$

This condition can be rewritten by using the periodicity and arbitrariness of P:

$$\sum_{i=0}^{\infty} \sqrt{w+i}\int_{S^2} G(\sqrt{w+i}\,\omega)d\omega = 0 \qquad \text{for a.e. } w \in (0,1). \tag{2.14}$$

Since $\int_{S^2} G(\sqrt{u}\,\omega)d\omega = \sqrt{4\pi}\,G_{00}(u)$ we obtain the necessary condition for the solvability of the recursion (2.7) for $l = m = 0$ in $L^1\big((0,\infty);\ \sqrt{u}\,du\big)$:

$$\sum_{i=0}^{\infty} \sqrt{w+i}\,G_{00}(w+i) = 0 \qquad \text{for a.e. } w \in (0,1). \tag{2.15}$$

We prove:

Lemma 2.3 *Assume that there exist constants $A, B > 0$, $\beta \ge \frac{1}{2}$, such that*

$$\frac{B}{1+u^\beta} \le k_0(u) \le \frac{A}{1+\sqrt{u}}\,, \qquad u > 0. \tag{2.16}$$

Also let $G_{00} \in L^2\big((0,\infty);\ \frac{\sqrt{u}}{r(u)} a^{(1+\delta)u} du\big)$ for some $0 < \delta < 1$ satisfy (2.15). Then there exists a unique solution F_{00} of (2.7) for $l = m = 0$, which satisfies

$$\int_0^\infty \sqrt{u}\, r(u) a^{(1-\delta)u} |F_{00}(u)|^2 du \le C \int_0^\infty \frac{\sqrt{u}}{r(u)} a^{(1+\delta)u} |G_{00}(u)|^2 du \,,$$

$$\begin{aligned} \int_0^\infty \sqrt{u}\, r(u) F_{00}(u) P(u) du = 0 \qquad & \forall\, P \in L^\infty(0,\infty) \\ \textit{with } P(u+1) = P(u) \ \textit{a.e. in } (0,\infty), & \end{aligned} \tag{2.17}$$

where C is independent of G_{00}.

Proof. We consider the recursion (2.10) with

$$\lambda(u) = \lambda_n(u) = 1 - \frac{1}{n}, \qquad u > -1,$$

for $n = 2, 3, \ldots$ The corresponding quadratic form then reads

$$\begin{aligned} a_{\lambda_n}(f,\varphi) &= \frac{1}{n} \int_0^\infty \sqrt{u}\, r(u) a^u f(u) \overline{\varphi(u)} du + \left(1 - \frac{1}{n}\right) \\ & \quad \times \int_0^\infty \sqrt{u}\, p(u) a^u \big(f(u) - a f(u+1)\big)\big(\overline{\varphi(u)} - a\overline{\varphi(u+1)}\big) du \,. \end{aligned}$$

Now let $f_n \in L^2\big((0,\infty);\ \sqrt{u}\, r(u) a^u du\big)$ be the unique solution of

$$a_{\lambda_n}(f_n,\varphi) = G(\varphi) \qquad \forall\, \varphi \in L^2\big((0,\infty);\ \sqrt{u}\, r(u) a^u du\big).$$

Setting $\varphi(u) = a^{-u}\overline{P(u)}$, where $P \in L^\infty(0,\infty)$ is 1-periodic, we conclude

$$\int_0^\infty \sqrt{u}\, r(u) f_n(u) P(u) du = -n \int_0^\infty \sqrt{u}\, g(u) P(u) du = 0 \,,$$

because $g(u) = G_{00}(u)$ satisfies (2.15). Thus $f_n(u)$ satisfies (2.17).

In order to obtain a uniform bound on f_n we estimate

$$a_{\lambda_n}(f_n, f_n) \ge \frac{1}{2} \int_0^\infty \sqrt{u}\, p(u) a^u |f_n(u) - a f_n(u+1)|^2 du \,.$$

Therefore we obtain the bound

$$\int_0^\infty \sqrt{u}\, r(u) a^{(1-\delta)u} |f_n(u)|^2 du \le (2D)^2 \int_0^\infty \frac{\sqrt{u}}{r(u)} a^{(1+\delta)u} |g(u)|^2 du \,, \tag{2.18}$$

if we show the estimate

$$\begin{aligned} & \int_0^\infty \sqrt{u}\, r(u) a^{(1-\delta)u} |\varphi(u)|^2 du \\ & \le D \int_0^\infty \sqrt{u}\, p(u) a^u |\varphi(u) - a\varphi(u+1)|^2 du \end{aligned} \tag{2.19}$$

for all $\varphi \in L^2\big((0,\infty);\ \sqrt{u}\,r(u)a^{(1-\delta)u}du\big)$ which satisfy

$$\sum_{i=0}^{\infty} \sqrt{w+i}\,r(w+i)\varphi(w+i) = 0 \qquad \text{for a.e. } w \in (0,1). \tag{2.20}$$

To prove (2.19), (2.20) we set $\varphi(u) = a^{-u}\Phi(u)$ and

$$E(u) = \Phi(u) - \Phi(u+1)\,. \tag{2.21}$$

Then (2.19), (2.20) can be written as

$$\begin{aligned}
&\sum_{i=0}^{\infty}\int_0^1 \sqrt{w+i}\,r(w+i)a^{-(1+\delta)(w+i)}|\Phi(w+i)|^2 dw \\
&\quad \le D\sum_{i=0}^{\infty}\int_0^1 \sqrt{w+i}\,p(w+i)a^{-w-i}|E(w+i)|^2 dw
\end{aligned} \tag{2.22}$$

and

$$\sum_{i=0}^{\infty} \sqrt{w+i}\,r(w+i)a^{-w-i}\Phi(w+i) = 0 \qquad \text{for a.e. } w \in (0,1). \tag{2.23}$$

Defining

$$\sigma_l(w) = \sum_{j=0}^{l} \sqrt{w+j}\,r(w+j)a^{-j} \Big/ \sum_{j=0}^{\infty} \sqrt{w+j}\,r(w+j)a^{-j}\,,$$

we can write the solution of (2.21), (2.23) as

$$\Phi(w+i) = -\sum_{j=0}^{i-1} E(w+j) + \sum_{j=0}^{\infty} E(w+j)\big(1-\sigma_j(w)\big)\,, \qquad i \ge 0, \tag{2.24}$$

(with the obvious definition $\sum_{j=0}^{-1} a_j = 0$). Inserting (2.24) into the left hand side of (2.22) gives

$$\begin{aligned}
&\int_0^1 \sqrt{w}\,r(w)a^{-(1+\delta)w}\left|\big(1-\sigma_0(w)\big)E(w) + \sum_{j=1}^{\infty} E(w+j)\big(1-\sigma_j(w)\big)\right|^2 dw \\
&+ \int_0^1 \sum_{i=1}^{\infty} \sqrt{w+i}\,r(w+i)a^{-(1+\delta)(w+i)} \\
&\qquad \times \left|\sigma_0(w)E(w) - \sum_{j=1}^{\infty} E(w+j)\big(1-\sigma_j(w)\big) + \sum_{j=1}^{i-1} E(w+j)\right|^2 dw \\
&=: I_1 + I_2\,.
\end{aligned}$$

We estimate in a straightforward way:

$$\begin{aligned}
I_1 &\leq 2\int_0^1 \sqrt{w}\, p(w)a^{-w}|E(w)|^2 dw \\
&+2\sup_{0<w<1}\left(\sqrt{w}\, r(w)a^{-\delta w}\sum_{l=1}^{\infty}\frac{(1-\sigma_l(w))^2a^l}{\sqrt{w+l}\, p(w+l)}\right) \\
&\times \int_0^1\sum_{l=1}^{\infty}\sqrt{w+l}\, p(w+l)a^{-w-l}|E(w+l)|^2 dw\,.
\end{aligned}$$

Using the assumption (2.16) we obtain

$$\begin{aligned}
&1-\sigma_l(w)\leq K_1 a^{-l} \qquad \text{and} \\
&\sqrt{w}\, r(w)a^{-\delta w}\sum_{l=1}^{\infty}\frac{(1-\sigma_l(w))^2a^l}{\sqrt{w+l}\, p(w+l)}\leq K_2 \qquad \text{on } (0,1).
\end{aligned}$$

Therefore,

$$I_1\leq K_3\sum_{l=0}^{\infty}\int_0^1 \sqrt{w+l}\, p(w+l)a^{-w-l}|E(w+l)|^2 dw\,.$$

To estimate I_2 we proceed analogously:

$$\begin{aligned}
I_2 &\leq K_4\int_0^1 \sqrt{w}\, p(w)|E(w)|^2 dw \\
&+K_5\sum_{l=1}^{\infty}\int_0^1 \sqrt{w+l}\, p(w+l)a^{-w-l}|E(w+l)|^2 dw \\
&+K_6\sup_{0<w<1}\left(\sum_{i=1}^{\infty}\sqrt{w+i}\, p(w+i)a^{-(1+\delta)(w+i)}\sum_{j=1}^{i-1}\frac{a^{w+j}}{\sqrt{w+j}\, p(w+j)}\right) \\
&\times\int_0^1\sum_{l=1}^{\infty}\sqrt{w+l}\, p(w+l)a^{-w-l}|E(w+l)|^2 dw\,.
\end{aligned}$$

By again employing the assumption (2.16) we obtain an estimate for I_2 which is analogous to the one for I_1 and (2.22) follows.

Therefore, the estimate (2.18) holds and we conclude the existence of a subsequence n_k such that

$$f_{n_k}\overset{k\to\infty}{\longrightarrow} f \qquad \text{in } L^2\big((0,\infty);\ \sqrt{u}\, r(u)a^{(1-\delta)u}du\big) \text{ weakly,}$$

where f also satisfies (2.18).

It is immediate that f satisfies (2.10) with $\lambda=1$. $\square$

We remark that the recursion (2.7) for $l=m=0$ can be solved explicitly. Simple manipulations give

$$F_{00}(w+j) \;=\; a^{-j}F_{00}(w)+\sum_{i=0}^{j-1}\frac{a^{i-j}}{\sqrt{w+i}\, p(w+i)}$$

$$\times \sum_{l=0}^{i} \sqrt{w+l}\, G_{00}(w+l)\,, \qquad 0 < w < 1,$$

where $F_{00}(w)$ has to be chosen such that (2.17) holds. Lemma 2.3 can also be proven using this explicit solution representation, however the necessary calculations seem more involved.

We collect the results in

Theorem 2.2 *Assume that the overlap factor k satisfies the following assumptions:*

- $k \in C\big([0,\infty)^2 \times [-1,1] \setminus \{(u,u,1) \mid u \geq 0\}\big)$, $k(u,u+1,\cdot) \in C^\infty([-1,1])$ *and* $\frac{\partial^j}{\partial s^j} k(u,u+1,s)$ *is continuous in* $[0,\infty)^2 \times [-1,1]$ *for all* $j \in \mathbb{N} \cup \{0\}$,
- $k(u,u',s) = k(u',u,s)$ *for* $u, u' \geq 0$, $u \neq u'$, $-1 \leq s \leq 1$,
- *there exist constants* $A, B, D > 0$, $\beta \geq \frac{1}{2}$, $0 < \delta < 1$, $U > 0$, *such that*

$$\frac{B}{1+u^\beta} \leq \int_{-1}^{1} k(u,u+1,s)ds \leq \frac{A}{1+\sqrt{u}}\,, \qquad \text{for } u \geq 0,$$
$$k(u,u+1,-1) \geq D \int_{-1}^{1} k(u,u+1,s)ds a^{-\delta u}\,, \qquad \text{for } u \geq U,$$

- $\frac{\partial^j}{\partial s^j} k(u,u+1,s) \geq 0$ *for* $j \geq 0$, $u \geq 0$, $-1 \leq s \leq 1$.

Then, if $G \in L^1(\mathbb{R}^3_v)$, *the condition*

$$\int_{\mathbb{R}^3_v} G(v)P(|v|^2)dv = 0 \qquad \forall\, P \in L^\infty(0,\infty)$$
$$\text{with } P(u+1) = P(u) \text{ a.e. in } (0,\infty) \tag{2.25}$$

is necessary for the existence of a solution $F \in L^1(\mathbb{R}^3_v)$ *of the equation*

$$Q(F) = G\,. \tag{2.26}$$

If additionally $G \in L^2\big(\mathbb{R}^3_v;\ \frac{a^{(1+\delta)|v|^2}}{r(|v|^2)}dv\big)$ *holds then there exists a unique solution* $F \in L^2\big(\mathbb{R}^3_v;\ r(|v|^2)a^{(1-\delta)|v|^2}dv\big)$ *of (2.26) which satisfies*

$$\int_{\mathbb{R}^3_v} r(|v|^2)a^{(1-\delta)|v|^2}F(v)^2dv \leq C\int_{\mathbb{R}^3_v} \frac{a^{(1+\delta)|v|^2}}{r(|v|^2)}G(v)^2dv\,,$$
$$\int_{\mathbb{R}^3_v} r(|v|^2)F(v)P(|v|^2)dv = 0 \qquad \forall\, P \in L^\infty(0,\infty)$$
$$\text{with } P(u+1) = P(u) \text{ a.e. in } (0,\infty), \tag{2.27}$$

where the constant C is independent of G.

Proof. Let $\varphi = \varphi(v)$ have the spherical harmonics expansion

$$\begin{aligned} \varphi(\sqrt{u}\,\omega) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \varphi_{lm}(u) Y_{lm}(\omega)\,, \\ \varphi_{lm}(u) &= \int_{S^2} \varphi(\sqrt{u}\,\omega)\overline{Y_{lm}(\omega)}d\omega\,. \end{aligned} \tag{2.28}$$

Then, for a given function $a = a(u) \geq 0$ we have

$$\int_{\mathbb{R}_v^3} a(|v|^2)\varphi(v)^2 dv = \frac{1}{2}\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} \sqrt{u}\, a(u)|\varphi_{lm}(u)|^2 du\,. \tag{2.29}$$

Thus, the assertions of the theorem follow immediately from the above. □

We remark that the overlap factors of the form (2.8) satisfy the assumptions of the theorem.

3. The Drift-Diffusion Expansion — Formal Asymptotics

We now consider the Boltzmann equation (1.1) for small values of the parameter α. The electric potential $\Phi = \Phi(x,t)$ is assumed to be given and we impose an initial condition

$$F(t=0) = F_I\,. \tag{3.1}$$

In this Section we are only concerned with the formal Hilbert expansion of the IVP (1.1), (3.1) as $\alpha \to 0$. We assume that all the involved functions are sufficiently regular and that the overlap factor satisfies the assumptions of Theorem 2.2.

We expand the solution in powers of α:

$$F = F_0 + \alpha F_1 + \alpha^2 F_2 + O(\alpha^3)\,.$$

Inserting the expansion into the Boltzmann equation and equating $O(\alpha^0)$-terms gives

$$Q(F_0) = 0\,. \tag{3.2}$$

Thus, by Theorem 2.1 we can set

$$F_0(x,v,t) = a^{\Phi(x,t)-|v|^2} L_0\big(x, |v|^2 - \Phi(x,t), t\big)\,,$$

where $L_0 = L_0(x,z,t)$ is 1-periodic in the variable z. We remark that the particular form of L_0 was chosen to simplify as much as possible the subsequent calculations.

Equating $O(\alpha^1)$-terms gives

$$v \cdot \nabla_x F_0 + \frac{1}{2}\nabla_x \Phi \cdot \nabla_v F_0 = Q(F_1)\,.$$

A simple calculation yields

$$v \cdot \nabla_x F_0 + \frac{1}{2}\nabla_x \Phi \cdot \nabla_v F_0 = a^{\Phi-|v|^2} v \cdot \nabla_x L_0(x, |v|^2 - \Phi, t)\,,$$

where ∇_x denotes differentiation with respect to the first argument of L_0 only.

Thus we have to solve the equation

$$Q(F_1) = a^{\Phi-|v|^2} v \cdot \nabla_x L_0(x, |v|^2 - \Phi, t)\,. \tag{3.3}$$

Lemma 3.1 *Every solution of (3.3) has the form*

$$\begin{aligned} F_1(x,v,t) &= a^{\Phi-|v|^2}\Big(-\mu(|v|^2)\frac{v}{|v|} \cdot \nabla_x L_0(x, |v|^2 - \Phi, t) \\ &\quad + L_1(x, |v|^2 - \Phi, t)\Big)\,, \end{aligned} \tag{3.4}$$

where $L_1 = L_1(x,z,t)$ is an arbitrary function, which is 1-periodic in z and $\mu = \mu(u) \geq 0$ is the unique solution in $L^2\big((0,\infty);\ \sqrt{u}\, r(u) a^{-(1+\delta)u} du\big)$, $\delta > 0$, of the recursion

$$p(u)\lambda_1(u)\mu(u+1) + aq(u)\lambda_1(u-1)\mu(u-1) - r(u)\mu(u) = -\sqrt{u}\,, \qquad u > 0\,. \tag{3.5}$$

An explicit calculation gives

$$\lambda_1(u) = \int_{-1}^{1} k(u, u+1, s) s\, ds \Big/ \int_{-1}^{1} k(u, u+1, s) ds\,.$$

Proof. Theorem 2.1 (2), (3) imply that the general solution of (3.3) is given by

$$F_1(x,v,t) = a^{\Phi} M(v) \cdot \nabla_x L_0 + a^{-|v|^2} P(|v|^2)\,,$$

where P is an arbitrary 1-periodic function and $M(v)$ is a (vector valued) solution of

$$Q(M) = a^{-|v|^2} v\,.$$

Since $a^{-|v|^2} v$ satisfies the solvability condition (2.25), Theorem 2.2 implies the existence of a unique solution M satisfying (2.27). We write

$$a^{-|v|^2} v = a^{-u}\sqrt{u}\,\omega\,.$$

Denoting the components of ω by $\omega_1, \omega_2, \omega_3$, we have

$$Y_{1,\pm 1}(\omega) = \sqrt{\frac{3}{8\pi}}(\mp\omega_1 - i\omega_2)\,, \qquad Y_{10}(\omega) = \sqrt{\frac{3}{4\pi}}\omega_3\,.$$

Thus, only the polynomials $\omega_1, \omega_2, \omega_3$ appear in the spherical harmonics expansion of M and we can set

$$M = -a^{-u}\mu(u)\omega\,.$$

The recusion (3.5) then follows immediately from (2.7) with $l = 1$. $\square$

We shall analyze the properties of μ later on. In this Section we assume that $\mu = \mu(u)$ is sufficiently regular to be able to carry out the subsequent calculations.

Equating $O(\alpha^2)$-terms then gives the equation for F_2:

$$\frac{\partial}{\partial t} F_0 + v \cdot \nabla_x F_1 + \frac{1}{2} \nabla_x \Phi \cdot \nabla_v F_1 = Q(F_2) . \tag{3.6}$$

A lengthy computation using (3.2) and (3.4) with $L_1 = 0$ yields

$$\begin{aligned} \frac{\partial}{\partial t} F_0 + v \cdot \nabla_x F_1 + \frac{1}{2} \nabla_x \Phi \cdot \nabla_v F_1 = a^{\Phi - |v|^2} \Bigg[& \frac{\partial \Phi}{\partial t} \left(L_0 \ln a - \frac{\partial L_0}{\partial z} \right) \\ & + \frac{\partial L_0}{\partial t} - \frac{\mu(|v|^2)}{|v|} \sum_{j,l=1}^{3} v_j v_l \frac{\partial^2 L_0}{\partial x_j \partial x_l} - \frac{\mu(|v|^2)}{2|v|} \nabla_x L_0 \cdot \nabla_x \Phi \\ & - \left(\frac{\mu'(|v|^2)}{|v|} - \frac{\mu(|v|^2)}{2|v|^3} \right) \sum_{j,l=1}^{3} v_j v_l \frac{\partial L_0}{\partial x_j} \frac{\partial \Phi}{\partial x_l} \Bigg] . \end{aligned} \tag{3.7}$$

The necessary condition for solvability of (3.6) then is (2.13) or, equivalently, (2.14), where now G stands for the left hand side of (3.6). Inserting the right hand side of (3.7) into (2.14), carrying out the integration over the unit sphere and taking into account the periodicity of L_0 with respect to the second variable $z = |v|^2 - \Phi$ gives

$$\frac{\partial L_0}{\partial t} + \frac{\partial \Phi}{\partial t} \left(L_0 \ln a - \frac{\partial L_0}{\partial z} \right) = A(|v|^2) \Delta_x L_0 + B(|v|^2) \nabla_x L_0 \cdot \nabla_x \Phi , \tag{3.8}$$

where $A = A(u)$, $B = B(u)$ are the 1-periodic extensions of

$$\begin{aligned} A(u) &= \frac{\sum_{k=0}^{\infty} (u+k) \mu(u+k) a^{-k}}{3 \sum_{k=0}^{\infty} (u+k)^{1/2} a^{-k}} , \qquad 0 < u < 1 , \\ B(u) &= \frac{\sum_{k=0}^{\infty} \frac{d}{du} \left[(u+k) \mu(u+k) \right] a^{-k}}{3 \sum_{k=0}^{\infty} (u+k)^{1/2} a^{-k}} , \qquad 0 < u < 1 . \end{aligned}$$

An $O(\alpha)$-approximation of the position density is obtained by taking

$$n_0(x,t) := \int_{\mathbb{R}_v^3} F_0(x,v,t) dv .$$

Since $\int_{\mathbb{R}_v^3} v F_0 dv = 0$, the current density is $O(\alpha)$. Thus, we define

$$J_0(x,t) := \int_{\mathbb{R}_v^3} v F_1(x,v,t) dv ,$$

and — at least formally — we have

$$J = \alpha J_0 + O(\alpha^2) .$$

Simple computations using (3.2) and (3.4) then give

$$n_0 = \int_{-\Phi}^{1-\Phi} C(z+\Phi) a^{\Phi} L_0(x,z,t)\,dz\,, \tag{3.9}$$

$$J_0 = -\int_{-\Phi}^{1-\Phi} D(z+\Phi) a^{\Phi} \nabla_x L_0(x,z,t)\,dz\,, \tag{3.10}$$

where C, D are the 1-periodic extensions of the functions

$$C(u) = 2\pi \sum_{k=0}^{\infty} a^{-u-k}(u+k)^{1/2}\,, \qquad 0 < u < 1\,,$$

$$D(u) = \frac{2\pi}{3} \sum_{k=0}^{\infty} a^{-u-k}(u+k)\mu(u+k)\,, \qquad 0 < u < 1\,.$$

Carrying out the variable transformation $z = |v|^2 - \Phi$ in the equation (3.8) gives the 'conservation form'

$$C(z+\Phi)a^{\Phi}\left[\frac{\partial L_0}{\partial t} + \left(L_0 \ln a - \frac{\partial L_0}{\partial z}\right)\frac{\partial \Phi}{\partial t}\right] = \nabla_x \cdot \left(D(z+\Phi)a^{\Phi}\nabla_x L_0\right)\,. \tag{3.11}$$

We impose an initial condition on L_0:

$$L_0(x,z,0) = L_I(x,z)\,, \tag{3.12}$$

which corresponds to assuming that the initial datum for the Boltzmann equation is of the form

$$F_I(x,v) = a^{\Phi(x,0)-|v|^2} L_I(x, |v|^2 - \Phi(x,0))\,.$$

Thus, assuming that L_I is defined for $x \in \mathbb{R}^3$, $z \in \mathbb{R}$ and 1-periodic in z, we have to solve the IVP (3.11), (3.12) for a function $L_0 = L_0(x,z,t)$, defined for $x \in \mathbb{R}^3$, $t > 0$ and 1-periodic in $z \in \mathbb{R}$. Then the position and current densities (3.9) and (3.10), respectively, can be computed.

Note that both the functions $C(u)$ and $D(u)$ assume the same values at $u = 0$ and at $u = 1$. Thus, no additional transmission condition for $\nabla_x L_0$ is required when passing from (3.8) to (3.11). Also, the conservation law

$$\frac{\partial n_0}{\partial t} + \nabla_x \cdot J_0 = 0$$

follows by integrating (3.11) with respect to z from $-\Phi(x,t)$ to $1-\Phi(x,t)$ and taking into account the equality of $C(u)$, $D(u)$ at $u = 0$ and $u = 1$ and the periodicity of L_0 in z.

The equation (3.11) can easily be restated in a form which more resembles the standard drift-diffusion equations [5]. For this purpose we set

$$N_0(x,u,t) := a^{\Phi} L_0(x, u - \Phi(x,t), t)\,,$$

and compute the densities

$$
\begin{aligned}
n_0 &= \int_0^1 C(u) N_0(x,u,t)\,du\,, \\
J_0 &= -\int_0^1 D(u) \left(\left\{ \nabla_x + \nabla_x \Phi \frac{\partial}{\partial u} \right\} N_0 - \ln a N_0 \nabla_x \Phi \right) du\,.
\end{aligned}
$$

The drift-diffusion equation then reads

$$
\begin{aligned}
C(u)\frac{\partial N_0}{\partial t} &= \left\{ \nabla_x + \nabla_x \Phi \frac{\partial}{\partial u} \right\} \\
&\quad \cdot \left[D(u) \left(\left\{ \nabla_x + \nabla_x \Phi \frac{\partial}{\partial u} \right\} N_0 - \ln a N_0 \nabla_x \Phi \right) \right]. \qquad (3.13)
\end{aligned}
$$

It is subject to 1-periodic boundary conditions in u and to the initial condition

$$
N_0(x,u,0) = N_I(x,u) = a^{\Phi(x,0)} L_I(x, u - \Phi(x,0))\,. \qquad (3.14)
$$

Obviously, compared to the standard drift-diffusion model the gradient in the x-direction is replaced by the operator $\nabla_x + \nabla_x \Phi \frac{\partial}{\partial u}$. Note that in terms of the variables (x,z,t) the gradient in the x-direction is recovered from this operator. Thus, a physical interpretation of (3.13) is that in energy-position space drift and diffusion occur in the z-direction, i.e., the direction of constant total energy $|v|^2 - \Phi$.

4. Rigorous Derivation of the Drift-Diffusion limit

At first we prove additional properties of the collision operator Q. Therefore we introduce the space

$$
\begin{aligned}
S &= \{ \varphi(v) = a^{-|v|^2} P(|v|^2) \in L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{|v|^2} dv) \mid \\
&\qquad P(u+1) = P(u) \text{ a.e. in } (0,\infty) \}\,, \qquad (4.1)
\end{aligned}
$$

and denote by Π the orthogonal projection of $L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{|v|^2} dv)$ onto S.

Lemma 4.1 *Let the overlap factor k satisfy the assumptions of Theorem 2.2. Then*

1. $Q:\ L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{|v|^2} dv) \to L^2\left(\mathbb{R}^3_v;\ \frac{a^{|v|^2}}{r(|v|^2)} dv\right)$ *is bounded,*

2. $$\int_{\mathbb{R}^3_v} Q(F_1) F_2 a^{|v|^2} dv = \int_{\mathbb{R}^3_v} Q(F_2) F_1 a^{|v|^2} dv$$

   for all $F_1, F_2 \in L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{|v|^2} dv)$,

3. *There exists a constant $C > 0$ such that*

   $$\|F - \Pi F\|^2_{L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{(1-\delta)|v|^2} dv)} \le -C \int_{\mathbb{R}^3_v} Q(F) F a^{|v|^2} dv$$

   holds for all $F \in L^2(\mathbb{R}^3_v;\ r(|v|^2) a^{|v|^2} dv)$.

Proof. (1), (2) follow from the spherical harmonics expansion (2.4), (2.5) by using the formulas (2.28), (2.29).

To prove (3) we note that

$$\int_{\mathbb{R}^3_v} Q(F) F a^{|v|^2} dv = \int_{\mathbb{R}^3_v} Q(F - \Pi F)(F - \Pi F) a^{|v|^2} dv$$

because of the symmetry property (2) and since $Q(\Pi F) = 0$ holds (see Theorem 2.1, (2)). The statement then follows immediately from the proofs of the Lemmas 2.2 and 2.3. $\square$

We now consider the IVP for the Boltzmann equation

$$\alpha^2 F_t + \alpha \left(v \cdot \nabla_x F + \frac{1}{2} \nabla_x \Phi \cdot \nabla_v F \right) = Q(F) \,, \tag{4.2}$$

$$F(t=0) = F_I \,, \tag{4.3}$$

where we assumed that the potential Φ is in $W^{2,\infty}(\mathbb{R}^3_x \times (0,\infty))$. Multiplication of (4.2) by $F a^{|v|^2 - \Phi}$ and integration over $\mathbb{R}^3_x \times \mathbb{R}^3_v$ gives formally:

$$\begin{aligned} \frac{\alpha^2}{2} \frac{d}{dt} \int F^2 a^{|v|^2 - \Phi} dv dx &= \int Q(F) F a^{|v|^2 - \Phi} dv dx \\ &\quad - \alpha^2 \frac{\ln a}{2} \int F^2 \Phi_t a^{|v|^2 - \Phi} dv dx \,. \end{aligned} \tag{4.4}$$

Since the first term on the right hand side is nonpositive (see Theorem 2.1, (4)) and since $\|\Phi_t\|_{L^\infty(\mathbb{R}^3_x \times (0,\infty))} \le K$ we conclude from the Gronwall inequality

$$\int F(t)^2 a^{|v|^2 - \Phi(t)} dv dx \le a^{Kt} \int F_I^2 a^{|v|^2 - \Phi(t=0)} dv dx \,.$$

By using standard transport theory this argument can easily be made rigorous and, for an initial datum $F_I \in L^2(\mathbb{R}^6_{(x,v)};\ a^{|v|^2} dv dx)$, we obtain the existence of a unique solution $F = F(t) \ge 0$ uniformly bounded in $L^\infty_{loc}\big([0,\infty);\ L^2(\mathbb{R}^6_{(x,v)};\ a^{|v|^2} dv dx)\big)$ as $\alpha \to 0$.

Thus, for every sequence $\alpha \to 0$ there exists a subsequence (which we denote by the same symbol) and a function F_0 such that, as $\alpha \to 0$,

$$F \to F_0 \qquad \text{in } L^\infty_{loc}\big([0,\infty);\ L^2(\mathbb{R}^6_{(x,v)};\ a^{|v|^2} dv dx)\big) \text{ weak } *. \tag{4.5}$$

Integrating (4.4) over $(0,T)$ gives

$$\begin{aligned} -\int_0^T \int Q(F) F a^{|v|^2 - \Phi} dv dx dt &= -\alpha^2 \frac{\ln a}{2} \int_0^T \int F^2 \Phi_t a^{|v|^2 - \Phi} dv dx dt \\ &\quad + \frac{\alpha^2}{2} \int F_I^2 a^{|v|^2 - \Phi} dv dx - \frac{\alpha^2}{2} \int F^2 a^{|v|^2 - \Phi} dv dx \,, \end{aligned}$$

and

$$-\int_0^T \int Q(F) F a^{|v|^2} dv dx dt \le C_T \alpha^2$$

follows for some constant C_T independent of α.

Since r is in $L^\infty(\mathrm{IR}^3_v)$ we can apply the coercivity estimate (3) of Lemma 4.1 and obtain a uniform bound for

$$R := \frac{F - \Pi F}{\alpha}$$

in $L^2\big((0,T);\ L^2(\mathrm{IR}^6_{(x,v)};\ r(|v|^2)a^{(1-\delta)|v|^2}dvdx)\big)$ for every $T>0$. After maybe again extracting a subsequence we conclude the existence of a function R_0 such that, as $\alpha \to 0$,

$$R \to R_0 \qquad \text{in } L^2_{loc}\big([0,\infty);\ L^2(\mathrm{IR}^6_{(x,v)};\ r(|v|^2)a^{(1-\delta)|v|^2}dvdx)\big) \text{ weakly.} \tag{4.6}$$

Also, the definition of R and its uniform boundedness imply

$$F_0 = \Pi F_0$$

and, by the definition (4.1) of the subspace S there is a function $N_0 = N_0(x,u,t)$, 1-periodic in u, such that

$$F_0(x,v,t) = a^{-|v|^2} N_0(x,|v|^2,t) \tag{4.7}$$

holds.

Now let $P = P(u)$ be an arbitrary smooth 1-periodic function on $[0,\infty)$ and let $\vartheta = \vartheta(x,t) \in \mathcal{D}(\mathrm{IR}^3_x \times [0,T))$ be a test function. Multiplying the Boltzmann equation (4.2) by $P(|v|^2)\vartheta(x,t)$ and integrating by parts gives

$$\int_0^\infty \int\int FP(|v|^2)dv\,\vartheta_t dxdt + \int_0^\infty \int\int RP(|v|^2)vdv\ \cdot \nabla_x \vartheta dxdt$$
$$\int_0^\infty \int\int RP'(|v|^2)vdv\ \cdot \nabla_x \Phi \vartheta dxdt = -\int\int F_I P(|v|^2)dv\,\vartheta(x,0)dx\,,$$

since $\int (\Pi F) v P(|v|^2)dv = 0$ and since $P(|v|^2)$ is a collision invariant of Q. By (4.5), (4.6) we can pass to the limit $\alpha \to 0$ and obtain

$$\int_0^\infty \int\int F_0 P(|v|^2)dv\,\vartheta_t dxdt + \int_0^\infty \int\int R_0 P(|v|^2)vdv\ \cdot \nabla_x \vartheta dxdt$$
$$+\int_0^\infty \int\int R_0 P'(|v|^2)vdv\ \cdot \nabla_x \Phi \vartheta dxdt = -\int\int F_I P(|v|^2)dv\,\vartheta(x,0)dx\,. \tag{4.8}$$

For the identification of R_0 we divide (4.2) by α and use $Q(\Pi F) = 0$:

$$\alpha F_t + \nabla_x \cdot (vF) + \frac{1}{2}\nabla_v \cdot (F\nabla_x \Phi) = Q(R)\,.$$

Obviously, the left hand side converges to

$$\nabla_x \cdot (vF_0) + \frac{1}{2}\nabla_v \cdot (F_0 \nabla_x \Phi)$$

in $\mathcal{D}'\left(\mathbb{R}^3_x \times \mathbb{R}^3_v \times (0,\infty)\right)$. The weak continuity of Q is immediate and we obtain $Q(R_0)$ as limit of the right hand side. Thus, using (4.7), we have to solve

$$a^{-|v|^2} v \cdot \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] = Q(R_0)$$

for R_0. Since $\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi$ is 1-periodic in u, the reasoning of the proof of Lemma 3.1 can be applied and we find

$$\begin{aligned} R_0(x,v,t) &= -a^{-|v|^2} \mu(|v|^2) \frac{v}{|v|} \cdot \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] \\ &\quad + a^{-|v|^2} r_0(x, |v|^2, t)\,, \end{aligned} \tag{4.9}$$

where r_0 is 1-periodic in its second argument. μ satisfies the recursion (3.5).

Simple calculations now give

$$\begin{aligned} \int_{\mathbb{R}^3_v} R_0 v P(|v|^2) dv &= -\int_0^1 D(u) \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] P(u) du\,, \\ \int_{\mathbb{R}^3_v} R_0 v P'(|v|^2) dv &= -\int_0^1 D(u) \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] P'(u) du\,, \\ \int_{\mathbb{R}^3_v} F_0 P(|v|^2) dv &= \int_0^1 C(u) N_0 P(u) du\,, \end{aligned}$$

since $\int_{\mathbb{R}^3_v} v P(|v|^2) r_0 dv = 0$. Thus, (4.8) with the definition (4.9) of R_0 is the weak formulation of the IVP (3.13), (3.14):

$$\begin{aligned} &\int_0^\infty \int_{\mathbb{R}^3_x} \int_0^1 C(u) N_0 \sigma_t du dx dt \\ &- \int_0^\infty \int_{\mathbb{R}^3_x} \int_0^1 D(u) \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] \cdot \nabla_x \sigma du dx dt \\ &- \int_0^\infty \int_{\mathbb{R}^3_x} \int_0^1 D(u) \left[\nabla_x N_0 + \left(\frac{\partial N_0}{\partial u} - N_0 \ln a\right) \nabla_x \Phi\right] \cdot \nabla_x \Phi \frac{\partial \sigma}{\partial u} du dx dt \\ &= -\int_{\mathbb{R}^3_x} \int_0^1 C(u) N_I \sigma(x,u,0) du dx\,, \end{aligned} \tag{4.10}$$

where, by a usual density argument, $\sigma = \sigma(x,u,t)$ is an arbitrary test function in $\mathcal{D}_{per}\left(\mathbb{R}^3_x \times \mathbb{R}_u \times [0,\infty)\right)$ (1-periodic in u).

The initial function N_I is determined from the requirement

$$\int F_I(x,v) P(|v|^2) dv = \int_0^1 C(u) N_I(x,u) P(u) du$$

for all 1-periodic P. A straightforward computation shows

$$N_I(x,u) = \frac{1}{2C(u)} \sum_{k=0}^\infty \sqrt{u+k} \int_{S^2} F_I(x, \sqrt{u+k}\,\omega) d\omega\,. \tag{4.11}$$

We now formulate the main result of this Section:

Theorem 4.1 *Let $\Phi \in W^{2,\infty}(\mathbb{R}^3_x \times (0,\infty))$ and let $F_I \in L^2(\mathbb{R}^3_x \times \mathbb{R}^3_v;\ a^{|v|^2} dvdx)$. Then, for every sequence $\alpha \to 0$ there is a subsequence such that the unique mild solution F of the Boltzmann equation (4.2), (4.3) satisfies*

$$F \to a^{-|v|^2} N_0 \qquad in\ L^\infty_{loc}([0,\infty);\ L^2(\mathbb{R}^6_{(x,v)};\ a^{|v|^2} dvdx))\ weak\ *,$$

where $N_0 = N_0(x,u,t)$, 1-periodic in u, is a $\mathcal{D}'_{per}(\mathbb{R}^3_x \times \mathbb{R}_u \times [0,\infty))$-solution of (4.10), where N_I is given by (4.11).

We remark that strong convergence of the position and current densities can easily be obtained by averaging lemmas (see, e.g., [9]).

Finally, we remark that a minimum principle argument (similar to the proof of Lemma 2.2) can be applied to the recursion (3.5) to obtain a lower bound on μ:

$$\mu(u) \ge \frac{\sqrt{u}}{r(u)}\,.$$

Thus,

$$D(u) \ge \frac{2\pi}{3} \sum_{k=0}^{\infty} a^{-u-k} \frac{(u+k)^{3/2}}{r(u+k)} \ge c > 0\,, \qquad 0 < u < 1\,,$$

and the equation (3.13) is uniformly parabolic in the (x,t)-space and hyperbolic in the (u,t)-space.

Acknowledgment

The work of the first author has been supported by the "Human Capital and Mobility"-Project No. ERBCHRXCT 930413 entitled "Nonlinear Spatial-Temporal Structures in Semiconductors, Fluids and Oscillator Ensembles" funded by the E.U. and by the DFG-Project Ma 1662/1-1. The work of the second author has been supported by the Austrian "Fonds zur Förderung der wissenschaftlichen Forschung" under grant number P08571-PHY.

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