DISSERTATION

On two models for charged particle systems: The cometary flow equation and the Shockley-Read-Hall model.

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Kurzfassung

In dieser Arbeit beschäftigen wir uns mit zwei Modellgleichungen von Systemen geladener Teilchen: das erste Modell ist das kinetische Transportmodell, das die Ablenkung von Teilchen in einem Kometenschweif behandelt, während das zweite Modell Generation und Rekombination von Elektronen und Löchern in Halbleitern behandelt.

In Kapitel 1 untersuchen wir folgende Gleichung (die als 'Cometary flow'-Gleichung bekannt ist):

$$\partial_t f + v \cdot \nabla_x f =: Q_{u_f}(f) = P_{u_f}(f) - f. \tag{1}$$

Die Teilchenverteilungsfunktion $f(t, x, v)$ ist eine nichtnegative Funktion von Zeit, Ort und Geschwindigkeit. Wir schreiben $Q_{u_f}(f)$ für das Streuintegral, mit einem nichtlinearen Projektionsoperator P_{u_f} auf die Menge der isotropen Verteilungsfuntionen um die mittlere Geschwindigkeit u_f (S^{d-1} ist die Einheitskugel in $\mathbb{R}^d$).

$$P_{u_f}(f)(v) = \frac{1}{|S^{d-1}|} \int_{S^{d-1}} f(u_f + |v - u_f|\omega)\, d\omega. \tag{2}$$

Die Menge der Gleichgewichtsverteilungen mit $Q(f) = 0$ ist unendlichdimensional und besteht aus allen isotropen Geschwindigkeitsverteilungen um eine beliebige mittlere Geschwindigkeit. Es existiert unendlich viele Streuinvarianten, aber nur drei von diesen ergeben makroskopische Erhaltungssätze. Aus diesem Grund können Limiten von Lösungen von (1) für lange Zeiträume nicht eindeutig aus den Anfangsbedingungen indentifiziert werden. Als Konsequenz daraus beschränken wir uns auf die linearisierte Version der Gleichung (1). Für den linearisierten Kometenfluss wenden wir die Entropie-Entropie Dissipations Methode von Desvillettes und Villani (siehe [10] und [12] von Kapitel 1) an, die starke Konvergenz mit algebraischer Rate gewährleistet.

Für die linearisierte 'Cometary flow'- Gleichung folgt die Konvergenz gegen einen eindeutigen Gleichgewichtzustand aus zwei Komponenten: einerseits den dissipativen Effekten des Streuoperators, der die Lösung gegen einen die Entropie minimierenden lokalen Gleichgewichtszustand streben lässt, und andererseits den Transportoperator und die periodischen Randbedigungen, die die Lösung von der Menge der lokalen Gleichgewichtszustände abstoßen, solange der angestrebte lokale Gleichgewichtzustand nicht global ist.

Unser wesentliches Konvergenzresultat wird im Abschnitt 1.2 vorgestellt und in den Abschnitten 1.3 und 1.4 bewiesen. Im Abschnitt 1.4 wird dieses Verhalten quantifiziert in einem System von Differentialungleichungen von relativen Entropien bezüglich verschiedener (Teil)-mengen von lokalen bzw. globalen Gleichgewichtszuständen. Wir führen Projektionsoperatoren ein, um eine handhabbare Schreibweise zu erlangen. Im Abschnitt 1.5 wird ein Modell mit drei Geschwindigkeiten betrachtet, das einige Problemstellungen der 'Cometary flow'- Gleichung reproduziert. Dieses Modell zeigt, dass die Entropie Dissipations Methode mit einem analogen Resultat ausgeführt werden kann, jedoch ergibt die Spektralanalyse eine exponentielle Konvergenzgeschwindigkeit.

In Kapitel 2 betrachten wir ein Modell zur Beschreibung der Statistik der Generation-Rekombination von Löchern und Elektronen in Halbleitern. Dieses Modell wurde im Jahre 1952 durch Shockley und Read [22] bzw. Hall [14] eingeführt. Der Sprung zwischen dem Valenzband und dem Leitungsband ist für Halbleiter sehr groß, daher ist zum Übergang von Elektronen vom Valenzband zum Leitungsband viel Energie nötig. Dieser Prozess wird als Generation von Elektron-Loch-Paaren bezeichnet, während der umgekehrte Prozess als Rekombination von Elektron-Loch- Paaren bezeichnet wird. Zustände, die durch Verunreinigungen im Kristall hervorgerufen werden, existieren innerhalb des verbotenen Bandes. Da der Sprung in zwei kleineren Schritten zurückgelegt werden kann, wird er wahrscheinlich.

Wir betrachten zwei Verallgemeinerungen des klassischen SRH Modells: 1) Statt einem einzigen erlaubten Zustand existiert eine Verteilung solcher Zustände über das verbotene Band, 2) ein semiklassisches kinetisches Modell unter Berücksichtigung der Fermionen-Natur der Ladungsträger.

Das ist (nach meinem Wissensstand) der erste Versuch ein 'kinetisches SRH Modell' einzuführen, obwohl die direkte Band-zu-Band Rekombination-Generation und Stoßionisation bereits vorher auf dem kinetischen Niveau betrachtet wurden (siehe z.B. [20], [6], [7] von Kapitel 2). Wir zeigen Existenz von Lösungen und begründen den quasistationären Limes rigoros für des Drift-Diffusions und das kinetische SRH Modell.

Abstract

In this work we are considering two models of charged particles; first model is a kinetic transport model which describes wave-particle interaction in cometary flows, and the second model describes the flow of electrons and holes through the trapped state.

In Chapter 1 we are investigating the following equation (called the cometary flow equation)

$$\partial_t f + v\cdot\nabla_x f =: Q_{u_f}(f) = P_{u_f}(f) - f. \tag{3}$$

The particle distribution function $f(t,x,v)$ is a nonnegative function, which depends on time, space, and on velocity. We denote with $Q_{u_f}(f)$ the collision operator, with a nonlinear projection operator P_{u_f} onto the set of distribution functions isotropic around the mean velocity u_f (S^{d-1} is the unit sphere in $\mathbb{R}^d$)

$$P_{u_f}(f)(v) = \frac{1}{|S^{d-1}|}\int_{S^{d-1}} f(u_f + |v-u_f|\omega)\,d\omega. \tag{4}$$

The set of equilibrium distributions satisfying $Q(f)=0$ is infinite dimensional, and consists of all velocity distributions isotropic around an arbitrary mean velocity. There are infinitely many collision invariants, but out of those only three produce macroscopic conservation laws. For this reason large time limits of solutions of (1) can not be identified uniquely from the initial data. As a consequence, we restrict our attention on the linearized version of (1). For the linearized cometary flow equation we apply the entropy-entropy dissipation approach developed by Desvillettes and Villani (see [10] and [12] from Chapter 1) which provides strong convergence at algebraic rates as time tends to infinity.

For linearized cometary flow equation, the convergence to a unique equilibrium state is the interplay between, firstly, the dissipative effects of the collision operator, which morphs the solution towards an entropy minimizing local equilibrium state, and secondly, the transport operator as well as the imposed periodic boundary conditions, which repulse the solution from the

set of local equilibria as long as the approached local equilibrium is not the global one.

Our main convergence result is stated in section 1.2, and proved in sections 1.3 and 1.4. In section 1.4 this behaviour is quantified in a system of differential inequalities of relative entropies with respect to different (sub)classes of local equilibria, respectively, the global equilibrium. We introduce projection operators leading to a convenient notation. In 1.5, a three velocity model which reproduces some of the difficulties found in the linearized cometary flow equation is considered. This model shows that the entropy dissipation approach can be carried out with an analogous result, however, a spectral analysis proves exponential convergence to equilibrium.

In Chapter 2 we are considering a model which describes the statistics of recombination and generation of holes and electrons in semiconductors occuring through the mechanism of trapping. This model was first introduced in 1952 by Shockley and Read [22], and Hall [14]. The bandgap between the valence and the conduction band is very large for semiconductors which means that a lot of energy is needed to transfer electrons from valence to the conduction band. This process is referred to as the generation of electron-hole pairs, whereas the inverse process is termed recombination of electron-hole pairs. Trap levels within the forbidden band are present, they are caused by crystal impurities. Since the jump can be split into two parts, each of them is 'cheaper' in terms of energy.

We consider two generalizations of the classical SRH model: 1) Instead of a single trapped state, a distribution of trapped states across the forbidden band is allowed, 2) a semiclassical kinetic model including the fermion nature of the charge carriers is introduced.

This is (to my knowledge) the first attempt to derive a 'kinetic SRH model', altough direct band-to-band recombination-generation and impact ionization have been done on the kinetic level before (see, e.g. [20], [6], [7] from Chapter 2).

We prove existence of solutions, and rigorously justify the quasistationary limit for both the drift-diffusion and the kinetic SRH model.

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Contents

Chapter 1

Convergence to Equilibrium for the Linearized Cometary Flow Equation

1.1 Introduction

We are interested in the following kinetic transport model called the cometary flow equation:

$$\partial_t f + v\cdot\nabla_x f = \frac{1}{|S^{d-1}|}\int_{S^{d-1}} f(u_f + |v - u_f|\omega)\,d\omega - f =: Q(f)\,, \qquad (1.1)$$

where $f(t,x,v)$ is a nonnegative particle distribution function depending on time $t > 0$, on position $x \in \mathbb{T}^d$ (the d-dimensional torus with periodic boundary conditions), and on velocity $v \in \mathbb{R}^d$. The collision operator Q is used in quasi-linear plasma theory as a simplified model for wave-particle interaction in cometary flows (see e.g. [7] and the references therein). The first term is a projection (with S^{d-1} and $|S^{d-1}|$ denoting the unit sphere in $\mathbb{R}^d$ and its $(d-1)$-dimensional Lebesgue measure, respectively) onto the set of distribution functions isotropic around the mean velocity $u_f(t,x)$, which is defined as the fraction of the momentum density $m_f(t,x)$ and the mass density $\rho_f(t,x)$:

$$\rho_f = \int_{\mathbb{R}^d} f\,dv\,, \qquad m_f = \rho_f u_f = \int_{\mathbb{R}^d} vf\,dv. \qquad (1.2)$$

Existence and uniqueness of solutions of initial value problems for (1.1) have been investigated in [7] and in [15], where also the long time behaviour is investigated. A weak convergence result on compact time intervals shifted to infinity is proven similarly to the corresponding result by Desvillettes [9] for the gas dynamics case. By entropy dissipation arguments it is shown that in the limit both the left hand side and the right hand side of (1.1) vanish.

The set of equilibrium distributions satisfying $Q(f) = 0$ is infinite dimensional. It consists of all velocity distributions which are isotropic around an arbitrary mean velocity. The collision invariants are the components of v as well as all functions of the form $\psi(|v-u_f|)$, i.e.

$$\int_{\mathbb{R}^d} Q(f)v\,dv = \int_{\mathbb{R}^d} Q(f)\psi(|v-u_f|)\,dv = 0\,,$$

for all f. Out of those, only 1,v, and $|v|^2 = |v-u_f|^2 + 2v\cdot u_f - |u_f|^2$ are independent of f and, thus, produce macroscopic conservation laws. For this reason it is not known how to identify large time limits of solutions of (1.1) uniquely from the initial data. This in twin prevents the applicability of the entropy dissipation approach for inhomogenous kinetic equations recently developed by Desvillettes and Villani [10], [12] (see also [14]) which provides strong convergence at algebraic rates as time tends to infinity.

As a consequence, we restrict our attention in this work to a linearized version of (1.1), which still posseses an infinite dimensional set of equilibrium distributions, but however also posseses enough macroscopic conservation laws such that the limit as $t \to \infty$ can be uniquely determined from the initial data. For the linearized cometary flow equation, presented in the following section, the Desvillettes-Villani approach is carried out. Our main convergence result is stated in section 1.2 and proved in sections 1.3 and 1.4. In section 1.3 a system of differential inequalities is derived for a number of relative entropies with respect to certain partial equilibria. In section 1.4 it is proved that these inequalities imply convergence to equilibrium at arbitrary algebraic rates.

Finally, in section 1.5, a simple three velocity model is considered which reproduces some of the difficulties found in the linearized cometary flow equation. The entropy dissipation approach can also be carried out with an analogous result. A spectral analysis, however, proves exponential convergence to equilibrium. This example is an extension of the two velocity model considered in [14].

1.2 The Linearized Cometary Flow Equation

We linearize (1.1) around an equilibrium steady state of the form $F(|v|^2/2)$, normalized such that $\int_{\mathbb{R}^d} F dv = 1$. Denoting the perturbation by g, the cometary flow equation becomes (see e.g. [6])

$$\partial_t g + v\cdot\nabla_x g = P(g) - g =: LQ(g)\,, \tag{1.3}$$

with the projection

$$P(g) = \overline{P}(g) - F'\, v\cdot m_g\,, \tag{1.4}$$

and the spherical average

$$\overline{P}(g)(v) = \frac{1}{|S^{d-1}|}\int_{S^{d-1}} g(|v|\omega)\,d\omega\,. \tag{1.5}$$

In (1.3) LQ denotes the linearized collision operator. It is easily seen that the components of v and all functions of the form $\psi(|v|)$ are collision invariants, i.e.,

$$\int_{\mathbb{R}^d} LQ(g)v\,dv = \int_{\mathbb{R}^d} LQ(g)\psi(|v|)\,dv = 0\,,$$

providing (with $\psi(|v|) = \delta(|v| - |v_0|)$) the global conservation laws

$$\frac{d}{dt}\int_{\mathbb{T}^d}\int_{\mathbb{R}^d} v\,g(t,x,v)\,dv\,dx = 0\,, \tag{1.6}$$

$$\frac{d}{dt}\int_{\mathbb{T}^d}\int_{S^{d-1}} g(t,x,|v_0|\omega)\,d\omega\,dx = 0, \tag{1.7}$$

for every $|v_0| \geq 0$.

The kernel of the collision operator LQ consists of all velocity distributions of the form $G(|v|^2/2) - F'(|v|^2/2)\,v\cdot m$ with an arbitrary function G of one variable and an arbitrary vector $m \in \mathbb{R}^d$. Thus, we assume that, as $t \to \infty$, g converges to an equilibrium distribution

$$g_\infty(x,v) = G_\infty\left(x, \frac{|v|^2}{2}\right) - F'\left(\frac{|v|^2}{2}\right) v\cdot m_\infty(x)\,. \tag{1.8}$$

It is a consequence of the stationary version of (1.3) that g_∞ is x-independent:

Lemma 1.2.1. *Assume that G_∞ and m_∞ are smooth and that g_∞, given by (2.61), solves (1.3) subject to periodic boundary conditions in x. Then G_∞ and m_∞ are independent of x.*

Proof. Substituting (2.61) into (1.3) yields

$$v\cdot\nabla_x G_\infty - F' v^{tr}\cdot\nabla_x m_\infty\cdot v = 0\,. \tag{1.9}$$

Now we set $v = |v|\omega$ and obtain

$$\omega\cdot\nabla_x G_\infty - F'|v|\,\omega^{tr}\cdot\nabla_x m_\infty\cdot\omega = 0\,, \qquad \forall\ \omega \in S^{d-1}\,, \tag{1.10}$$

implying that $\nabla_x G_\infty = 0$ holds and that $\nabla_x m_\infty$ is skew-symmetric. Now, a result of Desvillettes [8] implies that $m_\infty(x) = \Lambda x + C$, which can only satisfy periodic boundary conditions iff $\Lambda = 0$. $\square$

We consider (1.3) for $t > 0$, $x \in \mathbb{T}^d$, $v \in \mathbb{R}^d$, subject to the initial conditions

$$g(0,x,v) = g_I(x,v)\,, \tag{1.11}$$

where, without loss of generality, we assume vanishing initial total momentum, i.e.

$$\int_{\mathbb{T}^d}\int_{\mathbb{R}^d} v g_I(x,v)\,dv\,dx = 0\,. \tag{1.12}$$

Then, the conservation of momentum (1.6) implies vanishing total momentum for all $t > 0$ and, together with the family of conservation laws (1.7), uniquely determines the global equilibrium g_∞ as

$$g_\infty(v) = G_\infty\left(|v|^2/2\right) = \frac{1}{|\mathbb{T}^d|}\int_{\mathbb{T}^d} \overline{P}(g_I)\left(x, |v|^2/2\right)\,dx\,. \tag{1.13}$$

However, the smoothness assumption in lemma 1.2.1 cannot be proven in general although it is necessary: Formally, a distribution $g_\infty(x,v) = \rho(x)\delta(v)$ with an arbitrary x-periodic function $\rho(x)$ is also a stationary solution of (1.3). Moreover, we conjecture that even for smooth solutions, which are close to a delta distribution centered at the origin in velocity space, convergence to equilibrium can be arbitrarily slow. In order to avoid this problem, we make strong assumptions on the data :

Assumption 1.2.1. *There exists a lower "cutoff-velocity" $v_0 > 0$ such that*

$$F'\left(\frac{|v|^2}{2}\right) = 0\,, \quad g_I(x,v) = 0\,, \qquad \text{for} \quad |v| < v_0\,, \tag{1.14}$$

and

$$F'\left(\frac{|v|^2}{2}\right) < 0\,, \qquad \text{for} \quad |v| > v_0\,. \tag{1.15}$$

Furthermore, $|F'|$ has moments of all orders, i.e. $\int_{\mathbb{R}^d} |v|^k |F'(|v|^2/2)| dv < \infty$, for all $k \geq 0$.

It is an immediate consequence of (1.14) that $g(t,x,v) = 0$ for $|v| < v_0$, i.e., no perturbation of the nonlinear equilibrium distribution $F(|v|^2/2)$ occurs around $v = 0$.

We remark that assumption (1.15) is needed for the definition of an entropy: Introducing the measure

$$d\mu = \frac{dxdv}{|F'(|v|^2/2)|}\,, \tag{1.16}$$

on the phase space $R = \mathbb{T}^d \times \{v \in \mathbb{R}^d : |v| > v_0\}$, an easy computation shows - provided (1.15) - the basic entropy inequality

$$\frac{d}{dt}\int_R g^2\, d\mu = -2\int_R (LQ(g))^2\, d\mu \le 0\,, \tag{1.17}$$

which is the starting point of our analysis below.

Our main convergence result is proven under assumptions of boundedness and smoothness of solutions, which we are unable to prove. Nevertheless, similar properties have been shown recently for simpler models ([14], [17]).

Assumption 1.2.2. *The initial value problem (1.3), (1.11) has a unique solution satisfying*

$$|g(t,x,v)| \le C\sqrt{1+|v|^2}\left|F'\left(\frac{|v|^2}{2}\right)\right|,$$

for $t > 0$ and $(x,v) \in R$, and uniformly in t for all multiindices $(k_1,\dots,k_d)$

$$\int_R \left(\frac{\partial^{k_1+\dots+k_d} g}{\partial x_1^{k_1}\dots\partial x_d^{k_d}}\right)^2 d\mu < \infty\,.$$

Theorem 1.2.2. *Let the initial data $g_I(x,v)$ satisfy (1.12) and suppose that the assumptions 1.2.1 and 1.2.2 hold. Let g_∞ denote the global equilibrium given by (1.13). Then, for every $\varepsilon > 0$ there exists $C(\varepsilon, v_0, F) > 0$ such that for all $t > 0$*

$$\int_R (g-g_\infty)^2\, d\mu \le C(\varepsilon, v_0, F)\, t^{-1/\varepsilon}\,.$$

1.3 The Entropy Dissipation Approach

The basic entropy equality (1.17) suggests to introduce the scalar product

$$\langle f, g\rangle_\mu := \int_R f\, g\, d\mu\,,$$

and the corresponding weighted L^2-space with the induced norm $||\cdot||_\mu$. We also introduce the relative entropy of f with respect to g by

$$H(f|g) := ||f-g||_\mu^2 \,.$$

In particular, the following entropy dissipation equality is derived analogously to (1.17) as a consequence of the symmetry of LQ with respect to $\langle\cdot,\cdot\rangle_\mu$:

$$\frac{d}{dt}H(g|g_\infty) = -2H(g|P(g))\,. \tag{1.18}$$

In this context we use the terminology 'global equilibrium' for g_∞ and 'local equilibrium' for $P(g)$. Equation (1.18) already shows the basic difficulty of the entropy dissipation approach for inhomogenous kinetic equations: The decay of the entropy tends to stop, whenever the solution is approaching local equilibrium even without having reached the global equilibrium yet. The central idea of the method introduced in [10], [12] is to quantify how g cannot stay close to a local equilibrium as long as this is not the unique global equilibrium.

This was done in [10], [14], [18] for models with a single conservation law by deriving a second order differential inequality for $H(g|P(g))$ of the form

$$\frac{d^2}{dt^2}H(g|P(g)) \geq \kappa H(g|g_\infty) - C(\varepsilon)H(g|P(g))^{1-\varepsilon}\,, \tag{1.19}$$

with positive constants κ and $C(\varepsilon)$. Note that, whenever g is sufficiently close to $P(g)$ in relative entropy, (1.19) implies convexity in time and $H(g|P(g))$ will return to dissipate entropy in (1.18) as long as global equilibrium is not reached.

In the present situation, as for the Boltzmann equation [12], such an inequality does not hold, since (see below) an intermediate equilibrium between $P(g)$ and g_∞ has to be quantified as well.

However, we start by calculating the second order time derivative of the relative entropy with respect to the local equilibrium

$$\begin{aligned}\frac{d^2}{dt^2}H(g|P(g)) \;=\; & -2\langle LQ(v\cdot\nabla_x g), v\cdot\nabla_x g\rangle_\mu + 4H(g|P(g)) \\ & -6\langle LQ(g), v\cdot\nabla_x g\rangle_\mu + 2\langle LQ(\nabla_x g)\cdot v, v\cdot\nabla_x g\rangle_\mu.\end{aligned} \tag{1.20}$$

Note that if g is in local equilibrium, i.e. when we set $g = P(g)$ in the right hand side of (1.20), then all the terms vanish, except for the first, which we rewrite as

$$\begin{aligned}-\langle LQ(v\cdot\nabla_x g), v\cdot\nabla_x g\rangle_\mu &= \|\nabla_x\cdot LQ(vg)\|_\mu^2 \\ = \|\nabla_x\cdot LQ(vP(g))\|_\mu^2 &+ \langle\nabla_x\cdot LQ(v(g-P(g))), \nabla_x\cdot LQ(v(g+P(g))\rangle_\mu\end{aligned} \tag{1.21}$$

Considering the first term in the right-hand-side of (1.21), we denote the energy $e_g(t,x) = \int_{\mathbb{R}^d} |v|^2 \overline{P}(g)\, dv = \int_{\mathbb{R}^d} |v|^2 g\, dv$ and recall (1.4) to derive the following identities :

$$\begin{aligned} P(vP(g)) &= -\tfrac{|v|^2}{d} m_g F' - \tfrac{v}{d} F' e_g \,, \\ LQ(vP(g)) &= \left(v \otimes v - \tfrac{|v|^2}{d} \right) m_g F' - v\overline{P}(g) - \tfrac{v}{d} F' e_g \,, \\ \nabla_x \cdot LQ(vP(g)) &= \left(v \otimes v - \tfrac{|v|^2}{d} \right) : AF' - \nabla_x \cdot \left(v\overline{P}(g) + \tfrac{v}{d} F' e_g \right) , \end{aligned} \tag{1.22}$$

where

$$A = \{\nabla_x m_g\} = \frac{1}{2}(\nabla_x m_g + \nabla_x m_g^{tr}) - \frac{1}{d}(\nabla_x \cdot m_g) I_d \,.$$

Hence, since the two terms of the last identity in (1.22) are orthogonal with respect to $\langle \cdot, \cdot \rangle_\mu$,

$$\|\nabla_x \cdot LQ(vP(g))\|_\mu^2 = \left\| \left(v \otimes v - \frac{|v|^2}{d} \right) : AF' \right\|_\mu^2 + \left\| v \cdot \nabla_x \left(\overline{P}(g) + \frac{e_g}{d} F' \right) \right\|_\mu^2 . \tag{1.23}$$

For the first term on the right-hand side of (2.5), we use $I_{ijk} = \int_{\mathbb{R}^d} v_i v_j v_k^2 |F'|\, dv$ and $I_{ijk} = 0$ for $i \neq j$, $I_{iik} = \frac{e_F}{d}$ for $i \neq k$, $I_{kkk} = \frac{3e_F}{d}$, where $e_F = \int_{\mathbb{R}^d} |v|^2 F dv$:

$$\begin{aligned} \left\| \left(v \otimes v - \frac{|v|^2}{d} \right) : AF' \right\|_\mu^2 &= \frac{e_F}{d} \int_{\mathbb{T}^d} \left[3 \sum_i {A_{ii}}^2 + 2 \sum_{i<j} A_{ii} A_{jj} + 2 \sum_{i<j} {A_{ij}}^2 \right] dx \\ &= \frac{e_F}{d} \int_{\mathbb{T}^d} \left[\sum_{i,j} {A_{ij}}^2 + 2 \sum_i {A_{ii}}^2 + \sum_{i \neq j} A_{ii} A_{jj} \right] dx \\ &= \frac{e_F}{d} \int_{\mathbb{T}^d} \left[\sum_{i,j} {A_{ij}}^2 + 2 \sum_i {A_{ii}}^2 - \sum_i {A_{ii}}^2 \right] dx \\ &\geq \frac{e_F}{d} \int_{\mathbb{T}^d} |A|^2 dx \,. \end{aligned}$$

Collecting these estimates, we have

$$\frac{d^2}{dt^2} H(g|P(g))\Big|_{g=P(g)} \geq \frac{2e_F}{d} \int_{\mathbb{T}^d} |\{\nabla_x m_g\}|^2\, dx + 2 \left\| v \cdot \nabla_x \left(\overline{P}(g) + \frac{e_g}{d} F' \right) \right\|_\mu^2 . \tag{1.24}$$

The first term can be estimated from below by $\frac{2e_F}{d} \int_{\mathbb{T}^d} |\nabla_x m_g| dx$ using a Korn inequality (see [12, proposition 11]), which shows that this term only vanishes for x-independent m_g. The second term, instead of controlling $\nabla_x \overline{P}(g)$, contains the projection

$$P_0(g) = -\frac{e_g}{d} F' = \frac{e_g}{d} |F'| \,, \tag{1.25}$$

and therefore vanishes whenever $(I - P_0)(\overline{P}(g))$ is x-independent, which allows still an x-dependent contribution $P_0(\overline{P}(g))$ and (1.24) is not sufficient to conclude convergence to the equilibrium g_∞ (1.13). A similar difficulty occurs also for the Boltzmann equation in [12], which motivates the following procedure.

Our strategy is to decompose $P(g)$ as

$$P(g) = P_0(g) + P_1(g)\,, \tag{1.26}$$

and then to introduce an intermediate (between local and global) equilibrium, defined as

$$\widetilde{P}(g) = P_0(g) + P_1(g_\infty)\,, \tag{1.27}$$

which can alternatively be written as

$$\widetilde{P}(g) = P_0(g) + P(g_\infty) - P_0(g_\infty) = g_\infty + P_0(g - g_\infty)\,, \tag{1.28}$$

which will be used below.

Lemma 1.3.1.

$$H(\widetilde{P}(g)|g_\infty) \geq \frac{1}{2}H(g|g_\infty) - H(g|\widetilde{P}(g))\,. \tag{1.29}$$

Proof. The proof is immediate from the fact that

$$H(\widetilde{P}(g)|g_\infty) = H(g|g_\infty) + H(g|\widetilde{P}(g)) - 2\langle g - g_\infty, g - \widetilde{P}(g)\rangle_\mu\,.$$

□

We now estimate the second term on the right hand side of (1.24)

$$\begin{aligned}
\|v\cdot\nabla_x(\overline{P} - P_0)(g)\|_\mu^2 &= \sum_{i,j=1}^{d}\int_R v_i v_j \frac{\partial}{\partial x_i}(\overline{P} - P_0)(g)\frac{\partial}{\partial x_j}(\overline{P} - P_0)(g)\,d\mu \\
&= \sum_i \int_R {v_i}^2 \left(\frac{\partial}{\partial x_i}(\overline{P} - P_0)(g)\right)^2 d\mu \\
&= \frac{1}{d}\int_R |v|^2|\nabla_x(\overline{P} - P_0)(g)|^2\,d\mu.
\end{aligned} \tag{1.30}$$

At this point we need assumption 1.2.1 in order to prevent that (1.30) vanishes in case of g concentrating around $v = 0$. By the lower bound $|v| \geq v_0$ on the phase space R, we continue to estimate

$$\begin{aligned}
\|v\cdot\nabla_x(\overline{P} - P_0)(g)\|_\mu^2 &\geq C\|\nabla_x(\overline{P} - P_0)(g)\|_\mu^2 = C\|\nabla_x(\overline{P} - P_0)(g - g_\infty)\|_\mu^2 \\
&\geq C\|(\overline{P} - P_0)(g - g_\infty)\|_\mu^2\,,
\end{aligned} \tag{1.31}$$

by a Poincare inequality on $\mathbb{T}^d$, using that $\int_{\mathbb{T}^d}(\overline{P}-P_0)(g-g_\infty)\,dx=0$, pointwise in v. Similarly, $\int_{\mathbb{T}^d}|\nabla_x m_g|^2\,dx \geq C\int_{\mathbb{T}^d}|m_g|^2\,dx$ holds since $\int_{\mathbb{T}^d} m_g\,dx = 0$ by the conservation of momentum. Thus, from (1.24) and (1.31) it follows with $P_1(g)=(\overline{P}-P_0)(g)-m_g\cdot vF'$ (and these two terms being orthogonal) for a constant κ_1 depending on v_0 and F that

$$\frac{d^2}{dt^2}H(g|P(g))\Big|_{g=P(g)} \geq \kappa_1\|P_1(g-g_\infty)\|_\mu^2 = \kappa_1\,H(g|\widetilde{P}(g))\,, \tag{1.32}$$

since, for $g=P(g)$, we have by (1.28) that $g-\widetilde{P}(g)=g-g_\infty-P_0(g-g_\infty)=P_1(g-g_\infty)$.

In the following, we apply the same strategy as for (1.18): first compute the second derivative of the relative entropy with respect to $\widetilde{P}$,

$$\begin{aligned}\frac{d^2}{dt^2}H(g|\widetilde{P}(g)) \;=\;& 2\langle (I-P_0)(v\cdot\nabla_x g - LQ(g)), (I-P_0)(v\cdot\nabla_x g) - LQ(g)\rangle_\mu\\ &+2\langle g-\widetilde{P}(g), \nabla_x\cdot(v(v\cdot\nabla_x g)-vLQ(g)) \qquad (1.33)\\ &-LQ(v\cdot\nabla_x g)+LQ(g)+\nabla_x\cdot P_0(-v(v\cdot\nabla_x g)+vLQ(g))\rangle_\mu\end{aligned}$$

and then consider (1.33) for $g=\widetilde{P}(g)$ with $\widetilde{P}(g)(x,v,t)=\frac{e_g(t,x)}{d}F'(|v|^2/2)+P_1(g_\infty)(|v|^2/2)$

$$\begin{aligned}\frac{d^2}{dt^2}H(g|\widetilde{P}(g))\Big|_{g=\widetilde{P}(g)} &= \frac{2}{d^2}\|(I-P_0)(v\cdot\nabla_x e_g F')\|_\mu^2 = \frac{2}{d^2}\|v\cdot\nabla_x e_g F'\|_\mu^2\\ &= \frac{2}{d^2}\sum_{i,j}\int_R v_i v_j \frac{\partial e_g}{\partial x_i}\frac{\partial e_g}{\partial x_j}|F'|\,dv\,dx = \frac{2}{d}\int_{\mathbb{T}^d}|\nabla_x e_g|^2\,dx\\ &= \frac{2}{d\int_{\mathbb{R}^d}|F'|\,dv}\|\nabla_x e_g F'\|_\mu^2\\ &= \frac{2}{d\int_{\mathbb{R}^d}|F'|\,dv}\|\nabla_x(\widetilde{P}(g)-g_\infty)\|_\mu^2\,.\end{aligned} \tag{1.34}$$

Finally by the Poincare inequality on $\mathbb{T}^d$, we obtain

$$\frac{d^2}{dt^2}H(g|\widetilde{P}(g))\Big|_{g=\widetilde{P}(g)} \geq C\,H(\widetilde{P}(g)|g_\infty)\,. \tag{1.35}$$

Thus, at least formally, the entropy equation (1.18) and the inequalities (1.32) and (1.35) imply that the decay of $H(g|g_\infty)$ can only stop when global equilibrium is reached. In order to quantify this formal information, we generalize (1.32) and (1.35) to all $g\neq P(g)$ and $g\neq\widetilde{P}(g)$, respectively. Herein, we will use the following lemma :

Lemma 1.3.2. *Let Assumption 1.2.1 be satisfied. Then the operators* $\overline{P}, P_0, P_1$, *and, consequently,* P *- defined in (1.5), (1.25), (1.26), and (1.4) - are bounded with respect to* $\|.\|_\mu$.

Proof. The operator $\overline{P}(g)$ is bounded by Jensen's inequality:

$$\|\overline{P}(g)\|_\mu^2 \le \int_R \overline{P}(g^2)\, d\mu = \int_R g^2\, d\mu = \|g\|_\mu^2 \,. \tag{1.36}$$

As for the operator P_0,

$$\|P_0(g)\|_\mu^2 = \frac{\int_{\mathbb{R}^d} |F'|\, dv}{d^2} \int_{\mathbb{T}^d} \left(\int_{\mathbb{R}^d} |v|^2 \overline{P}(g)\, dv \right)^2 dx \,,$$

we obtain the desired estimate with the Cauchy-Schwartz inequality

$$\begin{aligned} \|P_0(g)\|_\mu^2 &\le \frac{\int_{\mathbb{R}^d} |F'|\, dv}{d^2} \int_{\mathbb{T}^d} \int_{\mathbb{R}^d} |v|^4 |F'|\, dv \int_{\mathbb{R}^d} \frac{\overline{P}(g)^2}{|F'|}\, dv\, dx \\ &= C \|\overline{P}(g)\|_\mu^2 \le C\|g\|_\mu^2 \,. \end{aligned}$$

In order to show that P is bounded, we apply again the Cauchy-Schwartz inequality :

$$\begin{aligned} \|F' v \cdot m_g\|_\mu^2 &\le \int_R |F'||v|^2 |m_g|^2\, dv\, dx = C \int_{\mathbb{T}^d} \left(\int_{\mathbb{R}^d} vg\, dv \right)^2 dx \\ &\le \int_{\mathbb{R}^d} |v|^2 |F'|\, dv \int_R \frac{g^2}{|F'|}\, dv\, dx = C\, \|g\|_\mu^2 \,. \end{aligned} \tag{1.37}$$

Finally, the equations (1.36) and (1.37) bound P, and, thus, P_1. □

Theorem 1.3.3. *Let assumptions 1.2.1 and 1.2.2 be satisfied. Then,*

$$\frac{d^2}{dt^2} H(g|P(g)) \ge \kappa_1 H(g|\widetilde{P}(g)) - \delta H(g|g_\infty) - C_1(\varepsilon)\, \delta^{\varepsilon-1} H(g|P(g))^{1-\varepsilon} \tag{1.38}$$

holds for arbitrarily small $1 > \varepsilon > 0$, *and* $\delta > 0$, *and for positive constants* κ_1, *and* $C_1(\varepsilon)$.

Proof. From (1.20) und (1.21),

$$\begin{aligned} \frac{d^2}{dt^2} H(g|P(g)) &= 2\|\nabla_x \cdot LQ(vP(g))\|_\mu^2 - 6\langle LQ(g), v \cdot \nabla_x g\rangle \\ &\quad -2\, \langle \nabla_x \cdot LQ(vLQ(g)), \nabla_x \cdot LQ(v(g+P(g)) \rangle_\mu \\ &\quad +4H(g|P(g)) + 2\langle v \cdot LQ(\nabla_x g), v \cdot \nabla_x g\rangle_\mu \\ &= I_1 + I_2 + I_3 + I_4 + I_5 \,. \end{aligned}$$

For the first term, it follows from (1.32) that $I_1 \geq \kappa_1 H(g|\widetilde{P}(g))$.

As for the remaining terms, we begin by estimating I_3, and for the other integrals similar arguments will apply. For I_3, the x-independence of g_∞ and integration by parts yields

$$I_3 = 2\langle \nabla_x(\nabla_x \cdot LQ(vLQ(g))), LQ(v(I+P)(g-g_\infty))\rangle_\mu . \tag{1.39}$$

Before we are going to apply Hölder's inequality for (1.39), we estimate the two factors as (with ∇_x^2 denoting the gradient tensor product)

$$\begin{aligned} |LQ(\nabla_x^2 LQ(g)v)| &\leq |v| \Big((I+\overline{P})(|\nabla_x{}^2 LQ(g)|) \\ &\qquad + \frac{e_g}{d}|F'|\, \|\nabla_x^2 LQ(g)\|_\mu \Big) , \qquad (1.40) \\ |LQ(v(I+P)(g-g_\infty))| &\leq |v| \Big((I+\overline{P})(I+P)(|g-g_\infty|) \\ &\qquad + \frac{e_g}{d}|F'| \|g-g_\infty\|_\mu \Big) . \qquad (1.41) \end{aligned}$$

Note that for the right hand side of (1.41) assumption 1.2.2 implies $|g|, |g_\infty| \leq C\sqrt{1+|v|^2}|F'|$, and, thus, $(I+\overline{P})(I+P)(|g-g_\infty|) \leq C\sqrt{1+|v|^2}|F'|$. Therefore, splitting $(1.41) = (1.41)^{\varepsilon'}(1.41)^{1-\varepsilon'}$ for all $1 > \varepsilon' > 0$:

$$\begin{aligned} |I_3| \leq C \int_R & |v|^2 (1+|v|^2)^{\frac{\varepsilon'}{2}} |F'|^{\frac{\varepsilon'}{2}} \\ & \times |F'|^{\frac{\varepsilon'-1}{2}} \Big((I+\overline{P})(I+P)(|g-g_\infty|) + \frac{e_g}{d}|F'| \|g-g_\infty\|_\mu \Big)^{1-\varepsilon'} \\ & \times |F'|^{-\frac{1}{2}} \Big((I+\overline{P})(|\nabla_x^2 LQ(g)|) + \frac{e_g}{d}|F'| \|\nabla_x^2 LQ(g)\|_\mu \Big) \, dv \, dx \end{aligned}$$

and Hölder's inequality with the exponents $\frac{2}{\varepsilon'}$, $\frac{2}{1-\varepsilon'}$, and 2 yields (with $\int |v|^{\frac{4}{\varepsilon'}}(1+|v|^2)|F'| \, dv < \infty$ by assumption 1.2.2) :

$$\begin{aligned} |I_3| &\leq C(\varepsilon') \left\| (I+\overline{P})(I+P)(|g-g_\infty|) + \frac{e_g}{d}|F'| \|g-g_\infty\|_\mu \right\|_\mu^{1-\varepsilon'} \\ &\qquad \times \left\| (I+\overline{P})(|\nabla_x^2 LQ(g)|) + \frac{e_g}{d}|F'| \|\nabla_x^2 LQ(g)\|_\mu \right\|_\mu . \end{aligned}$$

Furthermore, by lemma 1.3.2 and Young's inequality with exponents $\frac{2}{1-\varepsilon'}$ and $\frac{2}{1+\varepsilon'}$

$$\begin{aligned} |I_3| &\leq C(\varepsilon') \|g-g_\infty\|_\mu^{1-\varepsilon'} \|\nabla_x^2 LQ(g)\|_\mu , \\ &\leq \Big(\delta H(g|g_\infty) + C(\varepsilon') \delta^{\frac{\varepsilon'-1}{\varepsilon'+1}} \|\nabla_x^2 (LQ(g))\|_\mu^{\frac{2}{1+\varepsilon'}} \Big) , \end{aligned}$$

for all $\delta > 0$. Finally, the global smoothness assumption 1.2.2 permits (compare [10]) to control the derivatives of $LQ(g) = P(g) - g$ by the interpolation

$$\|\nabla_x^2 u\|_{L^2(\mathbb{T}^d)} \leq C(\varepsilon')\, \|u\|_{L^2(\mathbb{T}^d)}^{1-\varepsilon'}\, \|u\|_{H^n(\mathbb{T}^d)}^{\varepsilon'}\,, \qquad \text{for } \; n > \frac{2}{\varepsilon'}\,,$$

and with $\frac{1-\varepsilon'}{1+\varepsilon'} = 1 - \varepsilon$:

$$|I_3| \leq \delta H(g|g_\infty) + C(\varepsilon)\delta^{\varepsilon-1} H(g|P(g))^{1-\varepsilon}.$$

In the same manner, we estimate the terms I_2 and I_5 as

$$\begin{aligned} |I_2| &\leq C(\varepsilon')\,\langle |v||\nabla_x LQ(g)|, |g - g_\infty|\rangle_\mu\,, \\ |I_5| &\leq C(\varepsilon')\,\langle |v|^2|\nabla_x^2 LQ(g)|, |g - g_\infty|\rangle_\mu\,, \end{aligned}$$

and we interpolate the derivatives as above for I_3 to match (1.38).

Finally for I_4, we note that $H(g|P(g) \leq CH(g|P(g))^{1-\varepsilon}$ holds by the bounds of assumption 1.2.2. □

Theorem 1.3.4. *Let assumptions 1.2.1 and 1.2.2 be satisfied. Then,*

$$\frac{d^2}{dt^2} H(g|\widetilde{P}(g)) \geq \kappa_2 H(g|g_\infty) - C_2(\varepsilon)\, H(g|\widetilde{P}(g))^{1-\varepsilon} \tag{1.42}$$

holds for arbitrarily small $1 > \varepsilon > 0$, and for positive constants κ_2 and $C_2(\varepsilon)$.

Proof. We rewrite (1.33) with respect to (1.34) as

$$\begin{aligned} \frac{d^2}{dt^2} H(g|\widetilde{P}(g)) &= 2\|(I - P_0)(v\cdot\nabla_x \widetilde{P}(g))\|_\mu^2 \\ &\quad +2\langle v\cdot\nabla_x P_0(g - g_\infty), (I - P_0)(v\cdot\nabla_x(g - \widetilde{P}(g))\rangle_\mu \\ &\quad +2\langle (I - P_0)(v\cdot\nabla_x(g - \widetilde{P}(g))), v\cdot\nabla_x g - \nabla_x\cdot P_0(vg)\rangle_\mu \\ &\quad +2H(g|P(g)) - 4\langle (I - P_0)(v\cdot\nabla_x g), LQ(g)\rangle_\mu \\ &\quad +2\langle g - \widetilde{P}(g), \nabla_x\cdot(v(v\cdot\nabla_x g)) - \nabla_x\cdot(vLQ(g)) \\ &\quad -LQ(v\cdot\nabla_x g) + LQ(g) - \nabla_x\cdot P_0(v(v\cdot\nabla_x g) - vLQ(g))\rangle_\mu \\ &= \sum_{i=1}^{10} I_i\,. \end{aligned} \tag{1.43}$$

and estimate I_1 with (1.35) and lemma 1.3.1 as :

$$I_1 \geq C(H(g|g_\infty) - H(g|\widetilde{P}(g)))\,.$$

Analogously to the previous proof we estimate I_2:

$$
\begin{aligned}
|I_2| &\leq C \int_R |v|^2 |P_0(g-g_\infty)| |\nabla_x{}^2 (g - \widetilde{P}(g))| \, d\mu \,, \\
&\leq \delta H(g|g_\infty) + C(\varepsilon)\delta^{\varepsilon-1} H(g|\widetilde{P}(g))^{1-\varepsilon}. \qquad (1.44)
\end{aligned}
$$

For I_3, we apply Hölder's inequality similarily to (1.41) and (1.40) after estimating the factors

$$
\begin{aligned}
|(I-P_0)(\nabla_x^2(g-\widetilde{P}(g))v)| &\leq C\Big(|v||\nabla_x{}^2(g-\widetilde{P}(g))| \\
&\qquad + |F'| \int |\nabla_x^2(g-\widetilde{P}(g))|^2 \frac{dv}{|F'|}\Big)\,, \\
|(I-P_0)(v(g-g_\infty))| &\leq C\Big(|v||g-g_\infty| + |F'| \int |g-g_\infty|^2 \frac{dv}{|F'|}\Big)\,,
\end{aligned}
$$

and the second order derivatives are controlled using the same interpolation idea with the global smoothness assumption 1.2.2 as in the previous proof.

Moreover, $|I_4| \leq H(g|\widetilde{P}(g))$ is a consequence of lemma 1.3.5 below. All the remaining terms I_5–I_{10} are estimated with similar arguments as in the proof of the previous theorem and yield bounds of the form (1.44). The proof is completed by choosing δ small enough. □

Lemma 1.3.5. *Let assumptions 1.2.1 and 1.2.2 be satisfied. Then, the inequalities*

$$
\begin{aligned}
H(g|\widetilde{P}(g)) - H(g|P(g)) &\geq 0\,, \qquad (1.45) \\
\frac{d}{dt}\Big(H(g|\widetilde{P}(g)) - H(g|P(g))\Big) &\leq C(\varepsilon)\, H(g|g_\infty)^{1-\varepsilon}\,, \qquad (1.46)
\end{aligned}
$$

hold for arbitrarily small $1 > \varepsilon > 0$ *with a positive constant* $C(\varepsilon)$.

Proof. The identity $H(g|\widetilde{P}(g)) - H(g|P(g)) = ||P_1(g-g_\infty)||_\mu^2 \geq 0$ proves the first inequality. Differentiation with respect to time gives

$$
\frac{d}{dt}||P_1(g-g_\infty)||_\mu^2 = 2\langle P_1(g-g_\infty), P_1(-v\cdot\nabla_x(g-g_\infty) + LQ(g-g_\infty))\rangle_\mu\,,
$$

which is estimated in the same way as in the previous two proofs. □

1.4 A System of Ordinary Differential Inequalities

We introduce $x := H(g|g_\infty)$, $y := H(g|P(g))$, $z := H(g|\widetilde{P}(g))$, and $w := z-y$ in (1.18), (1.38), (1.42), (1.45), and (1.46), and denote time-derivatives by $\frac{d}{dt} = \,'\,$:

$$
\begin{aligned}
x' &= -2y\,, && (1.47)\\
y'' &\geq \kappa_1 z - \delta x - \delta^{\varepsilon_y - 1} C_1(\varepsilon_y)\, y^{1-\varepsilon_y}\,, && (1.48)\\
z'' &\geq \kappa_2 x - C_2(\varepsilon_z)\, z^{1-\varepsilon_z}\,, && (1.49)\\
|w'| &\leq C_3(\varepsilon_w)\, x^{1-\varepsilon_w}\,, && (1.50)
\end{aligned}
$$

where $1 > \varepsilon_y$, ε_z, $\varepsilon_w > 0$ and $\delta > 0$ are arbitrarily small, x, y, z, $w \geq 0$, and κ_1, κ_2, C_1, C_2, and C_3 are positive constants.

We want to deduce decay of $x(t)$ with an arbitrarily high algebraic rate according to arbitrarily small ε_y, ε_z, $\varepsilon_w > 0$. Note that the first three inequalities could be seen as a 'closed' system for x, y, and z. However, the additional information contained in the fourth inequality shall be needed.

The presented proof is quite particular in quantifing different regimes of (1.47)–(1.49) and using (1.50) to prevent rapid oscillations inbetween.

As a preliminary technical result on second-order differential inequalities, we reformulate [12, Lemma 12], which discusses time-averages of the entropy production :

Lemma 1.4.1. *Let $h \in C^2([0,L])$ be nonnegative and satisfy*

$$
h''(t) + C\,h(t)^{1-\varepsilon} \geq \alpha\,, \qquad \text{for } \; 0 \leq t \leq L\,,
$$

with positive constants C, α and $\varepsilon \in (0, \frac{1}{10})$. Then,

- *either L is small : $L \leq 50\, C^{-\frac{1}{2(1-\varepsilon)}}\, \alpha^{\frac{\varepsilon}{2(1-\varepsilon)}}$,*
- *or h is large on the average : $\langle h \rangle_{(0,L)} = \frac{1}{L}\int_0^L h(t)\,dt \geq \frac{1}{100}\left(\frac{\alpha}{C}\right)^{\frac{1}{1-\varepsilon}}$.*

Proof. By introducing the rescaling $\tau = t\sqrt{A}$, $\alpha' = \frac{\alpha}{A}$, we obtain

$$
\frac{d^2 h}{d\tau^2} + h^{1-\varepsilon} \geq \alpha',
$$

where $\tau \in [0, L\sqrt{A}]$ and $L\sqrt{A} = L'$. It then follows from [12, Lemma 12] that

- either L' is small,

$$L' \leq 50\alpha'^{\frac{\varepsilon}{2(1-\varepsilon)}}$$

- or h is large on the average,

$$\langle h\rangle_{(0,L')} \geq \frac{1}{100}\alpha'^{\frac{1}{1-\varepsilon}}.$$

The result now follows by returning to the original variables.

□

Our main result theorem 1.2.2 is a direct consequence of

Theorem 1.4.2. *Let x, y, z, and $w = z - y \geq 0$ be smooth and, for $t > 0$, satisfy (1.47)–(1.50), where $1 > \varepsilon_y$, ε_z, $\varepsilon_w > 0$, and $\delta > 0$ are arbitrarily small. Then, for every sufficiently small $\varepsilon > 0$, there exists a constant $C(\varepsilon) > 0$ such that*

$$x(t) \leq C(\varepsilon)\, t^{-1/\varepsilon}\,. \tag{1.51}$$

Proof. We view (1.51) in the following way: let $t_0 > 0$ be arbitrary with $\alpha_0 = x(t_0)$. The aim is to find an upper bound of the form

$$T_0 \leq C{\alpha_0}^{-\varepsilon} \tag{1.52}$$

on a time T_0 such that $x(t_0 + T_0) = \gamma\alpha_0$, where $\gamma < 1$ is given.

Once such a bound is proven, (1.51) follows as in [10], [12].

At first, we consider (1.48) using $z = w + y \geq w$:

$$y'' \geq \kappa_1 w - \delta x - \delta^{\varepsilon_y - 1}\, C_1\, y^{1-\varepsilon_y}. \tag{1.53}$$

The idea of the following is to deduce 'big' $\langle y\rangle_{(0,L)}$-averages from lemma 2.81, where we distinguish between the cases where w is 'big' in (1.53), and the cases where w is 'small' but y is close to $z = y + w$ and lemma 1.4.1 is used for (1.49). However, the realization of this concept requires some care.

Step 1: We define the set Ω_z (quantifying w 'small') by

$$t \in \Omega_z \Leftrightarrow \mathrm{dist}\,(\mathrm{t}, \{\mathrm{t_0} \leq \tau \leq \mathrm{t_0} + \mathrm{T_0} : \mathrm{w}(\tau) \geq \widetilde{\mathrm{w}}(\alpha_0)\}) \geq \mu(\alpha_0)\,, \tag{1.54}$$

where $\widetilde{w}(\alpha_0)$ and $\mu(\alpha_0)$ are to be chosen later. On the interval $[t_0, t_0 + T_0]$, the set Ω_z and its complement devide into unions of intervals : $\Omega_z = \cup I_z$ and $[t_0, t_0 + T_0]\backslash\Omega_z = \cup I_y$ (where w is 'big'), and lemma 1.4.1 will be applied to (1.48) and (1.49) for I_y and I_z, respectively.

Moreover on I_y, we quantify w 'big' using (1.50), which controls the derivative $|w'|$ in terms of $x \leq x(t_0) = \alpha_0$ (by (1.47))

$$\begin{aligned} w &\geq \widetilde{w}(\alpha_0) - \mu(\alpha_0) \sup_{t_0<\tau<t_0+T_0} |w'(\tau)| \\ &\geq \widetilde{w}(\alpha_0) - C_3\, {\alpha_0}^{1-\varepsilon_w}\, \mu(\alpha_0) =: \widehat{w}(\alpha_0) > 0\,. \end{aligned} \tag{1.55}$$

Step 2: For nonempty intervals I_y, we have by construction of Ω_z (1.54) that the length $\ell(I_y) \geq min\{\mu(\alpha_0), T_0\}$. The following three cases are possible :

Case 1) $[t_0, t_0 + T_0] = \Omega_z$ and there are no intervals I_y,

Case 2) $T_0 \leq \mu(\alpha_0)$ will satisfy (1.52) for suitable $\mu(\alpha_0)$ to be chosen below,

Case 3) $\ell(I_y) \geq \mu(\alpha_0)$: Firstly, we consider $\delta = \delta(\alpha_0)$ to be fixed below, for which estimate with $\alpha(\alpha_0)$ to be chosen below

$$\kappa_1 w - \delta x \geq \kappa_1 \widehat{w}(\alpha_0) - \delta(\alpha_0)\alpha_0 =: \alpha(\alpha_0) > 0\,. \tag{1.56}$$

Then, for (1.48), lemma 1.4.1 applies with $C = C_1/\delta(\alpha_0)^{1-\varepsilon_y}$, $\alpha = \alpha(\alpha_0)$, and $L = \ell(I_y)$. Moreover, due to $\ell(I_y) \geq \mu(\alpha_0)$, we rule out the first case in lemma 2.81 by setting

$$\mu(\alpha_0) \geq 50 \left(C_1 \delta(\alpha_0)^{\varepsilon_y - 1}\right)^{-\frac{1}{2(1-\varepsilon_y)}} \alpha(\alpha_0)^{\frac{\varepsilon_y}{2(1-\varepsilon_y)}}\,. \tag{1.57}$$

Therefore, the second case of lemma 1.4.1 yields

$$\langle y \rangle_{I_y} \geq \frac{1}{100} \left(C_1 \delta^{\varepsilon_y - 1}\right)^{-\frac{1}{1-\varepsilon_y}} \alpha(\alpha_0)^{\frac{1}{1-\varepsilon_y}}\,.$$

Step 3: Next, for the intervals $I_z \subseteq \Omega_z$, it follows by (1.47) that

$$\kappa_2\, x \geq \kappa_2\, x(t_0 + T_0) = \kappa_2 \gamma \alpha_0.$$

Then, applying lemma 1.4.1 to (1.49) yields

- either : $\ell(I_z) \leq 50\, C_2^{-\frac{1}{2(1-\varepsilon_z)}} (\kappa_2 \gamma \alpha_0)^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}}$,
- or : $\langle z \rangle_{I_z} \geq \frac{1}{100} \left(\frac{\kappa_2 \gamma \alpha_0}{C_2}\right)^{\frac{1}{1-\varepsilon_z}}$.

In the second case, equation (1.54) implies with the constant $a_1 = \frac{1}{100}\left(\frac{\kappa_2\gamma}{C_2}\right)^{\frac{1}{1-\varepsilon_z}}$

$$\langle y\rangle_{I_z} = \langle z-w\rangle_{I_z} \geq a_1 {\alpha_0}^{\frac{1}{1-\varepsilon_z}} - \widetilde{w}(\alpha_0) \geq \frac{a_1}{2}\alpha_0^{\frac{1}{1-\varepsilon_z}} ,$$

where we have chosen $\widetilde{w}(\alpha_0) = \frac{a_1}{2}\alpha_0^{\frac{1}{1-\varepsilon_z}}$. Moreover, we set in the definition of Ω_z (1.54) and in (1.56) the choices

$$\begin{aligned} \mu(\alpha_0) &= \frac{a_1}{4C_3}\alpha_0^{\frac{\varepsilon_z}{1-\varepsilon_z}+\varepsilon_w} &\implies \quad \widehat{w}(\alpha_0) &= \frac{a_1}{4}\alpha_0^{\frac{1}{1-\varepsilon_z}} , \\ \delta(\alpha_0) &= \frac{\kappa_1 a_1}{8}\alpha_0^{\frac{\varepsilon_z}{1-\varepsilon_z}} &\implies \quad \alpha(\alpha_0) &= \frac{a_1}{8}\kappa_1\alpha_0^{\frac{1}{1-\varepsilon_z}} . \end{aligned} \tag{1.58}$$

By inserting (1.58) into (1.57) we get the constraint

$$ {\alpha_0}^{\frac{\varepsilon_y}{(1-\varepsilon_y)(1-\varepsilon_z)}-\frac{\varepsilon_z}{1-\varepsilon_z}-2\varepsilon_w} \leq C_1^{\frac{1}{1-\varepsilon_y}} a_2(\gamma,\kappa_1,\kappa_2,C_2,C_3) , \tag{1.59}$$

where - for small ε_y, ε_z, and ε_w - the constant a_2 can be chosen to depend only on γ, κ_1, κ_2, C_2, and C_3. In the following, we choose $\varepsilon_y \leq \frac{1}{2}$ and $\varepsilon_z = \varepsilon_w = \frac{\varepsilon_y}{4}$. Thus the exponent on the right-hand-side of (1.59) is positive, and (1.59) can be satisfy for all possible values of $\alpha_0 \in [0, x(t=0)]$ by making C_1 bigger if necessary (which does not conflict with (1.48)).

We summarize step 2 and step 3 that for every I_y

$$\langle y\rangle_{I_y} \geq a_3(\gamma,\kappa_1,\kappa_2,C_1,C_2)\, {\alpha_0}^{\frac{\varepsilon_z}{1-\varepsilon_z}+\frac{1}{(1-\varepsilon_y)(1-\varepsilon_z)}} , \tag{1.60}$$

and for every I_z that either

$$\ell(I_z) \leq 50\, {\alpha_0}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}} \quad \text{or} \quad \langle y\rangle_{I_z} \geq \frac{a_1}{2}\, {\alpha_0}^{\frac{1}{1-\varepsilon_z}} . \tag{1.61}$$

Step 4: We continue by combining pairs of intervals (I_y, I_z) to their union $\overline{I} := I_y \cup I_z$, where we restrict to the above case 3) : $\ell(I_y) \geq \mu(\alpha_0)$. Then,

$$\langle y\rangle_{\overline{I}} = \frac{\ell(I_y)\langle y\rangle_{I_y} + \ell(I_z)\langle y_z\rangle_{I_z}}{\ell(\overline{I})} = \frac{\ell(I_y)}{\ell(I_y)+\ell(I_z)}\langle y\rangle_{I_y} + \frac{\ell(I_z)}{\ell(I_y)+\ell(I_z)}\langle y\rangle_{I_z} . \tag{1.62}$$

and we consider the two cases according to (1.61) :

1. In the first case in (1.61), $\ell(I_z) \leq 50\, {\alpha_0}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}}$ implies

$$\frac{\ell(I_y)}{\ell(I_z)} \geq a_4(\gamma,\kappa_2,C_2,C_3)\, {\alpha_0}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}+\varepsilon_w} ,$$

with a constant a_4 (and all constants $a_{j=5,\dots}$ from now on) being independent from α_0, ε_y, ε_z, and ε_w. Consequently,

$$\frac{\ell(I_y)}{\ell(I_y)+\ell(I_z)} \geq a_5\,\alpha_0{}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}+\varepsilon_w}\,,$$

and, neglecting the last term in (1.62), we obtain with an exponent $\varepsilon_1(\varepsilon_y,\varepsilon_z,\varepsilon_w)>0$ tending to zero as $\varepsilon_y,\varepsilon_z,\varepsilon_w\to 0$ that

$$\langle y\rangle_{\overline{I}} \geq a_6\,\alpha_0{}^{1+\varepsilon_1}\,. \tag{1.63}$$

2. For the second case in (1.61) and (1.60), both the mean values on I_y and I_z satisfy already estimates of the form (1.63).

Step 5: Finally, we regard the complete interval $[t_0,t_0+T_0]$, where we detail further the cases 1) $-$ 3) from step 2 :

1a) $[t_0,t_0+T_0]=\Omega_z$ and $T_0\leq 50\,\alpha_0{}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}}$.

1b) $[t_0,t_0+T_0]=\Omega_z$ and

$$\langle y\rangle_{[t_0,t_0+T_0]} \geq \frac{a_1}{2}\,\alpha_0{}^{\frac{1}{2(1-\varepsilon_z)}} = a_7\,\alpha_0{}^{1+\varepsilon_1}. \tag{1.64}$$

Integration of (1.47) yields $\alpha_0(1-\gamma)=2T_0\langle y\rangle_{[t_0,t_0+T_0]}$ and, thus, for an $\varepsilon_2(\varepsilon_y,\varepsilon_z,\varepsilon_w)>0$ tending to zero as $\varepsilon_y,\varepsilon_z,\varepsilon_w\to 0$,

$$T_0 \leq a_8\alpha_0{}^{-\varepsilon_2}\,. \tag{1.65}$$

2) $T_0\leq\mu(\alpha_0)$ immediately implies an estimate of the form (1.65).

3a) $\ell(I_y)\geq\mu(\alpha_0)$ for all I_y, and $\#I_y\geq\#I_z$, (where $\#I_y$ and $\#I_z$ denote the numbers of I_y and, respectively, I_z). We can split $[t_0,t_0+T_0]$ into intervals $I=\overline{I}=I_y\cup I_z$ or $I=I_y$, where

$$\langle y\rangle_I \geq a_9\,\alpha_0{}^{1+\varepsilon_1},$$

holds by (1.60) and (1.63), which further implies (1.64) and, thus, (1.65).

3b) $\ell(I_y)\geq\mu(\alpha_0)$ for all I_y and $\#I_z=\#I_y+1$. According to the two cases in (1.61) for the one extra I_z, we either have the situation of case $3a$), or

$$\ell(I_z)\leq 50\,\alpha_0{}^{\frac{\varepsilon_z}{2(1-\varepsilon_z)}} \quad\Longrightarrow\quad \frac{T_0-\ell(I_z)}{T_0}\geq a_{10}\,\alpha_0^{\varepsilon_1}\,,$$

since $T_0-\ell(I_z)\geq\mu(\alpha_0)$. By splitting $[t_0,t_0+T_0]=([t_0,t_0+T_0]\backslash I_z)\cup I_z$ as in (1.62) we again obtain (1.64).

Thus, all cases lead to estimates of the form (1.65), which completes the proof. □

1.5 A Discrete Velocity Model

In this section, we introduce a one-dimensional linear discrete velocity model, for which the entropy dissipation approach leads to the same system of ordinary differential inequalities as for the linearized cometary flow equation. However, the discrete velocity model can be solved explicitly by Fourier expansion, which proves actually exponential convergence to equilibrium. It is interesting to compare the three-velocity model below to the two-velocity model discussed in [**?**], in which the entropy dissipation approach controls local equilibria already by one second order differential inequality like (1.19).

We consider the equation

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = Lf\,, \tag{1.66}$$

with

$$f = (f_+, f_0, f_-)\,, \tag{1.67}$$

periodic boundary conditions in $x \in [0,1)$, and initial condition $f(t=0) = f_I$. We use a matrix-vector notation, and collect the discrete velocities $1, 0$ and -1 in the diagonal matrix

$$v = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{1.68}$$

For the collision operator L, we choose

$$L = \begin{pmatrix} -1/6 & 1/3 & -1/6 \\ 1/3 & -2/3 & 1/3 \\ -1/6 & 1/3 & -1/6 \end{pmatrix}, \tag{1.69}$$

which can be written as $L = P_0 + P_1 - I = \psi_0 \otimes \psi_0 + \psi_1 \otimes \psi_1 - I$, with

$$\psi_0 = \frac{1}{\sqrt{3}}(1,1,1)\,, \qquad P_0 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

$$\psi_1 = \frac{1}{\sqrt{2}}(1,0,-1)\,, \qquad P_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}.$$

Pointing out the similarities between (1.66) and the linearized cometary flow equation, we define - in analogy to section 1.3 - the entropy for (1.66)

$$H(f|g) := ||f - g||^2 ,$$

where $\|\cdot\|$ denotes the norm induced by the scalar product

$$\langle f, g\rangle := \int_0^1 f\cdot g\, dx .$$

Note that ψ_0 and ψ_1 are collision invariants since

$$\psi_i{}^{tr} L = 0 \Leftrightarrow L\psi_i = 0 .$$

Multiplying (1.66) by ψ_i, $i = 0, 1$ yields the conservation laws

$$\frac{\partial}{\partial t}(\psi_i\cdot f) + \frac{\partial}{\partial x}(\psi_i^{tr} v f) = 0 ,$$

where $i = 0$ corresponds to the conservation of mass, and $i = 1$ to the conservation of momentum.

The global equilibrium f_∞ is given by

$$f_\infty = \langle f_I, \psi_0\rangle\psi_0 + \langle f_I, \psi_1\rangle\psi_1 .$$

The local equilibrium is denoted by Pf, where $Pf = P_0 f + P_1 f$.

The time-derivative of the relative entropies with respect to the global equilibrium

$$\frac{d}{dt}H(f|f_\infty) = -2H(f|Pf) ,$$

leads, as in section 1.3, to consider the second time-derivatives of the relative entropies with respect to the local equilibrium

$$\begin{aligned}\frac{d^2}{dt^2}H(f|Pf) &= -2\left\langle Lv\frac{\partial f}{\partial x}, v\frac{\partial f}{\partial x}\right\rangle + 4H(f|Pf) \\ &\quad -6\left\langle Lf, v\frac{\partial f}{\partial x}\right\rangle + 2\left\langle vL\frac{\partial f}{\partial x}, v\frac{\partial f}{\partial x}\right\rangle , \qquad (1.70)\end{aligned}$$

which has the same structure as (1.20) for cometary flow equation.

If we assume that f is in local equilibrium (i.e., $f = Pf$), only the first term on the right hand side of (1.70) contributes, since $v(-L)v = \frac{1}{3}P_1$:

$$\frac{d^2}{dt^2}H(f|Pf)\Big|_{f=Pf} = \frac{2}{3}\left\|\frac{\partial}{\partial x}P_1 f\right\|^2 .$$

However, as for the linearized cometary flow equation, this term may vanish without $f = f_\infty$, and we introduce the projection $\widetilde{P}f = P_0 f + P_1 f_\infty$, with the matrix representation $\widetilde{P} = P_0 + P_1 + P_1 P_0$. Note that $(P - \widetilde{P})f = P_1(f - f_\infty)$, whence

$$\frac{d^2}{dt^2} H(f|\widetilde{P}f) = \frac{d^2}{dt^2} H(f|Pf) + 2\left\| P_1\, v\, \frac{\partial f}{\partial x}\right\|^2 - 2\left\langle P_1 \frac{\partial f}{\partial x}, v^2 \frac{\partial f}{\partial x}\right\rangle . \tag{1.71}$$

By setting $f = \widetilde{P}f$ in (1.71), it immediately follows that

$$\frac{d^2}{dt^2} H(f|\widetilde{P}f)\Big|_{f=\widetilde{P}f} = \int_0^1 \left(\frac{\partial}{\partial x}(f_+ + f_-)\right)^2 dx = \frac{4}{3}\left\|\frac{\partial}{\partial x} P_0 f\right\|^2 \geq C H(f|f_\infty)\,, \tag{1.72}$$

which vanishes if and only if f is in global equilibrium. Now, arbitraily fast algebraic convergence to equilibrium follows from theorems analog to 1.3.3 and 1.3.4 as well as lemma 1.3.5, which can be proven analog to section 1.4.

On the other hand, exponential convergence is shown directly by Fourier expansion,

$$f(x,t) = \sum_{k=-\infty}^{\infty} c_k(t) e^{i2\pi kx}\,. \tag{1.73}$$

Substituting (1.73) into (1.66), the coefficients compare to

$$\partial_t c_k = (L - i2\pi kv) c_k\,,$$

and it follows from the definition of L and v that

$$L - i2\pi kv = \begin{pmatrix} -1/6 - i2\pi k & 1/3 & -1/6 \\ 1/3 & -2/3 & 1/3 \\ -1/6 & 1/3 & -1/6 + i2\pi k \end{pmatrix}. \tag{1.74}$$

The characteristic polynomial of (1.74) is given by

$$p_k(\lambda) = \lambda^3 + \lambda^2 + 4\pi^2 k^2 (\lambda + 2/3)\,.$$

For $k = 0$ (and, thus, $\mu_k = 0$) we recover the double zero eigenvalue corresponding to the two dimensional set of equilibrium distributions. The third eigenvalue for $k = 0$ is $\lambda = -1$. For $k \neq 0$, an application of the Routh-Hurwitz criterion shows that all remaining eigenvalues have negative real parts. It is easily shown that, as $|k| \to \infty$, the three zeroes of p_k are approximated by

$$\lambda_{k1} \approx -\frac{2}{3}\,, \qquad \lambda_{k2} \approx -\frac{1}{6} + 2\pi k i\,, \qquad \lambda_{k3} \approx -\frac{1}{6} - 2\pi k i\,.$$

This proves the existence of a spectral gap and, thus, exponential convergence to equilibrium for (1.66).

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Chapter 2

On the Shockley-Read-Hall Model: Generation-Recombination in Semiconductors

2.1 Introduction

The Shockley-Read-Hall (SRH-)model was introduced in 1952 [22], [14] to describe the statistics of recombination and generation of holes and electrons in semiconductors occurring through the mechanism of trapping.

The transfer of electrons from the valence band to the conduction band is referred to as the generation of electron-hole pairs (or pair-generation process), since not only a free electron is created in the conduction band, but also a hole in the valence band which can contribute to the charge current. The inverse process is termed recombination of electron-hole pairs. The bandgap between the upper edge of the valence band and the lower edge of the conuction band is very large in semiconductors, which means that a big amount of energy is needed for a direct band-to-band generation event. The presence of trap levels within the forbidden band caused by crystal impurities facilitates this process, since the jump can be split into two parts, each of them 'cheaper' in terms of energy. The basic mechanisms are illustrated in Figure 2.1: (a) hole emission (an electron jumps from the valence band to the trapped level), (b) hole capture (an electron moves from an occupied trap to the valence band, a hole disappears), (c) electron emission (an electron jumps from trapped level to the conduction band), (d) electron capture (an electron moves from the conduction band to an unoccupied trap).

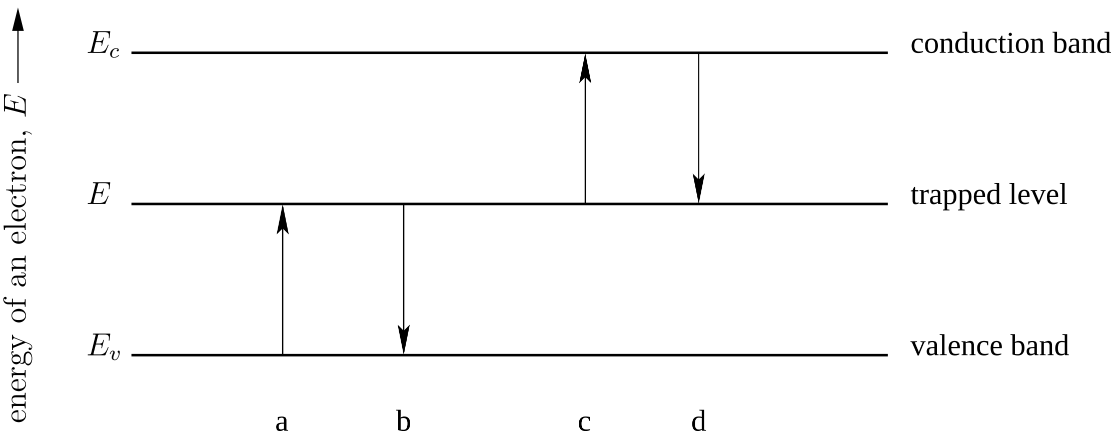

Figure 2.1: The four basic processes of electron-hole recombination.

Models for this process involve equations for the densities of electrons in the conduction band, holes in the valence band, and trapped electrons. Basic for the SRH model are the drift-diffusion assumption for the transport of electrons and holes, the assumption of one trap level in the forbidden band, and the assumption that the dynamics of the trapped electrons is quasistationary, which can be motivated by the smallness of the density of trapped states compared to typical carrier densities. This last assumption leads to the elimination of the density of trapped electrons from the system and to a nonlinear effective recombination-generation rate, reminiscent of Michaelis-Menten kinetics in chemistry. This model is an important ingredient of simulation models for semiconductor devices (see, e.g., [16], [21]).

In this work, two generalizations of the classical SRH model are considered: Instead of a single trapped state, a distribution of trapped states across the forbidden band is allowed and, in a second step, a semiclassical kinetic model including the fermion nature of the charge carriers is introduced. Although direct band-to-band recombination-generation (see, e.g., [20]) and impact ionization (e.g., [6], [7]) have been modelled on the kinetic level before, this is (to the knowledge of the authors) the first attempt to derive a 'kinetic SRH model'.

For both the drift-diffusion and the kinetic models with self consistent electric fields existence results and rigorous results concerning the quasistationary limit are proven. For the drift-diffusion problem, the essential estimate is derived similarly to [12], where the quasineutral limit has been carried out. For the kinetic model Degond's approach [8] for the existence of solutions of the Vlasov-Poisson problem is extended. Actually, the existence theory already provides the uniform estimates necessary for passing to the quasistationary limit.

In the following section, the drift-diffusion based model is formulated and nondimensionalized, and the SRH-model is formally derived. Section 3 contains the rigorous justification of the passage to the quasistationary limit. Section 4 corresponds to Section 2, dealing with the kinetic model, and in Section 5 existence of global solutions for the kinetic model is proven and the quasistationary limit is justified.

2.2 The drift-diffusion Shockley-Read-Hall model

We consider a semiconductor crystal with a forbidden band represented by the energy interval (E_v, E_c) with the valence band edge E_v and the conduction band edge E_c. The constant (in space) number density of trap states N_{tr} is obtained by summing up contributions across the forbidden band:

$$N_{tr} = \int_{E_v}^{E_c} M_{tr}(E)\, dE. \tag{2.1}$$

Here $M_{tr}(E)$ is the energy dependent density of available trapped states. The position density of occupied traps is given by

$$n_{tr}(f_{tr})(x,t) = \int_{E_v}^{E_c} M_{tr}(E) f_{tr}(x,E,t)\, dE, \tag{2.2}$$

where $f_{tr}(x,E,t)$ is the fraction of occupied trapped states at position $x \in \Omega$, energy $E \in (E_v, E_c)$, and time $t \geq 0$. Note that $0 \leq f_{tr} \leq 1$ should hold from a physical point of view.

The governing equations are given by

$$\partial_t f_{tr} = S_p - S_n, \quad S_p = \frac{1}{\tau_p N_{tr}}\big[p_0(1-f_{tr}) - p f_{tr}\big], \quad S_n = \frac{1}{\tau_n N_{tr}}\big[n_0 f_{tr} - n(1-f_{tr})\big] \tag{2.3}$$

$$\partial_t n = \nabla \cdot J_n + R_n, \quad J_n = \mu_n(U_T \nabla n - n\nabla V), \quad R_n = \int_{E_v}^{E_c} S_n M_{tr}\, dE \tag{2.4}$$

$$\partial_t p = -\nabla \cdot J_p + R_p, \quad J_p = -\mu_p(U_T \nabla p + p\nabla V), \quad R_p = \int_{E_v}^{E_c} S_p M_{tr}\, dE \tag{2.5}$$

$$\varepsilon_s \Delta V = q(n + n_{tr}(f_{tr}) - p - C). \tag{2.6}$$

Here $n(x,t) \geq 0$ denotes the density of electrons in the conduction band, whereas $p(x,t) \geq 0$ is the density of holes in the valence band, with electrons and holes being oppositely charged. For the current densities J_n, J_p we use the simplest possible model, the drift diffusion ansatz, with constant mobilities μ_n, μ_p, and with thermal voltage U_T. Moreover, since the trapped states have fixed positions, no flux appears in (2.3).

By R_n and R_p we denote the recombination-generation rates for n and p, respectively. The rate constants are $\tau_n(E)$, $\tau_p(E)$, $n_0(E)$, $p_0(E)$, where $n_0(E)p_0(E) = {n_i}^2$ with the energy independent intrinsic density n_i.

In the Poisson equation (2.6), $V(x,t)$ is the electrostatic potential, ε_s the permittivity of the semiconductor material, q the elementary charge, and $C = C(x)$ the given doping profile.

Note that if τ_n, τ_p, n_0, p_0 are independent from E, or if there exists only one trap level E_{tr} with $M_{tr}(E) = N_{tr}\delta(E-E_{tr})$, then $R_n = \frac{1}{\tau_n}[n_0\frac{n_{tr}}{N_{tr}} - n(1-\frac{n_{tr}}{N_{tr}})]$, $R_p = \frac{1}{\tau_p}[p_0(1-\frac{n_{tr}}{N_{tr}}) - p\frac{n_{tr}}{N_{tr}}]$, and the system for n,p, and n_{tr} is closed by integration of (2.3):

$$\partial_t n_{tr} = R_p - R_n. \tag{2.7}$$

By adding equations (2.4),(2.5),(2.7), we obtain the continuity equation

$$\partial_t(p - n - n_{tr}) + \nabla \cdot (J_n + J_p) = 0, \tag{2.8}$$

with the total charge density $p-n-n_{tr}$ and the total current density $J_n + J_p$.

We now introduce a scaling of n, p, and f_{tr} in order to render the equations (2.4)-(2.6) dimensionless:

Scaling of parameters:

i. $M_{tr} \to \frac{N_{tr}}{E_c - E_v} M_{tr}$.

ii. $\tau_{n,p} \to \bar{\tau}\tau_{n,p}$, where $\bar{\tau}$ is a typical value for τ_n and τ_p.

iii. $\mu_{n,p} \to \bar{\mu}\mu_{n,p}$, where $\bar{\mu}$ is a typical value for $\mu_{n,p}$.

iv. $(n_0, p_0, n_i, C) \to \bar{C}(n_0, p_0, n_i, C)$, where $\bar{C}$ is a typical value of C.

Scaling of unknowns:

v. $(n,p) \to \bar{C}(n,p)$.

vi. $n_{tr} \to N_{tr} n_{tr}$.

vii. $V \to U_T V$.

viii. $f_{tr} \to f_{tr}$.

Scaling of independent variables:

ix. $E \to E_v + (E_c - E_v)E$.

x. $x \to \sqrt{\bar{\mu} U_T \bar{\tau}}\, x$, where the reference length is a typical diffusion length before recombination.

xi. $t \to \bar{\tau} t$, where the reference time is a typical carrier life time.

Dimensionless parameters:

xii. $\lambda = \sqrt{\frac{\varepsilon_s}{q\bar{C}\bar{\mu}\bar{\tau}}} = \frac{1}{\bar{x}}\sqrt{\frac{\varepsilon_s U_T}{q\bar{C}}}$ is the scaled Debye length.

xiii. $\varepsilon = \frac{N_{tr}}{\bar{C}}$ is the ratio of the density of traps to the typical doping density, and will be assumed to be small: $\varepsilon \ll 1$.

The scaled system reads:

$$\varepsilon \partial_t f_{tr} = S_p(p, f_{tr}) - S_n(n, f_{tr}), \quad S_p = \frac{1}{\tau_p}\big[p_0(1 - f_{tr}) - p f_{tr}\big], \quad S_n = \frac{1}{\tau_n}\big[n_0 f_{tr} - n(1 - f_{tr})\big], \tag{2.9}$$

$$\partial_t n = \nabla \cdot J_n + R_n(n, f_{tr}), \quad J_n = \mu_n(\nabla n - n\nabla V), \quad R_n = \int_0^1 S_n M_{tr}\, dE\,, \tag{2.10}$$

$$\partial_t p = -\nabla \cdot J_p + R_p(p, f_{tr}), \quad J_p = -\mu_p(\nabla p + p\nabla V), \quad R_p = \int_0^1 S_p M_{tr}\, dE\,, \tag{2.11}$$

$$\lambda^2 \Delta V = n + \varepsilon n_{tr} - p - C\,, \qquad n_{tr}(f_{tr}) = \int_0^1 f_{tr} M_{tr}\, dE\,, \tag{2.12}$$

with $n_0(E)p_0(E) = n_i^2$ and $\int_0^1 M_{tr} dE = 1$.

By letting $\varepsilon \to 0$ in (2.9) formally, we obtain $f_{tr} = \frac{\tau_n p_0 + \tau_p n}{\tau_n(p+p_0)+\tau_p(n+n_0)}$, and the reduced system has the following form

$$\partial_t n = \nabla \cdot J_n + R(n, p), \tag{2.13}$$

$$\partial_t p = -\nabla \cdot J_p + R(n, p), \tag{2.14}$$

$$R = ({n_i}^2 - np)\int_0^1 \frac{M_{tr}(E)}{\tau_n(E)(p + p_0(E)) + \tau_p(E)(n + n_0(E))}\, dE, \tag{2.15}$$

$$\lambda^2 \Delta V = n - p - C. \tag{2.16}$$

Note that if τ_n, τ_p, n_0, p_0 are independent from E or if there exists only one trap level, then we would have the standard Shockley-Read-Hall model, with

$R = \frac{{n_i}^2 - np}{\tau_n(p+p_0)+\tau_p(n+n_0)}$. Existence and uniqueness of solutions of the limiting system (2.13)–(2.16) under the assumptions (2.21)–(2.25) stated below is a standard result in semiconductor modelling. A proof can be found in, e.g., [16].

2.3 Rigorous derivation of the drift-diffusion Shockley-Read-Hall model

We consider the system (2.9)–(2.12) with the position x varying in a bounded domain $\Omega \in \mathbb{R}^3$ (all our results are easily extended to the one- and two-dimensional situations), the energy $E \in (0,1)$, and time $t > 0$, subject to initial conditions

$$n(x,0) = n_I(x), \quad p(x,0) = p_I(x), \quad f_{tr}(x,E,0) = f_{tr,I}(x,E) \tag{2.17}$$

and mixed Dirichlet-Neumann boundary conditions

$$n(x,t) = n_D(x,t), \quad p(x,t) = p_D(x,t), \quad V(x,t) = V_D(x,t) \quad x \in \partial\Omega_D \subset \partial\Omega \tag{2.18}$$

and

$$\frac{\partial n}{\partial \nu}(x,t) = \frac{\partial p}{\partial \nu}(x,t) = \frac{\partial V}{\partial \nu}(x,t) = 0 \quad x \in \partial\Omega_N := \partial\Omega \setminus \partial\Omega_D, \tag{2.19}$$

where ν is the unit outward normal vector along $\partial\Omega_N$. We permit the special cases that either $\partial\Omega_D$ or $\partial\Omega_N$ are empty. More precisely, we assume that either $\partial\Omega_D$ has positive $(d-1)$-dimensional measure, or it is empty. In the second situation ($\partial\Omega_D$ empty) we have to assume total charge neutrality, i.e.,

$$\int_\Omega (n + \varepsilon n_{tr} - p - C)\, dx = 0\,, \qquad \text{if } \partial\Omega = \partial\Omega_N\,. \tag{2.20}$$

The potential is then only determined up to a (physically irrelevant) additive constant.

The following assumptions on the data will be used: For the boundary data

$$n_D, p_D \in W^{1,\infty}_{loc}(\Omega \times \mathbb{R}^+_t), \quad V_D \in L^\infty_{loc}(\mathbb{R}^+_t, W^{1,6}(\Omega)), \tag{2.21}$$

for the initial data

$$n_I, p_I \in H^1(\Omega) \cap L^\infty(\Omega), \quad 0 \le f_{tr,I} \le 1\,, \tag{2.22}$$

$$\textstyle\int_\Omega (n_I + \varepsilon n_{tr}(f_{tr,I}) - p_I - C)\, dx = 0\,, \qquad \text{if } \partial\Omega = \partial\Omega_N\,, \tag{2.23}$$

for the doping profile

$$C \in L^\infty(\Omega)\,, \tag{2.24}$$

for the recombination-generation rate constants

$$n_0, p_0, \tau_n, \tau_p \in L^\infty((0,1))\,, \quad \tau_n, \tau_p \geq \tau_{min} > 0\,. \tag{2.25}$$

We shall first prove local existence of solutions for fixed positive ε by a contraction argument, following the lines of [11], [16]. We define the fixed point map $F : \{n, p, f_{tr}\} \to \{u, v, u_{tr}\}$ by the following:

Step 1: For n,p, f_{tr} given (satisfying (2.20) if $\partial\Omega = \partial\Omega_N$), we obtain V by solving the problem (2.12),(2.18), (2.19); if $\partial\Omega_D$ has a positive measure, the solution exists and it is unique for all t. For empty $\partial\Omega_D$ the assumption (2.20) implies solvability and uniqueness up to a constant, whose value is unimportant for the following.

Step 2: We obtain the new trap occupancy u_{tr} from

$$\begin{gathered}\varepsilon\partial_t u_{tr} = \tfrac{1}{\tau_p}\big[p_0(1-u_{tr}) - p u_{tr}\big] - \tfrac{1}{\tau_n}\big[n_0 u_{tr} - n(1-u_{tr})\big]\,, \\ u_{tr}|_{t=0} = f_{tr,I}\,,\end{gathered} \tag{2.26}$$

the new electron density u from

$$\begin{gathered}\partial_t u = \nabla\cdot(\mu_n(\nabla u - n\nabla V)) + R_n(n, u_{tr})\,, \\ u|_{\partial\Omega_D} = n_D, \quad \tfrac{\partial u}{\partial\nu}|_{\partial\Omega_N} = 0, \quad u|_{t=0} = n_I\,,\end{gathered} \tag{2.27}$$

and the new hole density v from

$$\begin{gathered}\partial_t v = \nabla\cdot(\mu_p(\nabla v + p\nabla V) + R_p(p, u_{tr})\,, \\ v|_{\partial\Omega_D} = p_D, \quad \tfrac{\partial v}{\partial\nu}|_{\partial\Omega_N} = 0, \quad v|_{t=0} = p_I\,.\end{gathered}$$

For the fixed point argument we shall use the following norm:

$$\|(n,p,f_{tr})\|_T = \max_{0\leq t\leq T}\left\{\|n(t)\|_{L^2(\Omega)} + \|p(t)\|_{L^2(\Omega)} + \|f_{tr}(t)\|_{L^2(\Omega\times(0,1))}\right\} \tag{2.28}$$

$$+\left(\int_0^T\left(\|\nabla n(t)\|^2_{L^2(\Omega)} + \|\nabla p(t)\|^2_{L^2(\Omega)}\right)dt\right)^{1/2}. \tag{2.29}$$

Note that the property (2.20) is preserved in case of a pure Neumann problem. We now show that the map F is contractive for a sufficiently small time interval $(0,T)$ on a ball with sufficiently large radius a around the initial data (considered as constant functions of time):

$$M_a := \{(n,p,f_{tr}) :\ 0 \le f_{tr} \le 1,\ \|(n-n_I, p-p_I, f_{tr}-f_{tr,I})\|_T \le a\}. \tag{2.30}$$

First, let us show that F maps M_a into itself. We observe that the equation for u_{tr} preserves the natural bounds for the initial data: $0 \le u_{tr} \le 1$. Multiplication of (2.26) by $u_{tr} - f_{tr,I}$ and straightforward estimation gives

$$\max_{[0,T]} \|u_{tr} - f_{tr,I}\|_{L^2(\Omega\times(0,1))} \le \frac{T\gamma(a)}{\varepsilon} \le \frac{a}{5}\,, \tag{2.31}$$

for any a by choosing T small enough.

Multiplication of (2.27) by $u - n_D$ ($n_D = 0$ for the pure Neumann problem) and integration by parts gives

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega (u-n_D)^2\,dx = -\mu_n \int_\Omega |\nabla u|^2\,dx + \mu_n \int_\Omega \nabla u \cdot (n\nabla V + \nabla n_D) \\ - \mu_n \int_\Omega n\nabla V \cdot \nabla n_D\,dx + \int_\Omega (u-n_D)(R_n - \partial_t n_D)\,dx\end{aligned} \tag{2.32}$$

For estimating the right hand side we use the Cauchy-Schwarz inequality, the assumptions on boundary and initial data, the estimate $|R_n(n,u_{tr})| \le C(n+1)$, and the fact that $(n,p,f_{tr}) \in M_a$:

$$\frac{1}{2}\frac{d}{dt}\|u-n_D\|^2_{L^2(\Omega)} \le -\frac{\mu_n}{2}\|\nabla(u-n_I)\|^2_{L^2(\Omega)} + C(\gamma(a) + \|n\nabla V\|^2_{L^2(\Omega)} + \|u-n_D\|^2_{L^2(\Omega)})\,. \tag{2.33}$$

For estimating the nonlinear term $n\nabla V$ we employ the Hölder inequality, the Gagliardo-Nirenberg inequality, the Poisson equation, and the Sobolev imbedding theorem:

$$\begin{aligned}\|n\nabla V\|_{L^2(\Omega)} &\le \|n\|_{L^3(\Omega)}\|\nabla V\|_{L^6(\Omega)} \\ &\le (C(\delta)\|n\|_{L^2(\Omega)} + \delta\|\nabla n\|_{L^2(\Omega)})(\|n+p\|_{L^2(\Omega)} + \|f_{tr}\|_{L^2(\Omega\times(0,1))} + 1)\end{aligned} \tag{2.34}$$

for any $\delta > 0$, which leads to the estimate (using the definition of M_a)

$$\int_0^T \|n\nabla V\|^2_{L^2(\Omega)} dt \le \gamma(a)(TC(\delta) + \delta)\,. \tag{2.35}$$

As a consequence, the Gronwall lemma applied to (2.33) implies

$$\max_{[0,T]} \|u-n_D\|^2_{L^2(\Omega)} \le \|n_I - n_D\|^2_{L^2(\Omega)} + \gamma(a)(r(T)C(\delta) + \delta)\,, \tag{2.36}$$

with $r(T) \to 0$ for $T \to 0$, and, therefore,

$$\max_{[0,T]} \|u - n_I\|^2_{L^2(\Omega)} \leq 2\|n_I - n_D\|^2_{L^2(\Omega)} + \gamma(a)(r(T)C(\delta) + \delta) \leq \frac{a^2}{25}, \quad (2.37)$$

where the last inequality is achieved by first choosing a big enough, then δ small enough, and then T small enough.

Analogously, we prove

$$\max_{[0,T]} \|v - p_I\|_{L^2(\Omega)} \leq \frac{a}{5}. \quad (2.38)$$

As for the integral terms in the norm, we obtain from (2.33) after integration with respect to time

$$\frac{\mu_n}{2} \int_0^T \|\nabla(u - n_I)\|^2_{L^2(\Omega)} dt \leq \frac{1}{2}\|n_I - n_D\|^2_{L^2(\Omega)} + T\gamma(a) \leq \frac{\mu_n}{2}\frac{a^2}{25},$$

such that

$$\left(\int_0^T \|\nabla(u - n_I)\|^2_{L^2(\Omega)} dt\right)^{1/2} \leq \frac{a}{5}. \quad (2.39)$$

Note that again a has to be chosen big enough, and T small enough. The same estimate holds for $\nabla(v - p_I)$. Combining it with (2.31), (2.37), (2.38), and (2.39), $F:\ M_a \to M_a$ has been proven.

The next step is to prove that F is a contraction. For the components of the difference

$$(\delta u, \delta v, \delta u_{tr}) = F(n_1, p_1, f_{tr,1}) - F(n_2, p_2, f_{tr,2}) \quad (2.40)$$

we obtain the problems

$$\varepsilon \partial_t \delta u_{tr} = -\kappa \delta u_{tr} + A_n \delta n + A_p \delta p, \quad (2.41)$$
$$\delta u_{tr}|_{t=0} = 0,$$

with $\kappa = \frac{p_0+p_1}{\tau_p} + \frac{n_0+n_1}{\tau_n}$, $A_n = \frac{1-u_{tr,2}}{\tau_n}$, $A_p = -\frac{u_{tr,2}}{\tau_p}$, $\delta n = n_1 - n_2$ etc., for δu_{tr},

$$\partial_t \delta u = \nabla \cdot (\mu_n(\nabla \delta u - n_1 \nabla \delta V - \delta n \nabla V_2)) + R_n(n_1, u_{tr,1}) - R_n(n_2, u_{tr,2}) \quad (2.42)$$
$$\delta u|_{\partial\Omega_D} = 0, \quad \tfrac{\partial \delta u}{\partial \nu}|_{\partial\Omega_N} = 0, \quad \delta u|_{t=0} = 0,$$

for δu, and

$$\partial_t \delta v = \nabla \cdot (\mu_p(\nabla \delta v + p_1 \nabla \delta V + \delta p \nabla V_2)) + R_p(p_1, u_{tr,1}) - R_p(p_2, u_{tr,2}) \quad (2.43)$$
$$\delta v|_{\partial\Omega_D} = 0, \quad \tfrac{\partial \delta v}{\partial \nu}|_{\partial\Omega_N} = 0, \quad \delta v|_{t=0} = 0,$$

for δv.

The following estimates are very similar to the above. Multiplication of (2.41) by δu_{tr} and a simple estimation shows that

$$\max_{[0,T]} \|\delta u_{tr}\|_{L^2(\Omega\times(0,1))} \le \frac{r(T)}{\varepsilon}\|(\delta n, \delta p, \delta f_{tr})\|_T \,, \tag{2.44}$$

with $\lim_{T\to 0} r(T) = 0$.

Multiplying (2.42) with δu, integrating with respect to x and t, we obtain

$$\begin{aligned} &\frac{1}{2}\|\delta u(t)\|^2_{L^2(\Omega)} + \frac{\mu_n}{2}\int_0^t \|\nabla \delta u(s)\|^2_{L^2(\Omega)}\, ds \\ &\le C\int_0^t \left(\|\delta n \nabla V_2\|^2_{L^2(\Omega)} + \|n_1 \nabla \delta V\|^2_{L^2(\Omega)} + \|\delta n\|^2_{L^2(\Omega)} + \|\delta f_{tr}\|^2_{L^2(\Omega)} + \|\delta u\|^2_{L^2(\Omega)}\right) ds. \end{aligned} \tag{2.45}$$

The first two terms on the right hand side we estimate analogously to (2.34), leading to

$$\begin{aligned} &\int_0^t \left(\|\delta n \nabla V_2\|^2_{L^2(\Omega)} + \|n_1 \nabla \delta V\|^2_{L^2(\Omega)} + \|\delta n\|^2_{L^2(\Omega)} + \|\delta f_{tr}\|^2_{L^2(\Omega)}\right) ds \\ &\le (r(T)C(\delta) + \delta)\|(\delta n, \delta p, \delta f_{tr})\|_T \,. \end{aligned}$$

Application of the Gronwall lemma to (2.45), the analogous estimate for δv, and a combination of these results with (2.44) finally lead to

$$\|(\delta u, \delta v, \delta u_{tr})\|_T \le \left(\frac{r(T)C(\delta)}{\epsilon} + \delta\right))\|(\delta n, \delta p, \delta f_{tr})\|_T \,. \tag{2.46}$$

By choosing first δ and then T sufficiently small, F can be made contractive in M_a. Summarizing, the following local existence result has been proven.

Theorem 2.3.1. *Let the assumptions (2.21)–(2.25) hold. Then there exists $T > 0$, such that the problem (2.9)–(2.12), (2.17)–(2.19) has a unique solution with $n, p \in C([0,T], L^2(\Omega)) \cap L^2((0,T), H^1(\Omega))$, $f_{tr} \in C([0,T], L^2(\Omega \times (0,1)))$, $0 \le f_{tr} \le 1$.*

It is obvious from (2.46) that the local existence result does not come with a uniform in ϵ estimate. Even the guaranteed existence time tends to zero with ε. The following global existence result with uniform (in ε) bounds is a generalization of [12, Lemma 3.1], where the case of homogeneous Neumann boundary conditions and vanishing recombination was treated. Our proof uses a similar approach.

Lemma 2.3.2. *Let the assumptions of Theorem 2.3.1 be satisfied. Then, the solution of (2.9)–(2.12), (2.17)–(2.19) exists for all times and satisfies* $n, p \in L^\infty_{loc}((0,\infty), L^\infty(\Omega)) \cap L^2_{loc}((0,\infty), H^1(\Omega)))$ *uniformly in* ε *as* $\varepsilon \to 0$ *as well as* $0 \le f_{tr} \le 1$.

Proof. Global existence will be a consequence of the following estimates. Introducing the new variables $\widetilde{n} = n - n_D$, $\widetilde{p} = p - p_D$, $\widetilde{C} = C - \varepsilon n_{tr} - n_D + p_D$ the equations (2.10)–(2.12) take the following form:

$$\partial_t \widetilde{n} = \nabla \cdot J_n + R_n - \partial_t n_D, \quad J_n = \mu_n \big[\nabla \widetilde{n} + \nabla n_D - (\widetilde{n} + n_D)\nabla V\big], \tag{2.47}$$

$$\partial_t \widetilde{p} = -\nabla J_p + R_p - \partial_t p_D, \quad J_p = -\mu_p \big[\nabla \widetilde{p} + \nabla p_D + (\widetilde{p} + p_D)\nabla V\big], \tag{2.48}$$

$$\lambda^2 \Delta V = \widetilde{n} - \widetilde{p} - \widetilde{C}\,. \tag{2.49}$$

As a consequence of $0 \le f_{tr} \le 1$, $\widetilde{C} \in L^\infty((0,\infty) \times \Omega)$ holds. For $q \ge 2$ and even, we multiply (2.47) by $\widetilde{n}^{q-1}/\mu_n$, (2.48) by $\widetilde{p}^{q-1}/\mu_p$, and add:

$$\begin{aligned}
\frac{d}{dt} \int_\Omega \left[\frac{\widetilde{n}^q}{q\mu_n} + \frac{\widetilde{p}^q}{q\mu_p}\right] dx &= -(q-1) \int_\Omega \widetilde{n}^{q-2} \nabla \widetilde{n} \nabla n \, dx - (q-1) \int_\Omega \widetilde{p}^{q-2} \nabla \widetilde{p} \nabla p \, dx \\
&\quad + (q-1) \int_\Omega \left[\widetilde{n}^{q-2} n \nabla \widetilde{n} \, - \, \widetilde{p}^{q-2} p \nabla \widetilde{p}\right] \nabla V \, dx \\
&\quad + \int_\Omega \frac{\widetilde{n}^{q-1}}{\mu_n} (R_n - \partial_t n_D) + \int_\Omega \frac{\widetilde{p}^{q-1}}{\mu_p} (R_p - \partial_t p_D) \\
&=: I_1 + I_2 + I_3 + I_4 + I_5.
\end{aligned} \tag{2.50}$$

Using the assumptions on n_D, p_D and $|R_n| \le C(n+1)$, $|R_p| \le C(p+1)$, we estimate

$$I_4 \le C \int_\Omega |\widetilde{n}|^{q-1} (n+1) \, dx \le C \left(\int_\Omega \widetilde{n}^q \, dx + 1 \right), \quad I_5 \le C \left(\int_\Omega \widetilde{p}^q \, dx + 1 \right).$$

The term I_3 can be rewritten as follows:

$$\begin{aligned}
I_3 &= \int_\Omega \left[\widetilde{n}^{q-1} \nabla \widetilde{n} - \widetilde{p}^{q-1} \ \nabla \widetilde{p}\right] \nabla V \, dx \\
&\quad + \int_\Omega \left[\widetilde{n}^{q-2} \nabla \widetilde{n}\right] (n_D \nabla V) \, dx - \int_\Omega \left[\widetilde{p}^{q-2} \nabla \widetilde{p}\right] (p_D \nabla V) \, dx \\
&= -\frac{1}{\lambda^2 q} \int_\Omega \left[\widetilde{n}^q - \widetilde{p}^q\right] (\widetilde{n} - \widetilde{p} - \widetilde{C}) \, dx \\
&\quad - \frac{1}{\lambda^2 (q-1)} \int_\Omega \widetilde{n}^{q-1} \left(\nabla n_D \nabla V + \, n_D (\widetilde{n} - \widetilde{p} - \widetilde{C})\right) \, dx \\
&\quad + \frac{1}{\lambda^2 (q-1)} \int_\Omega \widetilde{p}^{q-1} \left(\nabla p_D \nabla V + \, p_D (\widetilde{n} - \widetilde{p} - \widetilde{C})\right) \, dx.
\end{aligned}$$

The second equality uses integration by parts and (2.49). The first term on the right hand side is the only term of degree $q+1$. It reflects the quadratic nonlinearity of the problem. Fortunately, it can be written as the sum of a term of degree q and a nonnegative term. By estimation of the terms of degree q using the assumptions on n_D and p_D as well as $\|\nabla V\|_{L^q(\Omega)} \leq C(\|\widetilde{n}\|_{L^q(\Omega)} + \|\widetilde{p}\|_{L^q(\Omega)} + \|\widetilde{C}\|_{L^q(\Omega)})$, we obtain

$$
\begin{aligned}
I_3 &\leq -\frac{1}{\lambda^2 q}\int_\Omega [\widetilde{n}^q - \widetilde{p}^q]\,(\widetilde{n} - \widetilde{p})\,dx + C\left(\int_\Omega (\widetilde{n}^q + \widetilde{p}^q)\,dx + 1\right) \\
&\leq C\left(\int_\Omega (\widetilde{n}^q + \widetilde{p}^q)\,dx + 1\right).
\end{aligned}
$$

The integral I_1 can be written as

$$
I_1 = -\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2 dx + \int_\Omega \widetilde{n}^{q-2}\nabla n_D \nabla n\,dx. \tag{2.51}
$$

By rewriting the integrand in the second integral as

$$
\widetilde{n}^{q-2}\nabla n_D \nabla n = \widetilde{n}^{\frac{q-2}{2}}\nabla n \widetilde{n}^{\frac{q-2}{2}}\nabla n_D
$$

and applying the Cauchy-Schwarz inequality, we have the following estimate for (2.51):

$$
\begin{aligned}
I_1 &\leq -\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2 dx + \sqrt{\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2 dx \int_\Omega \widetilde{n}^{q-2}|\nabla n_D|^2 dx} \\
&\leq -\frac{1}{2}\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2 dx + C\|\widetilde{n}\|_{L^q}^{q-2} \leq -\frac{1}{2}\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2 dx + C\left(\int_\Omega \widetilde{n}^q\,dx + 1\right).
\end{aligned} \tag{2.52}
$$

For I_2, the same reasoning (with n and n_D replaced by p and p_D, respectively) yields an analogous estimate. Collecting our results, we obtain

$$
\begin{aligned}
\frac{d}{dt}\int_\Omega \left[\frac{\widetilde{n}^q}{q\mu_n} + \frac{\widetilde{p}^q}{q\mu_p}\right] dx &\leq -\frac{1}{2}\int_\Omega \widetilde{n}^{q-2}|\nabla n|^2\,dx - \frac{1}{2}\int_\Omega \widetilde{p}^{q-2}|\nabla p|^2\,dx \\
&\quad + C\left(\int_\Omega (\widetilde{n}^q + \widetilde{p}^q)\,dx + 1\right).
\end{aligned} \tag{2.53}
$$

Since $q \geq 2$ is even, the first two terms on the right hand side are nonpositive and the Gronwall lemma gives

$$
\int_\Omega (\widetilde{n}^q + \widetilde{p}^q) dx \leq e^{qCt}\left(\int_\Omega (\widetilde{n}(t=0)^q + \widetilde{p}(t=0)^q) dx + 1\right).
$$

A uniform-in-q-and-ε estimate for $\|n\|_{L^q}$, $\|p\|_{L^q}$ follows, and the uniform-in-ε bound in $L^\infty_{loc}((0,\infty), L^\infty(\Omega))$ is obtained in the limit $q \to \infty$. The estimate in $L^2_{loc}((0,\infty), H^1(\Omega))$ is then derived by returning to (2.53) with $q = 2$. □

Now we are ready for proving the main result of this section.

Theorem 2.3.3. *Let the assumptions of Theorem 2.3.1 be satisfied. Then, as $\varepsilon \to 0$, for every $T > 0$, the solution (f_{tr}, n, p, V) of (2.9)–(2.12), (2.17)–(2.19) converges with convergence of f_{tr} in $L^\infty((0,T) \times \Omega \times (0,1))$ weak*, n and p in $L^2((0,T) \times \Omega)$, and V in $L^2((0,T), H^1(\Omega))$. The limits of n, p, and V satisfy (2.13)–(2.19)*

Proof. The L^∞-bounds for f_{tr}, n, and p, and the Poisson equation (2.12) imply $\nabla V \in L^2((0,T) \times \Omega)$. From the definition of J_n,J_p (see (2.4),(2.5)), it then follows that $J_n, J_p \in L^2((0,T) \times \Omega)$. Then (2.10) and (2.11) together with $R_n, R_p \in L^\infty((0,T) \times \Omega)$ imply $\partial_t n, \partial_t p \in L^2((0,T), H^{-1}(\Omega))$. The previous result and the Aubin lemma (see, e.g., Simon [23, Corollary 4, p. 85]) gives compactness of n and p in $L^2((0,T) \times \Omega)$.

We already know from the Poisson equation that $\nabla V \in L^\infty((0,T), H^1(\Omega))$. By taking the time derivative of (2.12), one obtains

$$\partial_t \Delta V = \nabla \cdot (J_n + J_p) \,,$$

with the consequence that $\partial_t \nabla V$ is bounded in $L^2((0,T) \times \Omega)$. Therefore, the Aubin lemma can again be applied as above to prove compactness of ∇V in $L^2((0,T) \times \Omega)$.

These results and the weak compactness of f_{tr} are sufficient for passing to the limit in the nonlinear terms $n\nabla V$, $p\nabla V$, nf_{tr}, and pf_{tr}. By the uniqueness result for the limiting problem (mentioned at the end of Section 2), the convergence is not restricted to subsequences. □

2.4 A kinetic Shockley-Read-Hall model

In this section we replace the drift-diffusion model for electrons and holes by a semiclassical kinetic transport model. It is governed by the system

$$\partial_t f_n + v_n(k) \cdot \nabla_x f_n + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f_n = Q_n(f_n) + Q_{n,r}(f_n, f_{tr}), \quad (2.54)$$

$$\partial_t f_p + v_p(k) \cdot \nabla_x f_p - \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f_p = Q_p(f_p) + Q_{p,r}(f_p, f_{tr}), \quad (2.55)$$

$$\partial_t f_{tr} = Q_{tr,r} = Q_{tr,p}(f_p, f_{tr}) - Q_{tr,n}(f_n, f_{tr}), \quad (2.56)$$

$$\varepsilon_s \Delta_x V = q(n + n_{tr} - p - C), \quad (2.57)$$

where $f_i(x,k,t)$ represents the particle distribution function (with $i=n$ for electrons and $i=p$ for holes) at time $t \geq 0$, at the position $x \in \mathbb{R}^3$, and at the wave vector (or generalized momentum) $k \in \mathbb{R}^3$. All functions of k have the periodicity of the reciprocal lattice of the semiconductor crystal. Equivalently, we shall consider only $k \in B$, where B is the Brillouin zone, i.e., the set of all k which are closer to the origin than to any other lattice point, with periodic boundary conditions on ∂B.

The coefficient functions $v_n(k)$ and $v_p(k)$ denote the electron and hole velocities, respectively, which are related to the electron and hole band diagrams by

$$v_n(k) = \nabla_k \varepsilon_n(k)/\hbar, \quad v_p(k) = -\nabla_k \varepsilon_p(k)/\hbar, \tag{2.58}$$

where $\hbar$ is the reduced Planck constant. The elementary charge is denoted by q.

The collision operators Q_n and Q_p describe the interactions between the particles and the crystal lattice. They involve several physical phenomena and can be written in the general form

$$Q_n(f_n) = \int_B \widetilde{\Phi}_n(k,k')[M_n f_n'(1-f_n) - M_n' f_n(1-f_n')]dk', \tag{2.59}$$

$$Q_p(f_p) = \int_B \widetilde{\Phi}_p(k,k')[M_p f_p'(1-f_p) - M_p' f_p(1-f_p')]dk', \tag{2.60}$$

with the primes denoting evaluation at k', with the nonnegative, symmetric scattering cross sections $\widetilde{\Phi}_n(k,k')$ and $\widetilde{\Phi}_p(k,k')$, and with the Maxwellians

$$M_n(k) = c_n \exp(-\varepsilon_n(k)/k_B T), \quad M_p(k) = c_p \exp(-\varepsilon_p(k)/k_B T),$$

where $k_B T$ is the thermal energy of the semiconductor crystal lattice and the constants c_n, c_p are chosen such that

$$\int_B M_n \, dk = \int_B M_p \, dk = 1.$$

The remaining collision operators $Q_{n,r}(f_n, f_{tr})$ and $Q_{p,r}(f_p, f_{tr})$ model the generation and recombination processes and are given by

$$Q_{n,r}(f_n, f_{tr}) = \int_{E_v}^{E_c} S_n(f_n, f_{tr}) M_{tr} \, dE \,, \tag{2.61}$$

with

$$S_n(f_n, f_{tr}) = \frac{\Phi_n(k,E)}{N_{tr}} \left[n_0 M_n f_{tr}(1-f_n) - f_n(1-f_{tr}) \right] \,,$$

and

$$Q_{p,r}(f_p, f_{tr}) = \int_{E_v}^{E_c} S_p(f_p, f_{tr}) M_{tr} \, dE \,, \tag{2.62}$$

with

$$S_p(f_p, f_{tr}) = \frac{\Phi_p(k,E)}{N_{tr}} \left[p_0 M_p(1-f_p)(1-f_{tr}) - f_p f_{tr}\right] ,$$

and where $M_{tr}(x,E)$ is the density of available trapped states as for the drift diffusion model, except that we allow for a position dependence now. This will be commented on below. The parameter N_{tr} is now determined as $N_{tr} = \sup_{x\in\mathbb{R}^3} \int_0^1 M_{tr}(x,E)dE$.

The right hand side in the equation for the occupancy $f_{tr}(x,E,t)$ of the trapped states is defined by

$$Q_{tr,n}(f_n, f_{tr}) = \int_B S_n \, dk = \lambda_n[n_0 M_n(1-f_n)]f_{tr} - \lambda_n[f_n](1-f_{tr}), \quad (2.63)$$

with $\lambda_n[g] = \int_B \Phi_n g \, dk$, and

$$Q_{tr,p}(f_p, f_{tr}) = \int_B S_p \, dk = \lambda_p[p_0 M_p(1-f_p)](1-f_{tr}) - \lambda_p[f_p]f_{tr}, \quad (2.64)$$

with $\lambda_p[g] = \int_B \Phi_p g \, dk$.

The factors $(1-f_n)$ and $(1-f_p)$ take into account the Pauli exclusion principle, which therefore manifests itself in the requirement that the values of the distribution function have to respect the bounds $0 \le f_n, f_p \le 1$.

The position densities on the right hand side of the Poisson equation (2.57) are given by

$$n(x,t) = \int_B f_n dk \, , \quad p(x,t) = \int_B f_p dk \, , \quad n_{tr}(x,t) = \int_{E_v}^{E_c} f_{tr} M_{tr} dE \, .$$

The following scaling, which is strongly related to the one used for the drift-diffusion model, will render the equations (2.54)- (2.57) dimensionless:

Scaling of parameters:

i. $M_{tr} \to \frac{N_{tr}}{E_v - E_c} M_{tr}$,

ii. $(\varepsilon_n, \varepsilon_p) \to k_B T(\varepsilon_n, \varepsilon_p)$, with the thermal energy $k_B T$,

iii. $(\Phi_n, \Phi_p, \widetilde{\Phi}_n, \widetilde{\Phi}_p) \to \overline{\tau}^{-1}(\Phi_n, \Phi_p, \widetilde{\Phi}_n, \widetilde{\Phi}_p)$, where $\overline{\tau}$ is a typical carrier life time,

iv. $(n_0, p_0, C) \to \overline{C}(n_0, p_0, C)$, where $\overline{C}$ is a typical value of $|C|$,

v. $(M_n, M_p) \to \overline{C}^{-1}(M_n, M_p)$.

Scaling of independent variables:

vi. $x \to k_B T \overline{\tau}\,\overline{C}^{-1/3} \hbar^{-1} x$,

vii. $t \to \overline{\tau} t$,

viii. $k \to \overline{C}^{1/3} k$,

ix. $E \to E_v + (E_c - E_v)E$,

Scaling of unknowns:

x. $(f_n, f_p, f_{tr}) \to (f_n, f_p, f_{tr})$,

xi. $V \to U_T V$, with the thermal voltage $U_T = k_B T/q$.

Dimensionless parameters:

xii. $\lambda = \frac{\hbar}{q\overline{\tau}\,\overline{C}^{1/6}} \sqrt{\frac{\varepsilon_s}{k_B T}}$,

xiii. $\varepsilon = \frac{N_{tr}}{\overline{C}}$, where again we shall study the situation $\varepsilon \ll 1$.

Finally, the scaled system reads

$$\partial_t f_n + v_n(k) \cdot \nabla_x f_n + \nabla_x V \cdot \nabla_k f_n = Q_n(f_n) + Q_{n,r}(f_n, f_{tr}), \tag{2.65}$$
$$\partial_t f_p + v_p(k) \cdot \nabla_x f_p - \nabla_x V \cdot \nabla_k f_p = Q_p(f_p) + Q_{p,r}(f_p, f_{tr}), \tag{2.66}$$
$$\varepsilon \partial_t f_{tr} = Q_{tr,r} = Q_{tr,p} - Q_{tr,n}, \tag{2.67}$$
$$\lambda^2 \Delta_x V = n + \varepsilon n_{tr} - p - C = -\rho, \tag{2.68}$$

with $v_n = \nabla_k \varepsilon_n$, $v_p = -\nabla_k \varepsilon_p$, with Q_n and Q_p still having the form (2.59) and, respectively, (2.60), with the scaled Maxwellians $M_n(k) = c_n \exp(-\varepsilon_n(k))$, $M_p(k) = c_p \exp(-\varepsilon_p(k))$, and with the recombination-generation terms

$$Q_{n,r}(f_n, f_{tr}) = \int_0^1 S_n M_{tr}\, dE\,, \qquad Q_{p,r}(f_p, f_{tr}) = \int_0^1 S_p M_{tr}\, dE\,, \tag{2.69}$$

with

$$S_n = \Phi_n[n_0 M_n f_{tr}(1-f_n) - f_n(1-f_{tr})]\,, \quad S_p = \Phi_p[p_0 M_p(1-f_{tr})(1-f_p) - f_p f_{tr}]\,. \tag{2.70}$$

The right hand side of (2.67) still has the form (2.63), (2.64). The position densities are given by

$$n = \int_B f_n\, dk\,, \qquad p = \int_B f_p\, dk\,, \qquad n_{tr} = \int_0^1 f_{tr}\, dE\,. \tag{2.71}$$

The system (2.65)–(2.67) conserves the total charge $\rho = p + C - n - \varepsilon n_{tr}$. With the definition

$$J_n = -\int_B v_n f_n \, dk \,, \quad J_p = \int_B v_p f_p \, dk \,,$$

of the current densities, the following continuity equation holds formally:

$$\partial_t \rho + \nabla_x \cdot (J_n + J_p) = 0 \,.$$

Setting formally $\varepsilon = 0$ in (2.67) we obtain

$$\overline{f}_{tr}(f_n, f_p) = \frac{p_0 \lambda_p [M_p(1-f_p)] + \lambda_n[f_n]}{p_0 \lambda_p [M_p(1-f_p)] + \lambda_p[f_p] + \lambda_n[f_n] + n_0 \lambda_n [M_n(1-f_n)]}$$

Substitution $\overline{f}_{tr}$ into (2.69) leads to the kinetic Shockley-Read-Hall recombination-generation operators

$$\overline{Q}_{n,r}(f_n, f_p) = \overline{g}_n[f_n, f_p](1-f_n) - \overline{r}_n[f_n, f_p] f_n \,, \qquad \overline{Q}_{p,r}(f_n, f_p) = \overline{g}_p[f_n, f_p](1-f_p) - \overline{r}_p[f_n, f_p] f_p \,, \tag{2.72}$$

with

$$\begin{aligned}
\overline{g}_n &= \int_0^1 \frac{\Phi_n M_n n_0 \Big(p_0 \lambda_p [M_p(1-f_p)] + \lambda_n[f_n] \Big) M_{tr}}{p_0 \lambda_p [M_p(1-f_p)] + \lambda_p[f_p] + \lambda_n[f_n] + n_0 \lambda_n [M_n(1-f_n)]} \, dE \,, \\
\overline{r}_n &= \int_0^1 \frac{\Phi_n \Big(\lambda_p[f_p] + n_0 \lambda_n [M_n(1-f_n)] \Big) M_{tr}}{p_0 \lambda_p [M_p(1-f_p)] + \lambda_p[f_p] + \lambda_n[f_n] + n_0 \lambda_n [M_n(1-f_n)]} \, dE \,, \\
\overline{g}_p &= \int_0^1 \frac{\Phi_p M_p p_0 \Big(n_0 \lambda_n [M_n(1-f_n)] + \lambda_p[f_p] \Big) M_{tr}}{p_0 \lambda_p [M_p(1-f_p)] + \lambda_p[f_p] + \lambda_n[f_n] + n_0 \lambda_n [M_n(1-f_n)]} \, dE \,, \\
\overline{r}_p &= \int_0^1 \frac{\Phi_p \Big(\lambda_n[f_n] + p_0 \lambda_p [M_p(1-f_p)] \Big) M_{tr}}{p_0 \lambda_p [M_p(1-f_p)] + \lambda_p[f_p] + \lambda_n[f_n] + n_0 \lambda_n [M_n(1-f_n)]} \, dE \,.
\end{aligned}$$

Of course, the limiting model still conserves charge, which is expressed by the identity

$$\int_B \overline{Q}_{n,r} \, dk = \int_B \overline{Q}_{p,r} \, dk \,.$$

Pairs of electrons and holes are generated or recombine, however, in general not with the same wave vector. This absence of momentum conservation is reasonable since the process involves an interaction with the trapped states fixed within the crystal lattice.

2.5 Rigorous derivation of the kinetic Shockley-Read-Hall model

The limit $\varepsilon \to 0$ will be carried out rigorously in an initial value problem for the kinetic model with $x \in \mathbb{R}^3$. Concerning the behaviour for $|x| \to \infty$, we shall require the densities to be in L^1 and use the Newtonian potential solution of the Poisson equation, i.e., (2.68) will be replaced by

$$E(x) = -\nabla_x V = \lambda^{-2} \int_{\mathbb{R}^3} \frac{x-y}{|x-y|^3} \rho(y,t)\, dy. \tag{2.73}$$

We define **Problem (K)** as the system (2.65)–(2.67), (2.73) with (2.59), (2.60), (2.69)–(2.71), (2.63), and (2.64), subject to the initial conditions

$$f_n(x,k,0) = f_{n,I}(x,k)\,, \quad f_p(x,k,0) = f_{p,I}(x,k)\,, \quad f_{tr}(x,E,0) = f_{tr,I}(x,E)\,.$$

We start by stating our assumptions on the data. For the velocities we assume

$$v_n, v_p \in W^{1,\infty}_{per}(B)\,, \tag{2.74}$$

where here and in the following, the subscript *per* denotes Sobolev spaces of functions of k satisfying periodic boundary conditions on ∂B. Further we assume that the cross sections satisfy

$$\widetilde{\Phi}_n, \widetilde{\Phi}_p \geq 0\,, \quad \widetilde{\Phi}_n, \widetilde{\Phi}_p \in W^{1,\infty}_{per}(B \times B)\,, \tag{2.75}$$

and

$$\Phi_n, \Phi_p \geq 0\,, \quad \Phi_n, \Phi_n \in W^{1,\infty}_{per}(B \times (0,1))\,. \tag{2.76}$$

A finite total number of trapped states is assumed:

$$M_{tr} \geq 0\,, \quad M_{tr} \in W^{1,\infty}(\mathbb{R}^3 \times (0,1)) \cap W^{1,1}(\mathbb{R}^3 \times (0,1))\,. \tag{2.77}$$

The L^1-assumption with respect to x is needed for controlling the total number of generated particles. For the initial data we assume

$$\begin{aligned} &0 \leq f_{n,I}, f_{p,I} \leq 1\,, \quad f_{n,I}, f_{p,I} \in W^{1,\infty}_{per}(\mathbb{R}^3 \times B) \cap W^{1,1}_{per}(\mathbb{R}^3 \times B)\,, \\ &0 \leq f_{tr,I} \leq 1\,, \quad f_{tr,I} \in W^{1,\infty}_{per}(\mathbb{R}^3 \times (0,1))\,. \end{aligned} \tag{2.78}$$

We also assume

$$n_0,\, p_0 \in L^\infty((0,1))\,, \qquad C \in W^{1,\infty}(\mathbb{R}^3) \cap W^{1,1}(\mathbb{R}^3)\,. \tag{2.79}$$

Finally, we need an upper bound for the life time of trapped electrons:

$$\int_B (\Phi_n \min\{1, n_0 M_n\} + \Phi_p \min\{1, p_0 M_p\})\, dk \geq \gamma > 0\,. \tag{2.80}$$

The reason for the various differentiability assumptions above is that we shall construct smooth solutions by an approach along the lines of [20], which goes back to [8].

An essential tool are the following potential theory estimates [24]:

$$\|E\|_{L^\infty(\mathbb{R}^3)} \le C\|\rho\|_{L^1(\mathbb{R}^3)}^{1/3}\|\rho\|_{L^\infty(\mathbb{R}^3)}^{2/3}\,, \tag{2.81}$$

$$\|\nabla_x E\|_{L^\infty(\mathbb{R}^3)} \le C\big(1+\|\rho\|_{L^1(\mathbb{R}^3)}+\|\rho\|_{L^\infty(\mathbb{R}^3)}\big[1+\log(1+\|\nabla_x\rho\|_{L^\infty(\mathbb{R}^3)})\big]\big)\,. \tag{2.82}$$

We start by rewriting the collision and recombination generation operators as

$$Q_i(f_i) = a_i[f_i](1-f_i) - b_i[f_i]f_i, \quad i=n,p\,, \tag{2.83}$$

and

$$Q_{i,r}(f_i,f_{tr}) = g_i[f_{tr}](1-f_i) - r_i[f_{tr}]f_i, \quad i=n,p\,, \tag{2.84}$$

with

$$a_i[f_i] = \int_B \widetilde{\Phi}_i M_i f_i'\,dk'\,, \quad b_i[f_i] = \int_B \widetilde{\Phi}_i M_i'(1-f_i')\,dk', \quad i=n,p \tag{2.85}$$

$$g_n[f_{tr}] = \int_0^1 \Phi_n n_0 M_n f_{tr} M_{tr}\,dE\,, \quad g_p[f_{tr}] = \int_0^1 \Phi_p p_0 M_p(1-f_{tr})M_{tr}\,dE\,, \tag{2.86}$$

$$r_n[f_{tr}] = \int_0^1 \Phi_n(1-f_{tr})M_{tr}\,dE\,, \quad r_p[f_{tr}] = \int_0^1 \Phi_p f_{tr} M_{tr}\,dE\,. \tag{2.87}$$

In order to construct an approximating sequence $(f_n^j, f_p^j, f_{tr}^j, E^j)$ we begin with

$$f_i^0(x,k,t) = f_{i,I}(x,k), \quad i=n,p\,, \quad f_{tr}^0(x,E,t) = f_{tr,I}(x,E) \tag{2.88}$$

The field always satisfies

$$E^j(x,t) = \int_{\mathbb{R}^3} \frac{x-y}{|x-y|^3}\rho^j(y,t)\,dy \tag{2.89}$$

Let $(f_n^j, f_p^j, f_{tr}^j, E^j)$ be given. Then the f_i^{j+1} are defined as the solutions of the following problem:

$$\begin{aligned}
\partial_t f_n^{j+1} &+ v_n(k)\cdot\nabla_x f_n^{j+1} - E^j\cdot\nabla_k f_n^{j+1} \\
&= (a_n[f_n^j] + g_n[f_{tr}^j])(1-f_n^{j+1}) - (b_n[f_n^j] + r_n[f_{tr}^j])f_n^{j+1}\,, \\
\partial_t f_p^{j+1} &+ v_p(k)\cdot\nabla_x f_p^{j+1} + E^j\cdot\nabla_k f_p^{j+1} \\
&= (a_p[f_p^j] + g_p[f_{tr}^j])(1-f_p^{j+1}) - (b_p[f_p^j] + r_p[f_{tr}^j])f_p^{j+1}\,, \\
\varepsilon\partial_t f_{tr}^{j+1} &= (p_0\lambda_p[M_p(1-f_p^j)] + \lambda_n[f_n^j])(1-f_{tr}^{j+1}) - (n_0\lambda_n[M_n(1-f_n^j)] + \lambda_p[f_p^j])f_{tr}^{j+1}\,,
\end{aligned} \tag{2.90}$$

subject to the initial conditions

$$f_n^{j+1}(x,k,0) = f_{n,I}(x,k)\,, \quad f_p^{j+1}(x,k,0) = f_{p,I}(x,k)\,, \quad f_{tr}^{j+1}(x,E,0) = f_{tr,I}(x,E)\,. \tag{2.91}$$

For the iterative sequence we state the following lemma, which is very similar to the Proposition 3.1 from [20]:

Lemma 2.5.1. *Let the assumptions (2.74)–(2.79) be satisfied. Then the sequence* $(f_n^j, f_p^j, f_{tr}^j, E^j)$*, defined by (2.88)-(2.91) satisfies for any time* $T > 0$

a) $0 \le f_i^j \le 1$, $i = n, p, tr$.

b) f_n^j *and* f_p^j *are uniformly bounded with respect to* $j \to \infty$ *and* $\varepsilon \to 0$ *in* $L^\infty((0,T), L^1(\mathbb{R}^3 \times B)$.

c) E^j *is uniformly bounded with respect to* j *and* ε *in* $L^\infty((0,T) \times \mathbb{R}^3)$.

Proof. The first two equations in (2.90) are standard linear transport equations, and the third equation is a linear ODE. Existence and uniqueness for the initial value problems are therefore standard results.

Note that the a_i, b_i, g_i, r_i, and λ_i in (2.90) are nonnegative if we assume that a) holds for j. Then a) for $j+1$ is an immediate consequence of the maximum principle.

To estimate the L^1-norms of the distributions, we integrate the first equation in (2.90) and obtain

$$\|f_n^{j+1}\|_{L^1(\mathbb{R}^3\times B)} \le \|f_{n,I}\|_{L^1(\mathbb{R}^3\times B)} + \int_0^t \|a_n[f_n^j] + g_n[f_{tr}^j]\|_{L^1(\mathbb{R}^3\times B)}(s)\,ds\,. \tag{2.92}$$

The boundedness of $\widetilde{\Phi}_n$, Φ_n, and f_{tr}^j, and the integrability of M_{tr} imply

$$\|a_n[f_n^j]\|_{L^1(\mathbb{R}^3\times B)} \le C\|f_n^j\|_{L^1(\mathbb{R}^3\times B)}\,, \quad \|g_n[f_{tr}^j]\|_{L^1(\mathbb{R}^3\times B)} \le C\,. \tag{2.93}$$

Now this is used in (2.92). Then an estimate is derived for f_n^j by replacing $j+1$ by j and using the Gronwall inequality. Finally, it is easily since that this estimate is passed from j to $j+1$ by (2.92). An analogous argument for f_p^j completes the proof of b).

A uniform-in-ε $(L^1 \cap L^\infty)$-bound for the total charge density $\rho^j = n^j + \varepsilon n_{tr}^j - p^j - C$ follows from b) and from the integrability of M_{tr}. The statement c) of the lemma is now a consequence of (2.81). □

For passing to the limit in the nonlinear terms some compactness is needed. Therefore we prove uniform smoothness of the approximating sequence.

Lemma 2.5.2. *Let the assumptions (2.74)–(2.80) be satisfied. Then for any time $T > 0$:*

a) *f_n^j and f_p^j are uniformly bounded with respect to j and ε in $L^\infty((0,T), W_{per}^{1,1}(\mathbb{R}^3 \times B) \cap W_{per}^{1,\infty}(\mathbb{R}^3 \times B))$,*

b) *f_{tr}^j is uniformly bounded with respect to j and ε in $L^\infty((0,T), W^{1,\infty}(\mathbb{R}^3 \times (0,1)))$,*

c) *E^j is uniformly bounded with respect to j and ε in $L^\infty((0,T), W_{1,\infty}(\mathbb{R}^3))$.*

Proof. We start by introducing $\nu^j = \nabla_{x,k} f_n^j = (\nu_x^j, \nu_k^j)$, $\pi^j = \nabla_{x,k} f_p^j = (\pi_x^j, \pi_k^j)$, $\phi^j = \nabla_x f_{tr}^j$ and by differentiating the last equation in (2.90) with respect to x:

$$\begin{aligned} \varepsilon \partial_t \phi^{j+1} &= (-p_0 \lambda_p [M_p \pi_x^j] + \lambda_n [\nu_x^j])(1 - f_{tr}^{j+1}) - (-n_0 \lambda_n [M_n \nu_x^j] + \lambda_p [\pi_x^j]) f_{tr}^{j+1} \\ &\quad - (p_0 \lambda_p [M_p (1 - f_p^j)] + \lambda_n [f_n^j] + n_0 \lambda_n [M_n (1 - f_n^j)] + \lambda_p [f_p^j]) \phi^{j+1} . \end{aligned}$$

The coefficient of ϕ^{j+1} on the right hand side is bounded below by the term appearing in assumption (2.80) and, thus, bounded away from zero. The maximum principle implies

$$\sup_{(0,t)} \|\phi^{j+1}\|_\infty \le C \left(\sup_{(0,t)} \|\nu_x^j\|_\infty + \sup_{(0,t)} \|\pi_x^j\|_\infty + 1 \right) ,$$

where here and in the following we use the symbol $\|\cdot\|_\infty$ for the L^∞-norm on $\mathbb{R}^3$, on $\mathbb{R}^3 \times B$ and on $\mathbb{R}^3 \times (0,1)$. The gradient of the first equation in (2.90) with respect to x and k can be written as

$$\partial_t \nu^{j+1} + v_n \cdot \nabla_x \nu^{j+1} - E^j \cdot \nabla_k \nu^{j+1} + (a_n + b_n + g_n + r_n) \nu^{j+1} = S_n^j ,$$

where it is easily seen that, using our assumptions,

$$\|S_n^j\|_\infty \le C \left(1 + \|\nu^j\|_\infty + \|\phi^j\|_\infty + \|\nu^{j+1}\|_\infty (1 + \|\nabla_x E^j\|_\infty)\right)$$

holds. The analogous treatment of the second equation in (2.90), the potential theory inequality (2.82), and the definition

$$\alpha^j(t) = \sup_{(0,t)} (\|\nu^j\|_\infty + \|\pi^j\|_\infty + \|\phi^j\|_\infty)$$

lead to

$$\alpha^{j+1} \le C \left(1 + \int_0^t (\alpha^j + \alpha^{j+1}(1 + \log(1 + \alpha^j)) ds \right)$$

implying boundedness of α^j on arbitrary bounded time intervals (as in [8]). This proves c) and the L^∞-part of a). The equation for $\partial_E f_{tr}^{j+1}$ can be treated as above completing the proof of b).

By $\int_{\mathbb{R}^3} n_{tr} dx \leq \int_{\mathbb{R}^3} M_{tr} dx$, it is trivial that the total number of trapped electrons is bounded. Therefore, the L^1-estimates in a) follow the line of [20]) since no coupling with the equation for the trapped electrons is necessary. □

With the previous results, the first two equations in (2.90) also give uniform bounds for the time derivatives of f_n^j and f_p^j. Thus, subsequences converge strongly locally in x and t. In the same way, the right hand side of the time derivative of the Poisson equation is bounded in L^1 and in L^∞, and (2.81) implies boundedness of the time derivative of the field. So the field also converges strongly. This and the (obvious) weak convergence of f_{tr}^j are sufficient for passing to the limit in the quadratic nonlinearities. Existence of a global solution of Problem (K) follows. By the same argument, however, the limit $\varepsilon \to 0$ can be justified, since all estimates are also uniform in ε.

Theorem 2.5.3. *Let the assumptions (2.74)–(2.80) be satisfied. Then Problem (K) has a global solution* (f_n, f_p, f_{tr}, E) *with* $f_n, f_p \in L^\infty_{loc}((0,\infty), W^{1,\infty}_{per}(\mathbb{R}^3 \times B))$, $f_{tr} \in L^\infty_{loc}((0,\infty), W^{1,\infty}(\mathbb{R}^3 \times (0,1)))$, $E \in L^\infty_{loc}((0,\infty), W^{1,\infty}(\mathbb{R}^3))$. *For* $\varepsilon \to 0$, *a subsequence of solutions converges to the formal limit problem. The convergence of* f_n *and* f_p *is in* $L^\infty_{loc}((0,\infty) \times \mathbb{R}^3 \times B)$, *that of* E *in* $L^\infty_{loc}((0,\infty) \times \mathbb{R}^3)$ *and that of* ${f_{tr}}^j$ *in* $L^\infty_{loc}((0,\infty) \times \mathbb{R}^3 \times (0,1))$ *weak*.*

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