Charge Transport in Semiconductors with Degeneracy Effects

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Abstract–It has been a common procedure to derive a model for charge transport in degenerate semiconductor material by incorporating a Fermi-Dirac distribution into the classical drift-diffusion model. In this work a Boltzmann equation with a nonlinear collision term is considered. A new fluid dynamical model is derived by considering small perturbations of thermal equilibrium. The analysis contains an existence and uniqueness proof for the Boltzmann equation, a justification of the perturbation argument and a study of initial-boundary value problems for the new fluid dynamical model.

1. Introduction

The basic equation of the kinetic theory of semiconductors is the *Boltzmann equation*

$$\partial_t f + \mathbf{v}.\nabla_{\mathbf{x}} f - \frac{q}{m}\mathbf{E}.\nabla_{\mathbf{v}} f = Q(f) \tag{1.1}$$

where the unknown $f = f(t, \mathbf{x}, \mathbf{v})$ can be interpreted as the fraction of occupied states at time $t \in [0, \infty)$ at the point $(\mathbf{x}, \mathbf{v}) \in R^3 \times R^3$ of the position-velocity space. The parameters in the Boltzmann equation are the charge q and the effective mass m of an electron, as well as the electric field $\mathbf{E} = \mathbf{E}(t, \mathbf{x}) \in R^3$.

The *collision operator* is defined by the relaxation time model

$$Q(f) = \frac{1}{\tau}\int_{\mathrm{R}^3} \big(Mf'(1-f) - M'f(1-f')\big)d\mathbf{v}'$$

where the prime denotes evaluation at $\mathbf{v}'$ instead of $\mathbf{v}$ and the *Maxwellian* is given by

$$M(\mathbf{v}) = \left(\frac{2\pi kT}{m}\right)^{-3/2} \exp\left(-\frac{m\mathbf{v}^2}{2kT}\right).$$

Here, τ denotes the relaxation time, k the Boltzmann constant and T the (constant) lattice temperature. The constant multiplying the exponential has been chosen such that the integral of the Maxwellian over the velocity space is equal to one:

$$\int M(\mathbf{v})d\mathbf{v} = 1$$

where here and in the following all integrations are over R^3 except when the domain of integration is indicated explicitely. The collision operator is modeled by a mass-action law where the rate of transitions from the velocity $\mathbf{v}'$ to the velocity $\mathbf{v}$ is proportional to the occupancy factor f' at velocity $\mathbf{v}'$, the fraction of unoccupied states $(1-f)$ at velocity $\mathbf{v}$, and the *scattering rate* M/τ.

Statistical mechanics dictates the requirement that the collision operator vanishes if the occupancy factor f is a *Fermi-Dirac distribution*:

$$f = \left(1 + \exp\left(\frac{m\mathbf{v}^2/2 - \mu}{kT}\right)\right)^{-1}$$

where μ denotes the *Fermi energy*. This requirement is satisfied whenever the scattering rate is the product of the Maxwellian and a collision cross section which is a symmetric function of $\mathbf{v}$ and $\mathbf{v}'$. Thus, our choice of a constant collision cross section is the simplest possible.

In (1.1), the *parabolic band approximation* has been used. This means it is assumed that the particles under consideration have energies close to an extremum of an energy band which therefore can be approximated by a paraboloid. This assumption also leads to the formula

$$\rho(t, \mathbf{x}) = 2\left(\frac{m}{2\hbar\pi}\right)^3 \int f(t, \mathbf{x}, \mathbf{v})d\mathbf{v}$$

for the position space number density of particles. The factor in front of the integral (containing the reduced Planck constant $\hbar$) represents the density of states (see e.g. [3]).

In this work, the initial value problem for the Boltzmann equation (1.1) is considered:

$$f(0,\mathbf{x},\mathbf{v}) = f_0(\mathbf{x},\mathbf{v}) \quad \text{for } (\mathbf{x},\mathbf{v}) \in R^3 \times R^3 \tag{1.2}$$

The electric field is assumed to be given and can be written as the negative gradient of an electrostatic potential:

$$\mathbf{E}(t,\mathbf{x}) = -\nabla_{\mathbf{x}} V(t,\mathbf{x})$$

The problem (1.1), (1.2) is nondimensionalized by choosing the thermal velocity $v_T = \sqrt{kT/m}$ and a characteristic length L as reference quantities for velocity and length. The reference field strength U_T/L is chosen by balancing the second and third terms on the left hand side of (1.1). Here, $U_T = kT/q$ denotes the thermal voltage. We point out that this scaling of the field corresponds to the low field case. A different scaling taking into account high field effects has been used in [16]. With the reference time $L^2/(\tau v_T^2)$ the nondimensionalized version of (1.1), (1.2) reads

$$\begin{aligned} &\alpha^2 \partial_t f + \alpha(\mathbf{v}.\nabla_{\mathbf{x}} f - \mathbf{E}.\nabla_{\mathbf{v}} f) = Q(f), \\ &f(0,\mathbf{x},\mathbf{v}) = f_0(\mathbf{x},\mathbf{v}) \end{aligned} \tag{1.3}$$

where $\alpha = \tau v_T/L$ is the scaled *mean free path* and the scaled collision operator is given by

$$Q(f) = \rho_f M(1-f) - \nu_f f. \tag{1.4}$$

The scaled Maxwellian is

$$M(\mathbf{v}) = (2\pi)^{-3/2} \exp(-\mathbf{v}^2/2)$$

and ρ_f and ν_f are defined by

$$\rho_f = \int f d\mathbf{v}, \qquad \nu_f = \int M(1-f) d\mathbf{v}.$$

Note that we used the same symbols for scaled and unscaled quantities. For more general models and details of the scaling we refer to [11].

In the following the situation where the mean free path is significantly smaller than the characteristic length L is analized. This means that α is a small parameter.

For low particle densities, the occupancy factor f is small compared to one, and the collision operator can be approximated by the linearized version

$$L(f) = \rho_f M - f. \tag{1.5}$$

This situation is commonly referred to as the *nondegenerate case*. From the resulting linear Boltzmann equation the classical drift-diffusion equation for charge transport in semiconductors can be derived. In the physical literature, the derivation is usually based on a moment method or a Legendre expansion of f with respect to the velocity (see e.g. [17]). However, from a mathematical point of view, it is easier to justify a procedure based on a perturbation analysis of (1.3) for small α. In gas dynamics this approach is known as the Hilbert expansion [7]. Mathematically rigorous applications to the neutron transport equation can be found in [2] and [10]. In the case of the linear collision operator (1.5), the Hilbert expansion has been carried out in [14]. It has been proved that for $\alpha \to 0$ the solution of (1.3) (with $Q(f)$ replaced by $L(f)$) converges to a Maxwellian

$$\exp\left(-\mathbf{v}^2/2 + \mu(t, \mathbf{x})\right)$$

where the scaled Fermi energy μ is a solution of the drift diffusion equation

$$\partial_t \rho(\mu) - \mathrm{div}_{\mathbf{x}} \left(\rho(\mu) \nabla_{\mathbf{x}} (\mu - V)\right) = 0 \tag{1.6}$$

with the scaled particle density being given by

$$\rho(\mu) = (2\pi)^{3/2} \mathrm{e}^{\mu}. \tag{1.7}$$

As pointed out above, the equilibrium in the general (degenerate) case is not given by a Maxwellian, but by a Fermi-Dirac distribution:

$$F(\mu, \mathbf{v}) = \frac{1}{1 + \exp(\mathbf{v}^2/2 - \mu)}$$

Now the particle density is given by

$$\rho(\mu) = \int F(\mu, \mathbf{v}) d\mathbf{v} = 4\pi\sqrt{2}\mathcal{F}_{1/2}(\mu) \tag{1.8}$$

where the Fermi integrals are defined by

$$\mathcal{F}_\gamma(\mu) = \int_0^\infty t^\gamma / \left(1 + \mathrm{e}^{t-\mu}\right) dt.$$

It has been a common procedure (see [13]) to derive an equation for the degenerate case by substituting (1.8) instead of (1.7) into the drift diffusion equation (1.6). However, the derivation of (1.6) depends strongly on the nondegeneracy assumption! It is the purpose of this paper to give a rigorous derivation of a fluid equation for the degenerate case.

As a first step, the Cauchy problem for the Boltzmann equation (1.3) is considered. Note that the analysis is simplified considerably by the assumption that the electric field is prescribed and smooth. The physically interesting case of a self consistent electric field, coupled to the Boltzmann equation via a Poisson equation, has been treated in [6], [15] and [12]. However, these analyses can not be straightforwardly applied in our context. The first two papers deal with a problem posed on the position-wave vector space for wave vectors in the (bounded) Brillouin zone. This corresponds to a bounded velocity space. Thus, the technical difficulties which appear for high velocities (as for the Vlasov-Poisson equation, see [1]) are avoided. More recently, Mustieles [12] has investigated a model with unbounded velocities. He has obtained global existence and uniqueness of smooth solutions in the 1- and 2-dimensional cases and global existence of weak solutions for 3-dimensional problems. But the particular assumptions on the collision cross section do not allow the application of his results to the relaxation time model.

Therefore section 2 of this work is concerned with an existence and uniqueness analysis for (1.3). Since the electric field is prescribed, the difficulties are not comparable to those encountered in [1] or [12]. The proof is based on an a priori estimate using an upper solution that seems not to have been pointed out before.

In section 3 the Hilbert expansion is carried out. It is shown that the occupancy factor converges to a Fermi-Dirac distribution $F(\mu, \mathbf{v})$. The Fermi energy μ satisfies the initial value problem

$$\begin{aligned} &\partial_t \rho(\mu) - \operatorname{div}_{\mathbf{x}} \left(D(\mu) \nabla_{\mathbf{x}} (\mu - V) \right) = 0 \\ &\mu(0, \mathbf{x}) = \mu_0(\mathbf{x}) \end{aligned} \tag{1.9}$$

where $\rho(\mu)$ is given by (1.8) and the diffusion coefficient by

$$D(\mu) = (2\pi)^{3/2} \frac{e^{\mu}}{2} \left(1 + \frac{\sigma(\mu)}{\rho(\mu)} \right). \tag{1.10}$$

The function $\sigma(\mu)$ is defined by

$$\sigma(\mu) = \int F(\mu, \mathbf{v}) \big(1 - F(\mu, \mathbf{v})\big)\, d\mathbf{v} = 2\pi\sqrt{2}\mathcal{F}_{-1/2}(\mu)$$

and the initial datum μ_0 is determined uniquely by the equation

$$\rho(\mu_0) = \rho_{f_0}. \tag{1.11}$$

The proof is similar to that in [6]. It is based on a recent regularity result for transport equations (see [4], [5]). The difficulties due to unbounded velocities are surmounted by employing two new properties: The existence of an upper solution and a stronger coerciveness result for the collision operator (compared to [15]).

Section 4 is concerned with initial-boundary value problems for a rescaled version of (1.9) for uniformly high densities. Existence and uniqueness is a consequence of standard results for quasilinear parabolic equations. Upper and lower solutions corresponding to the a priori estimates for (1.3) are obtained. Existence of steady state solutions and their uniqueness for sufficiently high densities is shown.

Finally, in section 5 an approximating problem for uniformly high densities is derived. Its most important property is that it does not contain integrals in the velocity direction. Error estimates for the transient as well as stationary problems are given.

2. Existence and Uniqueness for the Boltzmann Equation

The analysis of this section is based on the following assumptions:

A1. The electrostatic potential $V(t,\mathbf{x})$ is an element of $W^{2,\infty}((0,\infty)\times R^3)$.
A2. There is a constant β such that $0 \le f_0 \le F(\beta,\mathbf{v})$ holds for the initial datum $f_0(\mathbf{x},\mathbf{v})$.
A3. f_0 is in $L^1(R^6)$.

An essential ingredient of the existence proof are comparison functions. Suppose the functions $\gamma_1(t), \gamma_2(t)$ satisfy

$$\gamma_1'(t) = \operatorname{ess\,inf}\{\partial_t V(t,.)\}, \quad \gamma_2'(t) = \operatorname{ess\,sup}\{\partial_t V(t,.)\}.$$

Then, for the Fermi-Dirac function $F(\varphi_i,\mathbf{v})$ with $\varphi_i(t,\mathbf{x}) = \gamma_i(t) - V(t,\mathbf{x})$ we have

$$Q(F(\varphi_i,.)) = 0 \quad \text{and} \quad \mathbf{v}.\nabla_{\mathbf{x}} F(\varphi_i,\mathbf{v}) - \mathbf{E}.\nabla_{\mathbf{v}} F(\varphi_i,\mathbf{v}) = 0$$

since $F(\varphi_i,\mathbf{v})$ is a function of the energy $\mathbf{v}^2/2 - V$. Therefore, since obviously $\partial_t F(\varphi_1,\mathbf{v}) \le 0$ and $\partial_t F(\varphi_2,\mathbf{v}) \ge 0$ holds, $F(\varphi_1,\mathbf{v})$ is a lower solution and $F(\varphi_2,\mathbf{v})$ is an upper solution of the Boltzmann equation. By appropriate choices for the initial values of γ_1 and γ_2 comparison functions for the initial value problem (1.3) can be obtained. In particular, the function $F(\varphi_2,\mathbf{v})$ with $\gamma_2(0) = \beta + \operatorname{ess\,sup}\{V(0,.)\}$ will be used in the following.

Theorem 2.1. *The problem (1.3) has a unique weak solution in the set*

$$\mathcal{V} = \{f \in C(0,\infty; L^1(R^6)) \,|\, 0 \le f \le F(\varphi_2,\mathbf{v})\}.$$

Proof. For given $f \in \mathcal{V}$ let g be the solution of the linear transport equation

$$\begin{aligned} &\alpha^2 \partial_t g + \alpha(\mathbf{v}.\nabla_{\mathbf{x}} g - \mathbf{E}.\nabla_{\mathbf{v}} g) = \rho_f M(1-g) - \nu_f g, \\ &g(0,\mathbf{x},\mathbf{v}) = f_0(\mathbf{x},\mathbf{v}). \end{aligned}$$

Then we define the map Γ by $\Gamma(f) = g$. Obviously, fixed points of Γ correspond to solutions of (1.3). The proof of the theorem proceeds in two steps. First, we show that Γ maps $\mathcal{V}$ into itself, and then that Γ is a contraction for sufficiently small time intervals. In the following we use the notation $F_2(t,\mathbf{x},\mathbf{v}) = F(\varphi_2(t,\mathbf{x}),\mathbf{v})$.

The function $r = F_2 - g$ solves a linear transport problem of the form

$$\begin{aligned} &\alpha^2 \partial_t r + \alpha(\mathbf{v}.\nabla_{\mathbf{x}} r - \mathbf{E}.\nabla_{\mathbf{v}} r) + \lambda r = S, \\ &r(0,\mathbf{x},\mathbf{v}) = r_0(\mathbf{x},\mathbf{v}) \end{aligned}$$

where the initial datum $r_0 = F_2(0,.,.) - f_0$ and the collision frequency $\lambda = \rho_f M + \nu_f$ are obviously nonnegative. For the source term

$$S = \partial_t F_2 + \lambda F_2 - \rho_f M$$

we have

$$S = S - Q(F_2) = \partial_t F_2 + M(1-F_2)\big(\rho(\varphi_2) - \rho_f\big) + F_2\big(\nu_f - \nu(\varphi_2)\big) \ge 0$$

since $f \in \mathcal{V}$, and ρ_f and ν_f are monotonically increasing and resp. decreasing. It follows that r is nonnegative. Similarly we prove nonnegativity of g implying $g \in \mathcal{V}$.

For the second part of the proof, let f_1 and f_2 be two functions in $\mathcal{V}$. We define

$$g_1 = \Gamma(f_1), \quad g_2 = \Gamma(f_2), \quad r = g_2 - g_1.$$

Then r is a solution of the problem

$$\partial_t r + \mathbf{v}.\nabla_{\mathbf{x}} r - \mathbf{E}.\nabla_{\mathbf{v}} r + \lambda r = S, \tag{2.1}$$

$$r(0, \mathbf{x}, \mathbf{v}) = 0$$

with

$$\lambda = \rho_{f_1} M + \nu_{f_1} \geq 0,$$
$$S = M(1 - g_2)(\rho_{f_2} - \rho_{f_1}) + g_2(\nu_{f_1} - \nu_{f_2}).$$

Multiplication by $\mathrm{sign}(r)$ transforms (2.1) into an equation for $|r|$ with the inhomogeneity replaced by $\mathrm{sign}(r)S$. Integration of this equation implies

$$\frac{d}{dt}\|r(t,.,.)\|_{L^1(R^6)} \leq \|S(t,.,.)\|_{L^1(R^6)}.$$

For estimating the right hand side we use $g_2 \in \mathcal{V}$ and obtain for any time $t \leq T$

$$\|S(t,.,.)\|_{L^1(R^6)} \leq C_T \|f_2(t,.,.) - f_1(t,.,.)\|_{L^1(R^6)}.$$

This finally leads to the estimate

$$\|\Gamma(f_2)(t,.,.) - \Gamma(f_1)(t,.,.)\|_{L^1(R^6)} \leq C_T \int_0^t \|f_2(s,.,.) - f_1(s,.,.)\|_{L^1(R^6)} ds$$

concluding the proof.#

We conclude this section by stating a conservation and a regularity result:

Lemma 2.1. *For the solution f of (1.3)*

$$\|f(t,.,.)\|_{L^1(R^6)} = \|f_0\|_{L^1(R^6)}$$

holds. Furthermore, if f_0 belongs to $W^{1,p}(R^6)$, then f belongs to $C(0,\infty; W^{1,p}(R^6))$.

Proof. The property of mass conservation is a consequence of

$$\int Q(f) d\mathbf{v} = 0 \quad \text{for any } f \in L^1(R^3).$$

For proving the regularity of the solution we apply standard results of transport theory (see e.g. [1]) to differentiated versions of (1.3).#

3. Derivation of the fluid dynamical model

In this section we are concerned with limits of solutions of (1.3) as the scaled mean free path α tends to zero. In this context it is important that the a priori estimates

$$0 \le f \le F(\varphi_2, \mathbf{v}), \qquad \|f(t,.,.)\|_{L^1(R^6)} = \|f_0\|_{L^1(R^6)}$$

obtained above, are uniform with respect to α.

The assumptions from the beginning of the preceding section will be used with assumption A3 replaced by the stronger version

A3'. f_0 is in $W^{1,1}(R^6)$

and the additional assumption

A4. $\mathbf{E}$ belongs to $L^\infty_{loc}\big([0,\infty); L^2(R^3)\big)$.

We first examine the collision operator (1.4). For a given distribution of occupancy factors $f = f(\mathbf{v})$, an associated Fermi-Dirac function is defined by

$$F_f = \left(1 + \frac{\nu_f}{\rho_f M}\right)^{-1}.$$

As pointed out above, the collision operator vanishes when applied to Fermi-Dirac functions. The following lemma contains the reverse statement and a coercivity result.

Lemma 3.1. *a) $Q(f) = 0$ iff f is a Fermi-Dirac function. b) For any $f(\mathbf{v})$ with $0 \le f \le 1$ we define $\chi_f = M(1-f)/\big(f + M(1-f)\big)$. Then we have*

$$\nu_f^2 \int (f - F_f)^2/\big(f + M(1-f)\big)d\mathbf{v} \le \int Q^2(f)/\big(f + M(1-f)\big)d\mathbf{v}$$
$$\le 2(\rho_f + \nu_f)\int Q(f)\chi_f d\mathbf{v}.$$

Proof. a) The equation $Q(f) = 0$ is equivalent to $f = F_f$.
b) The integral on the right hand side above is given by

$$\int Q(f)\chi_f d\mathbf{v} = \int\int \frac{\big(M(1-f)f' - M'(1-f')f\big)M(1-f)}{f + M(1-f)} d\mathbf{v}\, d\mathbf{v}'.$$

By symmetrization it can be rewritten as

$$\int Q(f)\chi_f d\mathbf{v} = \int\int \frac{\big(M(1-f)f' - M'(1-f')f\big)^2}{2\big(f + M(1-f)\big)\big(f' + M'(1-f')\big)} d\mathbf{v}\, d\mathbf{v}'.$$

On the other hand, the Cauchy-Schwartz inequality implies

$$Q(f)^2 = \left(\int \big(M(1-f)f' - M'(1-f')f\big)d\mathbf{v}'\right)^2$$
$$\le \int \frac{\big(M(1-f)f' - M'(1-f')f\big)^2}{f' + M'(1-f')} d\mathbf{v}' \int \big(f' + M'(1-f')\big)d\mathbf{v}'.$$

Therefore, we get

$$\int Q(f)^2/(f+M(1-f))d\mathbf{v} \leq 2(\rho_f+\nu_f)\int Q(f)\chi_f d\mathbf{v}.$$

A simple computation shows that the collision term can be written as

$$Q(f) = (F_f - f)(\rho_f M + \nu_f)$$

implying

$$Q(f)^2 \geq (F_f - f)^2 \nu_f^2$$

which completes the proof.#

A second preliminary result is a slightly different version of a theorem of DiPerna and Lions [4]. Let $\mathcal{X}$ be the function space defined by

$$\mathcal{X} = \{f = f(t,\mathbf{x},\mathbf{v}) | \mathrm{e}^{\mathbf{v}^2/4} f \in L^2(R^7)\}.$$

Lemma 3.2. *Let f and g belong to bounded subsets of $\mathcal{X}$, and $\mathbf{h}$ belong to a bounded subset of $\mathcal{X}^3$. If f satisfies*

$$\alpha\partial_t f + \mathbf{v}.\nabla_{\mathbf{x}} f = g + \mathrm{div}_{\mathbf{v}}\mathbf{h},$$

then the density ρ_f is bounded in $L^2\big(-\infty,\infty;H^{1/5}(R^3)\big)$ uniformly with respect to α.

Proof. The proof is along the lines of that in [4].

We denote the Fourier transforms of f, g and $\mathbf{h}$ with respect to t and $\mathbf{x}$ by ϕ, γ and η, respectively. The Fourier variables are called τ and ξ. The functions ϕ, γ and the components of η belong to $\mathcal{X}$ and we have

$$(\alpha\tau + \mathbf{v}.\xi)\phi = \gamma + \mathrm{div}_{\mathbf{v}}\eta.$$

We have to show that $\left(1+|\xi|^{1/5}\right)\left|\int \phi d\mathbf{v}\right|$ belongs to $L^2(R_\tau \times R_\xi^3)$. For $|\xi| \leq 1$, the Cauchy-Schwartz inequality implies

$$\left(1+|\xi|^{1/5}\right)\left|\int \phi d\mathbf{v}\right| \leq 2\left|\int \phi d\mathbf{v}\right| \leq C\left(\int \phi^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2}.$$

The estimation for $|\xi| > 1$ is more involved. For each positive λ a function χ is introduced which satisfies

$$0 \leq \chi \leq 1, \quad \chi(z) = 0 \text{ if } |z| \leq \lambda, \quad \chi(z) = 1 \text{ if } |z| \geq 2\lambda, \quad |z\chi'(z)| \leq C\chi(z)$$

with C independent of λ (which is possible). With $z = (\alpha\tau + \mathbf{v}.\xi)$, we have

$$\begin{aligned}\left|\int \phi d\mathbf{v}\right| &\leq \left|\int \frac{\chi}{z}\gamma d\mathbf{v}\right| + \left|\int \frac{\chi}{z}\mathrm{div}_{\mathbf{v}}\eta d\mathbf{v}\right| + \left|\int (1-\chi)\phi d\mathbf{v}\right| \\ &= D + E + F.\end{aligned}$$

In the following estimation of the three integrals, C stands for generic constants independent of α and λ.

$$
\begin{aligned}
D &\le \left(\int \frac{\chi^2}{z^2} e^{-\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \left(\int \gamma^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \le \frac{C}{\lambda}\left(\int \gamma^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2}, \\
E &= \left|\int \frac{z\chi' - \chi}{z^2}\xi.\eta d\mathbf{v}\right| \le |\xi| \left(\int \frac{\chi^2}{z^4} e^{-\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \left(\int \eta^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \\
&\le C\frac{|\xi|}{\lambda^2}\left(\int \eta^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2}, \\
F &\le \left(\int (1-\chi)^2 e^{-\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \left(\int \phi^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2} \\
&\le C\sqrt{\frac{\lambda}{|\xi|}}\left(\int \phi^2 e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2}.
\end{aligned}
$$

If we now choose $\lambda = |\xi|^{3/5}$, we obtain for $|\xi| > 1$

$$
|\xi|^{1/5}\left|\int \phi d\mathbf{v}\right| \le C\left(\int (\phi^2 + \gamma^2 + \eta^2) e^{\mathbf{v}^2/2} d\mathbf{v}\right)^{1/2}
$$

which completes the proof.#

We are now in the position to prove the main result of this section.

Theorem 3.1. *As $\alpha \to 0$, the solution of (1.3) converges in $L^p_{loc}([0,\infty)\times R^6), 1 \le p < \infty$ to a Fermi-Dirac function $F(\mu, \mathbf{v})$ where the Fermi energy μ is a weak solution of (1.9).*

Proof. The proof is similar to that in [6]. It consists of three steps.

First step: Coercivity. It is our aim to prove the estimate

$$
\|(f - F_f)e^{\mathbf{v}^2/4}\|_{L^2([0,T]\times R^6)} \le C_T\alpha
$$

where here and in the following C_T denotes (possibly different) generic constants independent of α. Note that for a finite time interval $[0,T]$, $\varphi_2(t,\mathbf{x}) \le \varphi_T$ holds for the function φ_2 appearing in the a priori estimates. This implies

$$
\begin{aligned}
&0 < \nu_{F(\varphi_T,.)} \le \nu_f \le 1, \quad \rho_f \le \rho(\varphi_T) < \infty, \\
&f + M(1-f) \le F(\varphi_T,.) + M \le C_T e^{-\mathbf{v}^2/2}.
\end{aligned}
$$

Therefore the coercivity result Lemma 3.1.b leads to

$$
\begin{aligned}
&\int Q(f)^2 e^{\mathbf{v}^2/2} d\mathbf{v} \le C_T \int Q(f)\chi_f d\mathbf{v}, \\
&\int (f - F_f)^2 e^{\mathbf{v}^2/2} d\mathbf{v} \le C_T \int Q(f)\chi_f d\mathbf{v}.
\end{aligned}
\tag{3.1}
$$

We introduce the functions

$$G_f = \int_0^f \frac{M(\mathbf{v})(1-s)}{s+M(\mathbf{v})(1-s)} ds,$$
$$\mathbf{H}_f = \int_0^f \frac{\mathbf{v}M(\mathbf{v})s(1-s)}{\big(s+M(\mathbf{v})(1-s)\big)^2} ds.$$

With these notations we get

$$\partial_t G_f = \chi_f \partial_t f, \quad \nabla_{\mathbf{x}} G_f = \chi_f \nabla_{\mathbf{x}} f, \quad \nabla_{\mathbf{v}} G_f = \chi_f \nabla_{\mathbf{v}} f - \mathbf{H}_f.$$

Since f belongs to $C\big(0,T;W^{1,1}(R^6)\big)$ (Lemma 2.1), G_f belongs to the same space. This justifies all the integrations by parts which follow. Multiplication of (1.3) by χ_f and integration with respect to all variables gives

$$\begin{aligned}\int_0^T \int_{R^6} Q(f)\chi_f d\mathbf{x}\, d\mathbf{v}\, dt &= \alpha \int_0^T \int_{R^6} \mathbf{E}.\mathbf{H}_f d\mathbf{x}\, d\mathbf{v}\, dt \\ &+ \alpha^2 \left(\int_{R^6} G_f(T,.,.) d\mathbf{x}\, d\mathbf{v} - \int_{R^6} G_{f_0} d\mathbf{x}\, d\mathbf{v} \right).\end{aligned} \tag{3.2}$$

Since $0 \le \chi_f \le 1$ holds we have $0 \le G_f \le f$. This and the conservation property (Lemma 2.1) implies that the second term on the right hand side can be estimated by $\alpha^2 \|f_0\|_{L^1(R^6)}$. For estimating the first term on the right hand side we note that for any Fermi-Dirac function F, $\mathbf{H}_F$ is an odd function of $\mathbf{v}$. Therefore we have

$$\int \mathbf{E}.\mathbf{H}_f d\mathbf{v} = \int \mathbf{E}.\left(\mathbf{H}_f - \mathbf{H}_{F_f}\right) d\mathbf{v}.$$

Employing the estimate

$$\left|\mathbf{H}_f - \mathbf{H}_{F_f}\right| = \left| \int_f^{F_f} \frac{\mathbf{v}M(\mathbf{v})s(1-s)}{\big(s+M(\mathbf{v})(1-s)\big)^2} ds \right| \le \frac{1}{4} \left|\mathbf{v}(f-F_f)\right|$$

the Cauchy-Schwartz inequality leads to

$$\begin{aligned}&\int_0^T \int_{R^6} \mathbf{E}.\mathbf{H}_f d\mathbf{x}\, d\mathbf{v}\, dt \\ &\le \left(\int_0^T \int_{R^6} \mathbf{E}^2 \mathbf{v}^2 e^{-\mathbf{v}^2/2} d\mathbf{x}\, d\mathbf{v}\, dt \right)^{1/2} \left(\int_0^T \int_{R^6} (f-F_f)^2 e^{\mathbf{v}^2/2} d\mathbf{x}\, d\mathbf{v}\, dt \right)^{1/2} \\ &\le C_T \left(\int_0^T \int_{R^6} Q(f)\chi_f d\mathbf{x}\, d\mathbf{v}\, dt \right)^{1/2}.\end{aligned}$$

If this is used in (3.2), we obtain

$$\int_0^T \int_{R^6} Q(f)\chi_f d\mathbf{x}\, d\mathbf{v}\, dt - C_T\alpha \left(\int_0^T \int_{R^6} Q(f)\chi_f d\mathbf{x}\, d\mathbf{v}\, dt \right)^{1/2} \le C_T\alpha^2$$

and, thus,

$$\int_0^T \int_{R^6} Q(f)\chi_f d\mathbf{x}\, d\mathbf{v}\, dt \le C_T\alpha^2.$$

A combination of this result with the coercivity inequalities (3.1) finally gives

$$\int_0^T \int_{R^6} Q(f)^2 e^{\mathbf{v}^2/2} d\mathbf{x}\, d\mathbf{v}\, dt \le C_T\alpha^2, \tag{3.3}$$

$$\int_0^T \int_{R^6} \big(f - F_f\big)^2 e^{\mathbf{v}^2/2} d\mathbf{x}\, d\mathbf{v}\, dt \le C_T\alpha^2. \tag{3.4}$$

The functions f, F_f and $r = (f - F_f)/\alpha$ are uniformly bounded in $L^2((0,T)\times R^6)$ with the weight $e^{\mathbf{v}^2/2}$. Therefore, when $\alpha \to 0$, there is a subsequence such that

$$f \to \overline{F}, \quad F_f \to \overline{F}, \quad r \to \overline{r} \quad \text{weakly in } L^2((0,T)\times R^6)$$

holds for the corresponding functions f, F_f and r.

Second step: Strong convergence. Let $\kappa = \kappa(t) \in \mathcal{D}((0,\infty))$ be chosen such that $\kappa = 1$ on $[a,b]$, $0 < a < b < \infty$ holds. Then Lemma 3.2 with $g = \kappa' f + \kappa Q(f)/\alpha$ and $\mathbf{h} = \kappa f \mathbf{E}$ can be applied to a Boltzmann equation for κf. Note that here we use (3.3). We conclude that ρ_f is uniformly bounded in $L^2\big(a,b; H^{1/5}(R^3)\big)$.

On the other hand, by integration of (1.3) with respect to $\mathbf{v}$ we obtain the conservation law

$$\partial_t \rho_f + \frac{1}{\alpha}\mathrm{div}_{\mathbf{x}} \left(\int \mathbf{v} f\, d\mathbf{v} \right) = 0.$$

Since, obviously, $\int \mathbf{v} F_f d\mathbf{v} = 0$ holds ($\mathbf{v}F_f$ is an odd function of $\mathbf{v}$), we have

$$\partial_t \rho_f + \mathrm{div}_{\mathbf{x}} \left(\int \mathbf{v} r\, d\mathbf{v} \right) = 0. \tag{3.5}$$

In view of (3.4) it follows that ρ_f is uniformly bounded in $H^1\big(a,b; H^{-1}(R^3)\big)$. Now an interpolation allows to conclude that ρ_f is also uniformly bounded in $H^{1/6}((a,b)\times R^3)$. From the Rellich-Kondrakov theorem we deduce that for a convenient subsequence the concentration converges strongly in $L^2((a,b)\times K)$ for any compact set $K \in R^3$. Hence we can assume (always for a convenient subsequence) that the density converges almost everywhere in $[0,\infty)\times R^3$. Since ρ_f belongs to $L^\infty((0,T)\times K)$, the dominated convergence theorem implies that we have strong convergence $\rho_f \to \overline{\rho}$ in $L^p_{loc}\big([0,\infty)\times R^3\big)$, $1 \le p < \infty$.

Since the function $\rho(\mu) : R \to (0,\infty)$ given by (1.8) is strictly monotonically increasing and onto, there is a unique Fermi energy μ with $\rho(\mu) = \overline{\rho}$.

A straightforward estimation shows that for two Fermi-Dirac functions F_1, F_2 the inequality

$$\int |F_1 - F_2| d\mathbf{v} \le C|\rho_{F_1} - \rho_{F_2}|$$

holds, where the constant C only depends on an upper bound for ρ_{F_1} and ρ_{F_2}. Therefore we have

$$\int |F_f - F(\mu,\mathbf{v})|\, d\mathbf{v} \le |\rho_{F_f} - \rho_f| + |\rho_f - \rho(\mu)|.$$

In view of (3.4), $\rho_{F_f} - \rho_f$ converges to zero in $L^2\big((0,T)\times R^3\big)$, implying convergence of F_f in $L^1_{loc}\big([0,\infty)\times R^6\big)$. As above, the L^∞-estimates imply strong convergence of F_f and f to $F(\mu,\mathbf{v})$ in $L^p_{loc}\big([0,\infty)\times R^6\big)$.

Third step: Derivation of the fluid limit. We multiply the conservation law (3.5) by a test function $\theta = \theta(t,\mathbf{x}) \in \mathcal{D}(R^4)$ and integrate by parts:

$$\int_0^\infty \int_{R^3} \left(\rho_f \partial_t\theta + \left(\int \mathbf{v} r\, d\mathbf{v}\right).\nabla_{\mathbf{x}}\theta\right) d\mathbf{x}\, dt = \int_{R^3} \rho_{f_0}\theta(0,\mathbf{x})\, d\mathbf{x}$$

In view of our previous results, we can pass to the limit $\alpha \to 0$:

$$\int_0^\infty \int_{R^3} \left(\rho(\mu) \partial_t\theta + \left(\int \mathbf{v} \overline{r}\, d\mathbf{v}\right).\nabla_{\mathbf{x}}\theta\right) d\mathbf{x}\, dt = \int_{R^3} \rho_{f_0}\theta(0,\mathbf{x})\, d\mathbf{x} \qquad (3.6)$$

Now the problem is to compute $\overline{r}$. The left hand side of the Boltzmann equation

$$\alpha\partial_t f + \mathrm{div}_{\mathbf{x}}(\mathbf{v}f) - \mathrm{div}_{\mathbf{v}}(\mathbf{E}f) = Q(f)/\alpha$$

converges in $\mathcal{D}'(R^7)$ to

$$\mathrm{div}_{\mathbf{x}}\big(\mathbf{v}F(\mu,\mathbf{v})\big) - \mathrm{div}_{\mathbf{v}}\big(\mathbf{E}F(\mu,\mathbf{v})\big) = F(\mu,\mathbf{v})\big(1-F(\mu,\mathbf{v})\big)\mathbf{v}.\nabla_{\mathbf{x}}(\mu - V).$$

Straightforward algebra shows that the nonlinear term can be written as

$$Q(f)/\alpha = -(\rho_f M + \nu_f)r.$$

The strong convergence of f and the weak convergence of r allow to conclude that $Q(f)/\alpha$ converges weakly in $L^2\big((0,T)\times R^6\big)$ to

$$-\big(\rho(\mu)M + \nu_{F(\mu,.)}\big)\overline{r} = -\frac{\rho(\mu)M}{F(\mu,.)}\overline{r}.$$

From these relations we can compute $\overline{r}$ and therefore also the flux density

$$\int \mathbf{v}\overline{r}\, d\mathbf{v} = -D(\mu)\nabla_{\mathbf{x}}(\mu - V)$$

with the diffusion coefficient

$$D(\mu) = \frac{1}{\rho(\mu)} \int \frac{F(\mu,\mathbf{v})^2 \big(1 - F(\mu,\mathbf{v})\big)}{M(\mathbf{v})} v_j^2 \, d\mathbf{v}$$

which can be shown to be equal to (1.10) by straightforward manipulations. Finally, (3.6) can be written as

$$\int_0^\infty \int_{R^3} (\rho(\mu)\partial_t\theta - D(\mu)\nabla_{\mathbf{x}}(\mu - V).\nabla_{\mathbf{x}}\theta) \, d\mathbf{x} \, dt = \int_{R^3} \rho_{f_0}\theta(0,\mathbf{x}) \, d\mathbf{x}$$

which is a weak formulation of (1.9).#

4. The Fluid Dynamical Model for Uniformly High Densities

In this and the following sections we are concerned with initial-boundary value problems for the drift-diffusion equation (1.9) in the case of high particle densities. Obviously, high densities correspond to large values of the Fermi energy. For a piece of semiconductor material with uniformly high electron density we replace the Fermi energy μ by $\varepsilon^{-1} + \mu$ with a small positive parameter ε. It is a simple exercise in the asymptotic evaluation of integrals to show that

$$\lim_{\varepsilon\to 0} \big((\gamma + 1)\varepsilon^{\gamma+1}\mathcal{F}_\gamma(\varepsilon^{-1} + \mu)\big) = 1 \tag{4.1}$$

holds for the Fermi integrals. Therefore the quantities ρ, σ and D are replaced by the appropriately rescaled versions

$$\rho(\mu) = \varepsilon^{3/2}\mathcal{F}_{1/2}(\varepsilon^{-1} + \mu), \quad \sigma(\mu) = \frac{1}{2}\sqrt{\varepsilon}\mathcal{F}_{-1/2}(\varepsilon^{-1} + \mu), \quad D(\mu) = e^\mu \left(1 + \varepsilon\frac{\sigma(\mu)}{\rho(\mu)}\right).$$

Note that for fixed μ these definitions imply

$$\rho(\mu) = \frac{2}{3} + O(\varepsilon), \quad \sigma(\mu) = 1 + O(\varepsilon), \quad D(\mu) = e^\mu + O(\varepsilon),$$
$$\rho'(\mu) = O(\varepsilon), \quad \sigma'(\mu) = O(\varepsilon), \quad D'(\mu) = O(1).$$

After also rescaling the time by

$$t \to \frac{4}{\sqrt{\varepsilon\pi}} e^{-1/\varepsilon} t$$

the drift-diffusion equation reads

$$\sigma(\mu)\partial_t\mu - \operatorname{div}\left(D(\mu)\nabla(\mu - V)\right) = 0. \tag{4.2}$$

The analysis of (4.2) is facilitated by introducing the *quasi Fermi level* $\varphi = V - \mu$, which satisfies the equation

$$\sigma(V - \varphi)(\partial_t\varphi - \partial_t V) - \operatorname{div}\big(D(V - \varphi)\nabla\varphi\big) = 0. \tag{4.3}$$

The fact that the space operator is now formally self-adjoint will be used below.

In the following, initial-boundary value problems for (4.2)—or, equivalently, for (4.3)—will be considered. Thus, the differential equations hold for $(\mathbf{x}, t) \in \Omega_T = \Omega \times (0, T)$, where $\Omega \subset \mathrm{R}^3$ is a bounded domain. For simplicity, Dirichlet boundary conditions are assumed. The initial-boundary data $\tilde{\mu}$ and $\tilde{\varphi}$ for μ and, respectively, φ are given on $\Gamma_T = \big(\Omega \times \{0\}\big) \cup \big(\partial\Omega \times (0, T)\big)$. Since regularity considerations are not the subject of this work, we assume all given data, including the electrostatic potential, to be smooth. In particular, the initial-boundary data are assumed to possess smooth extensions to the interior of Ω_T. By the data being "smooth" we mean that any smoothness requirements which appear in the course of the subsequent analysis are satisfied.

The well-posedness of the initial-boundary value problem is the subject of the following theorem.

Theorem 4.1. *The problem* (4.3) *subject to the initial-boundary conditions*

$$\varphi = \tilde{\varphi} \quad \text{on } \Gamma_T \tag{4.4}$$

has a unique solution which is smooth and satisfies

$$\inf_{\Gamma_T} \tilde{\varphi} + \int_0^t \Big(\inf_{\Omega} \partial_t V\Big)(s)ds \le \varphi(\mathbf{x}, t) \le \sup_{\Gamma_T} \tilde{\varphi} + \int_0^t \Big(\sup_{\Omega} \partial_t V\Big)(s)ds \quad \text{in } \Omega_T. \tag{4.5}$$

Proof. The estimate (4.5) follows from a straightforward application of the maximum principle since the upper and lower bounds are upper and lower solutions, respectively. The remaining statements of the theorem follow from standard results for parabolic equations (see e.g. [8], Chapter V).#

The next result is concerned with the corresponding stationary problem consisting of the differential equation

$$\operatorname{div}\big(D(\psi - \varphi)\nabla\varphi\big) = 0 \quad \text{in } \Omega \tag{4.6}$$

subject to Dirichlet boundary conditions

$$\varphi = \varphi_D \quad \text{on } \partial\Omega. \tag{4.7}$$

The Dirichlet data φ_D are assumed to possess a smooth extension to the interior of Ω.

Theorem 4.2. *The problem* (4.6), (4.7) *has a smooth solution which satisfies*

$$\inf_{\partial\Omega} \varphi_D \le \varphi(\mathbf{x}) \le \sup_{\partial\Omega} \varphi_D \quad \text{in } \Omega. \tag{4.8}$$

There is a positive $\varepsilon_0 > 0$, which depends on the data, such that for $\varepsilon \le \varepsilon_0$ the solution is unique.

Proof. As above, the estimate (4.8) follows from the maximum principle. Existence and smoothness of a solution are standard results (see e.g. [9, Chapter 4]). For the proof of uniqueness for small ε we introduce the new variable $u = e^{-\varphi}$ and define the fixed point operator $\mathcal{T}u$ by solving the linear problem

$$\operatorname{div}\big(\tilde{D}(u)\nabla(\mathcal{T}u)\big) = 0 \quad \text{in } \Omega$$
$$\mathcal{T}u = e^{-\varphi_D} \quad \text{on } \partial\Omega$$

where $\tilde{D}$ is given by

$$\tilde{D}(u) = e^V \left(1 + \varepsilon \frac{\sigma(V + \ln u)}{\rho(V + \ln u)}\right).$$

Obviously, fixed points u^* of $\mathcal{T}$ correspond to solutions $\varphi = -\ln u^*$ of (4.6), (4.7). Our aim is to show that, in a subset of an appropriately chosen Banach space, $\mathcal{T}$ is a contraction. For the Banach space we choose $L^6(\Omega)$, and the operator $\mathcal{T}$ acts on the set $D_{\mathcal{T}}$ which is determined by the inequalities (4.8):

$$D_{\mathcal{T}} = \{\, u \in L^6(\Omega) \mid \exp(-\sup_{\partial\Omega} \varphi_D) \le u \le \exp(-\inf_{\partial\Omega} \varphi_D) \,\}$$

It is easy to see that

$$e^V \le \tilde{D}(u) \le 2e^V$$

holds. Therefore, the regularity theory for elliptic equations (see [9]) implies Hölder continuity of $\mathcal{T}u$ and, in particular, the uniform boundedness of the $L^3(\Omega)$-norm of the gradient:

$$\|\nabla(\mathcal{T}u)\|_3 \le c \tag{4.9}$$

where the $L^p(\Omega)$-norm is denoted by $\|\,.\,\|_p$. Here and in the following, c stands for (possibly different) generic constants independent from $u \in D_{\mathcal{T}}$ and from small ε.

For estimating the difference between the images of two functions u_1 and u_2 under the map $\mathcal{T}$, we multiply the difference of the corresponding differential equations by $\mathcal{T}u_1 - \mathcal{T}u_2$ and integrate by parts to obtain

$$\int_\Omega \tilde{D}(u_1)\big|\nabla(\mathcal{T}u_1) - \nabla(\mathcal{T}u_2)\big|^2 d\mathbf{x} = -\int_\Omega \big(\tilde{D}(u_1) - \tilde{D}(u_2)\big)\nabla(\mathcal{T}u_2).\big(\nabla(\mathcal{T}u_1) - \nabla(\mathcal{T}u_2)\big)d\mathbf{x}.$$

From this we get

$$\begin{aligned}\big\|\nabla(\mathcal{T}u_1) - \nabla(\mathcal{T}u_2)\big\|_2 &\le c\Big\|\big(\tilde{D}(u_1) - \tilde{D}(u_2)\big)\nabla(\mathcal{T}u_2)\Big\|_2 \\ &\le c\big\|\tilde{D}(u_1) - \tilde{D}(u_2)\big\|_6 \big\|\nabla(\mathcal{T}u_2)\big\|_3 \\ &\le \varepsilon^2 c\|u_1 - u_2\|_6\end{aligned}$$

where for the first estimate the Cauchy-Schwarz inequality was employed. The second estimate is an application of Hölder's inequality and the third estimate is a consequence of (4.9) and of the fact that the function $\tilde{D}$ is Lipschitz continuous with an $O(\varepsilon^2)$ Lipschitz constant.

Finally, the Sobolev imbedding theorem and a Poincaré inequality imply

$$\big\|\mathcal{T}u_1 - \mathcal{T}u_2\big\|_6 \le c\big\|\nabla(\mathcal{T}u_1) - \nabla(\mathcal{T}u_2)\big\|_2$$

which completes the proof since it is obvious now that the Lipschitz constant of $\mathcal{T}$ can be made smaller than 1 by choosing ε small enough.#

5. The Limiting Problem for High Densities

The Hilbert expansion method reduces the Boltzmann equation to an equation in position space. However, the fluid dynamical equation (4.3) contains integrals in the velocity direction. These integrals can be eliminated by the formal limit $\varepsilon \to 0$. It transforms problem (4.3), (4.4) into

$$\begin{aligned} \partial_t \varphi_0 - \partial_t V &= \operatorname{div}\left(e^{V-\varphi_0}\nabla\varphi_0\right) \quad \text{in } \Omega_T \\ \varphi_0 &= \tilde{\varphi} \quad \text{on } \Gamma_T. \end{aligned} \tag{5.1}$$

This section is concerned with a justification of the limiting procedure.

Theorem 5.1. *Problem (5.1) has a unique, smooth solution φ_0. For the solution φ of (4.3), (4.4)*

$$\sup_{(0,T)} \|\varphi - \varphi_0\|_2^2 + \int_0^T \|\nabla\varphi - \nabla\varphi_0\|_2^2(t)dt \le c_T\varepsilon^2$$

holds with a constant c_T independent of ε. In other words, the solution of (4.3), (4.4) converges to the solution of (5.1) in $L^\infty\big(0,T;L^2(\Omega)\big)$ and in $L^2\big(0,T;H^1(\Omega)\big)$.

Proof. Existence, uniqueness and smoothness for (5.1) follows in the same way as for (4.3), (4.4) in theorem 4.1.

For proving convergence we introduce the new variable

$$z = \int_0^\varphi \sigma(V-\xi)d\xi.$$

The property

$$\varphi(z) = z + O(\varepsilon)$$

of the transformation will be used below. Using the relations

$$\begin{aligned} \partial_t z &= \sigma(V-\varphi)(\partial_t\varphi - \partial_t V) + \sigma(V)\partial_t V, \\ \nabla z &= \sigma(V-\varphi)\nabla\varphi + \big(\sigma(V) - \sigma(V-\varphi)\big)\nabla V, \end{aligned}$$

the problem for z reads

$$\begin{aligned} \partial_t z - \sigma(V)\partial_t V &= \operatorname{div}\big(a(z)\nabla z\big) + \operatorname{div}\left(a(z)\big(\sigma(V-\varphi) - \sigma(V)\big)\nabla V\right) \quad \text{in } \Omega_T \\ z &= \tilde{z} \quad \text{on } \Gamma_T. \end{aligned}$$

With $\varepsilon \to 0$ in the differential equation we obtain the limiting problem

$$\begin{aligned} \partial_t z_0 - \partial_t V &= \operatorname{div}\big(a_0(z_0)\nabla z_0\big) \quad \text{in } \Omega_T \\ z_0 &= \tilde{z} \quad \text{on } \Gamma_T. \end{aligned}$$

The new diffusion coefficient and its formal limit are given by

$$a(z) = \frac{D\big(V-\varphi(z)\big)}{\sigma\big(V-\varphi(z)\big)} \quad \text{and} \quad a_0(z) = e^{V-z},$$

respectively. The approximation error $\delta z = z - z_0$ then solves the equation

$$\begin{aligned} &\partial_t(\delta z) - \operatorname{div}\big(a(z)\nabla(\delta z)\big) - \operatorname{div}\Big(\big(a(z) - a(z_0)\big)\nabla z_0\Big) \\ &\qquad = \big(\sigma(V) - 1\big)\partial_t V + \operatorname{div}\Big(\big(a(z_0) - a_0(z_0)\big)\nabla z_0\Big) + \operatorname{div}\big(a(z)\big(\sigma(V-\varphi) - \sigma(V)\big)\nabla V\big) \end{aligned} \tag{5.2}$$

subject to homogeneous initial-boundary data. By the Lipschitz continuity of a, the term $\big(a(z) - a(z_0)\big)\nabla z_0$ in this equation can be written as $(\delta z)\mathbf{b}$ with a vector field $\mathbf{b}$ which is uniformly bounded with respect to ε. Now (5.2) is multiplied by δz and integrated over Ω_t. Integration by parts and straightforward estimates imply the inequality

$$\begin{aligned} &\|\delta z\|_2^2(t) + c_1 \int_0^t \|\nabla(\delta z)\|_2^2 ds \\ &\qquad \le c_2 \int_{\Omega_t} |\delta z|\big|\nabla(\delta z)\big| d\mathbf{x}\, ds + c_3 \int_0^t \varepsilon \|\delta z\|_2 ds + c_4 \int_0^t \varepsilon \|\nabla(\delta z)\|_2 ds \end{aligned} \tag{5.3}$$

where the c_j-s are constants independent of ε. The last two terms reflect the fact that the right hand side of (5.2) is $O(\varepsilon)$. Applying Young's inequality, the right hand side of (5.3) is estimated by

$$\begin{aligned} \frac{c_2^2}{c_1}\int_0^t \|\delta z\|_2^2 ds + \frac{c_1}{4}\int_0^t \|\nabla(\delta z)\|_2^2 ds + \frac{c_3 t}{2}\varepsilon^2 + \frac{c_3}{2}\int_0^t \|\delta z\|_2^2 ds \\ + \frac{c_4^2 t}{c_1}\varepsilon^2 + \frac{c_1}{4}\int_0^t \|\nabla(\delta z)\|_2^2 ds \end{aligned}$$

implying

$$\|\delta z\|_2^2(t) + \frac{c_1}{2}\int_0^t \|\nabla(\delta z)\|_2^2 ds \le c_5 \int_0^t \|\delta z\|_2^2 ds + c_{1T}\varepsilon^2 \quad \text{for } 0 < t < T.$$

With the aid of the Gronwall lemma we conclude

$$\|\delta z\|_2^2(t) \le c_5 \int_0^t \|\delta z\|_2^2 ds + c_{1T}\varepsilon^2 \le c_{2T}\varepsilon^2.$$

Thus, we finally obtain

$$\sup_{(0,T)} \|\delta z\|_2^2 + \frac{c_1}{2}\int_0^T \|\nabla(\delta z)\|_2^2 dt \le c_{2T}\varepsilon^2.$$

The proof is completed by noting that the properties of the φ-z-transformation imply

$$\varphi - \varphi_0 = \delta z + O(\varepsilon), \quad \nabla(\varphi - \varphi_0) = \nabla(\delta z) + O(\varepsilon).\#$$

Our final result is for the stationary problem (4.6), (4.7). The formal limiting problem as $\varepsilon \to 0$ is

$$\operatorname{div}\left(e^{V-\varphi_0}\nabla\varphi_0\right) = 0 \quad \text{in } \Omega$$
$$\varphi_0 = \varphi_D \quad \text{on } \partial\Omega.$$

Theorem 5.2. *The limiting problem has a unique, smooth solution φ_0. For the solution φ of (4.6), (4.7)*

$$\|\varphi - \varphi_0\|_{H^1(\Omega)} = O(\varepsilon) \quad \text{as } \varepsilon \to 0$$

holds.

Proof. Since $u_0 = \exp(-\varphi_0)$ solves a linear problem, existence, uniqueness and smoothness of the limiting solution are obvious. The error

$$\delta u = e^{-\varphi} - u_0$$

satisfies the differential equation

$$\operatorname{div}\left(e^V \nabla(\delta u)\right) = \varepsilon \operatorname{div}\left(e^{V-\varphi}\frac{\sigma}{\rho}\nabla\varphi\right)$$

subject to homogeneous Dirichlet conditions. It is straightforward to show that the $H^1(\Omega)$-norm of φ is bounded uniformly in ε. This implies that

$$\|\delta u\|_{H^1(\Omega)} = O(\varepsilon)$$

holds, which completes the proof because of the Lipschitz continuity of the u-φ-transformation.#

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