Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Current Coupling of Drift-Diffusion Models and Dissipative Schrödinger-Poisson Systems: Dissipative Hybrid Models

Dedicated to H. Gajewski on the occasion of his 65^{th} ***birthday***

M. Baro, H. Neidhardt, J. Rehberg

submitted: July 15, 2004

Weierstrass Institute for Applied Analysis and Stochastics,
Mohrenstr. 39, D-10117 Berlin, Germany

E-Mail: baro@wias-berlin.de,
neidhard@wias-berlin.de,
rehberg@wias-berlin.de

No. 946
Berlin 2004

1991 *Mathematics Subject Classification.* 47B44,47E05, 35J05.

Key words and phrases. semi-conductors, quantum-classical coupling, hybrid models, drift-diffusion models, dissipative Schrödinger systems, Poisson equation, current coupling.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

A 1D coupled drift-diffusion dissipative Schrödinger model (hybrid model), which is capable to describe the transport of electrons and holes in semi-conductor devices in a non-equilibrium situation, is mathematically analyzed. The device domain is split into a part where the transport is well-described by the drift-diffusion equations (classical zone) and a part where a quantum description via a dissipative Schrödinger system (quantum zone) is used. Both system are coupled such that the continuity of the current densities is guaranteed. The electrostatic potential is self-consistently determined by Poisson's equation on the whole device. We show that the hybrid model is well-posed, prove existence of solutions and show their uniform boundedness provided the distribution function satisfy a so-called balance condition. The current densities are different from zero in the non-equilibrium case and uniformly bounded.

Contents

1 Introduction

A basic model for carrier transport in semi-conductors was originated in 1950 by van Roosbroeck [46]. It describes the transport of electron and holes by drift and diffusion processes in a self-consistent electrical field. This so-called drift-diffusion model was firstly used by Gummel, cf. [26], to calculate diodes. Since that time drift-diffusion models were intensively studied and there is an extensive literature on it, see [22, 41, 47] and references therein. However, modern semi-conductor devices inherently employ quantum effects in their operations like tunneling [15, 17, 49] which are well described by stationary or transient Wigner- or Schrödinger-Poisson systems [1, 9, 10, 12, 27, 28, 29, 33, 34, 35, 36, 38, 39, 43, 44, 45, 48]. Unfortunately, the numerical treatment of Wigner- or Schrödinger-Poisson systems is fairly expensive compared to classical models like drift-diffusion models. However, for several devices like resonant tunneling diodes [13, 14, 21, 42] the quantum effects occur only in some small spatial parts while other parts admit a quite reasonable description by approved "classical models" like drift-diffusion models etc. So one looks for a model which combines a quantum description in parts where it is necessary with a classical description in other parts. The aim is to obtain a model which allows an effective and fast numerical treatment, but describes the transport of electrons and holes in the semi-conductor device sufficiently accurate. Models of that type are usually called hybrid models, cf. [2, 6, 7, 16]. Numerical calculations carried out in [2, 16] for resonant tunneling diodes show that hybrid models are in a quite good agreement with experiments, in particular, the phenomenon of negative differentiable resistance reproduces well. In the following we are interested in an analytical treatment of such models under quite general assumptions but in a dissipative approximation.

In particular, we consider an one dimensional stationary hybrid model which consists of a stationary drift-diffusion model in the so-called "classical zone" and a stationary Schrödinger-Poisson system in the "quantum zone". Both systems are coupled by the conditions that the Fermi energies of the quantum zone are given by the electro-chemical potentials of the classical zone, the current densities are continuous at the interface points and the Poisson equation holds on the whole device domain.

The hybrid model approach evokes, however, several problems. In fact, if one is interested in a current density which is continuous over the whole device, then one has to consider an open system. Indeed, for Schrödinger operators with self-adjoint boundary conditions the current density is always zero since such operators commute with the complex conjugation. Thus, a continuous non-trivial net current flow through the interface between quantum and classical zones is impossible in this case. Consequently, hybrid models enforce at least non-selfadjoint boundary conditions for the Schrödinger operator to describe the particles in the quantum zone. Such models were introduced in [30, 31, 32]. Further, a non-trivial current density arises in the quantum zone only if the statistical behaviour of the quantum system is described by a density matrix which is different from those of the thermo-dynamical equilibrium. Hence, one has to find suitable non-equilibrium density matrices.

In more detail, we divide the one dimensional device domain $\Delta = [a_0, b_0] \subseteq \mathbb{R}$ into three subregions $\Sigma_a = [a_0, a]$, $\Omega = (a, b)$ and $\Sigma_b = [b, b_0]$, $a_0 < a < b < b_0$, where $\Sigma := \Sigma_a \cup \Sigma_b$ is called the classical zone and Ω is the quantum zone. In Σ we consider a stationary one dimensional drift-diffusion system, in short DD-system, without generation or recombination, [40]. That means, the carrier and current densities $u^{\pm}_{\nu}$ and $J^{\pm}_{\nu}$, $\nu = a, b$, for electrons "-" and holes "+" are given by the state equations

$$u_\nu^\pm(x) := f_\nu^\pm\left(\gamma_\nu^\pm(x)\right), \quad \text{and} \quad J_\nu^\pm(x) := -\mu_\nu^\pm u_\nu^\pm(x)\frac{d}{dx}z_\nu^\pm(x), \tag{1.1}$$

for $x \in \Sigma_\nu$, $\nu = a, b$, where $\gamma_\nu^\pm$ are the chemical energies, $z_\nu^\pm$ denote the electro-chemical potentials (energies) and $\mu_\nu^\pm$ are the mobilities of the carriers in Σ_ν, $\nu = a, b$. The electro-chemical potentials $z_\nu^\pm$ and the chemical energies $\gamma_\nu^\pm$ are related by

$$z_\nu^\pm = \pm\varphi + \gamma_\nu^\pm + E_\nu^\pm, \quad \nu = a, b, \tag{1.2}$$

where φ denotes the electrostatic potential and $E_\nu^\pm$ are the band edge-offsets in Σ_ν, $\nu = a, b$. In the following we choose the Boltzmann distribution

$$f_\nu^\pm(s) = N_\nu^\pm\, e^{s/k_BT}, \quad s \in \mathbb{R}, \tag{1.3}$$

where $N_\nu^\pm$, $\nu = a, b$, are the effective density of states, k_B is the Boltzmann constant, and T the temperature, which is assumed to be constant. In order to keep the notation as simple as possible we scale the factor k_BT to one in the following. Very often instead of the electro-chemical potentials $z_\nu^\pm$ the so-called quasi Fermi potentials $\phi_\nu^\pm := \pm z_\nu^\pm$ are used which we prefer to use also. In terms of quasi Fermi potentials one gets for the carrier and current densities the expressions

$$u_\nu^\pm = N_\nu^\pm\, e^{\mp(\varphi - \phi_\nu^\pm \pm E_\nu^\pm)} \quad \text{and} \quad J_\nu^\pm = \mp\mu_\nu^\pm u_\nu^\pm \frac{d}{dx}\phi_\nu^\pm, \quad \nu = a, b. \tag{1.4}$$

Since we exclude generation and recombination in this paper the current densities $J_\nu^\pm$, $\nu = a, b$, satisfy the continuity equations

$$\frac{d}{dx}J_\nu^\pm = 0, \quad \nu = a, b, \tag{1.5}$$

which yields that the current densities $J_\nu^\pm$ are constant on Σ_ν, $\nu = a, b$. Finally, one has to add boundary conditions

$$\phi_a^\pm(a_0) = \phi_{a_0}^\pm \in \mathbb{R}, \quad \text{and} \quad \phi_b^\pm(b_0) = \phi_{b_0}^\pm \in \mathbb{R}, \tag{1.6}$$

to the continuity equations (1.5).

To have a mathematically meaningful description the continuity equations require boundary conditions at the end points a and b of the classical zones Σ_a and Σ_b, too. However, for the hybrid model a and b are not boundary points but interface points at which the coupling of the drift-diffusion system with the quantum subsystem is realized. Hence the coupling conditions have to replace the boundary conditions at these interface points. We will develop these interface conditions later in the text.

In the quantum zone a dissipative Schrödinger system, in short a DS-system, is adopted, cf. [3, 30] and Appendix A.5, which is derived from a quantum transmitting Schrödinger system, in short QTS-system, see [4, 8] and Appendix B.1, B.3 and B.4. Dissipative Schrödinger systems, in short DS-systems, consist of two dissipative Schrödinger-type operators $h^\pm[\varkappa_a^\pm, \varkappa_b^\pm, v^\pm]$, cf. [31, 32] and Appendix A.1, arising from the differential expressions

$$h^\pm[\varkappa_a^\pm, \varkappa_b^\pm, v^\pm] = -\frac{1}{2}\frac{d}{dx}\frac{1}{m^\pm}\frac{d}{dx} + v^\pm \tag{1.7}$$

with

$$v^{\pm} := w^{\pm} \pm \varphi, \quad w^{\pm} \in L^{\infty}_{\mathbb{R}}(\Omega), \quad \varphi \in C_{\mathbb{R}}(\Omega), \tag{1.8}$$

on the Hilbert space $\mathfrak{h} = L^2(\Omega)$, where the index $\mathbb{R}$ of the function spaces indicates real-valued functions. The operators $h^{\pm}[\varkappa_a^{\pm}, \varkappa_b^{\pm}, v^{\pm}]$ are supplemented by the boundary conditions

$$\frac{1}{2m_a^{\pm}} g'(a) = -\varkappa_a^{\pm} g(a), \quad \text{and} \quad \frac{1}{2m_b^{\pm}} g'(b) = \varkappa_b^{\pm} g(b), \tag{1.9}$$

where $w^{\pm}$ are the band-edge offsets of the quantum zone and $\varkappa_a^{\pm}, \varkappa_b^{\pm} \in \mathbb{C}_+ := \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$. The other important ingredients of dissipative Schrödinger systems are the so-called density matrices $\rho^{\pm} \in L^{\infty}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$. Dissipative Schrödinger systems are indicated by the quadruple $\{h^{\pm}[\varkappa_a^{\pm}, \varkappa_b^{\pm}, v^{\pm}], \rho^{\pm}\} = \{h^{+}[\varkappa_a^{+}, \varkappa_b^{+}, v^{+}], h^{-}[\varkappa_a^{-}, \varkappa_b^{-}, v^{-}], \rho^{+}, \rho^{-}\}$ in the following. To dissipative Schrödinger systems one assigns carrier and current densities, cf. [3, 30] and Appendix A.3, A.4.

In contrast to [3, 30] where the coefficients $\varkappa_a^{\pm}, \varkappa_b^{\pm}$ were assumed to be constant we choose them now potential dependent,

$$\begin{aligned} \varkappa_a^{\pm}(\varphi) &:= i\sqrt{\tfrac{s^{\pm}(\varphi) - v^{\pm}(a)}{2m_a^{\pm}}}, \\ \varkappa_b^{\pm}(\varphi) &:= i\sqrt{\tfrac{s^{\pm}(\varphi) - v^{\pm}(b)}{2m_b^{\pm}}}, \end{aligned} \tag{1.10}$$

$\varphi \in C_{\mathbb{R}}(\Omega)$, where i denotes the imaginary unit, i.e. $i^2 = -1$,

$$v^{\pm}(a) := \pm\varphi(a) + E_a^{\pm}, \qquad v^{\pm}(b) := \pm\varphi(b) + E_b^{\pm} \tag{1.11}$$

and

$$s^{\pm}(\varphi) := v_{max}^{\pm}(\varphi) + \delta_0^{\pm}, \quad \delta_0^{\pm} > 0, \tag{1.12}$$

with

$$\begin{aligned} v_{max}^{+}(\varphi) &:= \max\{v^{+}(a), v^{+}(b)\}, \\ v_{max}^{-}(\varphi) &:= \max\{v^{-}(a), v^{-}(b)\} \end{aligned} \tag{1.13}$$

where $\delta_0^{\pm}$ are given positive constants. Notice that $\mathrm{Im}(\varkappa_a^{\pm}(\varphi)) > 0$ and $\mathrm{Im}(\varkappa_b^{\pm}(\varphi)) > 0$ for all $\varphi \in C_{\mathbb{R}}(\Omega)$. Hence the operators $h^{\pm}[\varphi] := h^{\pm}[\varkappa_a^{\pm}(\varphi), \varkappa_b^{\pm}(\varphi), w^{\pm} \pm \varphi]$ are maximal dissipative ones such that the multiplicity of their minimal self-adjoint dilations is two, cf. [32].

The density matrices $\rho_{\Lambda}^{\pm}[\varphi]$ of the DS-system are determined by

$$\Lambda^{\pm}[\varphi] := [v_{max}^{\pm}(\varphi), v_{max}^{\pm}(\varphi) + \delta^{\pm}), \quad 0 < \delta_0^{\pm} < \delta^{\pm} \leq \infty, \tag{1.14}$$

and

$$\rho^{\pm}(\lambda) := \rho^{\pm}_{\Lambda^{\pm}[\varphi]} = \begin{pmatrix} f^{\pm}(\lambda - \varepsilon_b^{\pm}) & 0 \\ 0 & f^{\pm}(\lambda - \varepsilon_b^{\pm}) \end{pmatrix} \chi_{\Lambda^{\pm}[\varphi]}(\lambda), \quad \lambda \in \mathbb{R}, \tag{1.15}$$

where $f^{\pm}$ are statistical distribution functions, cf. Appendix B.4. The real parameters $\mathfrak{A} := \{\delta_0^{\pm}, \delta\}$, $0 < \delta_0^{\pm} < \delta^{\pm} \leq \infty$, are called the approximation parameters. The interest to the semi-intervals $\Lambda^{\pm}[\varphi]$ is due to the fact that only energies above $v_{max}^{\pm}(\varphi)$ contribute to the current densities, cf. [30]. In the following we call them the current thresholds.

With each DS-system $\{h^{\pm}[\varphi], \rho^{\pm}\}$ one assigns carrier and current density operators $\mathcal{N}^{\pm}_{\rho^{\pm}}[\varphi]$ and $j^{\pm}_{\rho^{\pm}}[\varphi]$, see [3, 30] as well as Appendix A.3 and A.4. These operators define carrier densities $u^{\pm}_{Q} := \mathcal{N}^{\pm}_{\rho^{\pm}}[\varphi]$ and current densities $j^{\pm} := j^{\pm}_{\rho^{\pm}}[\varphi]$ for given electrostatic potentials $\varphi \in C_{\mathbb{R}}(\Omega)$ in the quantum zone. We recall that the current densities of the DS-system are constants for a given electrostatic potential, cf. [3, 30].

In a next step one couples the DS-system $\{h^{\pm}[\varphi], \rho^{\pm}\}$ to the drift-diffusion system by choosing the Fermi energies $\varepsilon^{\pm}_{a}$ and $\varepsilon^{\pm}_{b}$ in appropriate manner and demanding current continuity, i.e.

$$J^{\pm}_{a} = j^{\pm} = J^{\pm}_{b}. \tag{1.16}$$

To find the correct Fermi energies ε_a and ε_b one regards the semi-intervals $(-\infty, a)$ and (b, ∞) as carrier reservoirs which are characterized by carrier densities $u^{\pm}_{a}$ and $u^{\pm}_{b}$ and reservoir potential energies $v^{\pm}_{a}$ and $v^{\pm}_{b}$, respectively. Carrier densities $u^{\pm}_{a}$ and $u^{\pm}_{b}$ and reservoir potential energies $v^{\pm}_{a}$ and $v^{\pm}_{b}$ determine the Fermi energies $\varepsilon^{\pm}_{a}$ and $\varepsilon^{\pm}_{b}$ of these reservoirs. For the choice $u^{\pm}_{a} = u^{\pm}_{a}(a)$, $u^{\pm}_{b} = u^{\pm}_{b}(b)$, cf. (1.4) and $v^{\pm}_{a} = v^{\pm}(a)$ and $v^{\pm}_{b} = v^{\pm}(b)$, cf. (1.11), it turns out that the Fermi energies of the reservoirs are determined by

$$\varepsilon^{\pm}_{a} = z^{\pm}_{a}(a) = \pm\phi^{\pm}_{a}(a) \quad \text{and} \quad \varepsilon^{\pm}_{b} = z^{\pm}_{b}(b) = \pm\phi^{\pm}_{b}(b). \tag{1.17}$$

which yields the density matrices

$$\rho^{\pm}(\lambda) = \begin{pmatrix} f^{\pm}(\lambda \mp \phi^{\pm}_{b}(b)) & 0 \\ 0 & f^{\pm}(\lambda \mp \phi^{\pm}_{a}(a)) \end{pmatrix} \chi_{\Lambda^{\pm}[\varphi]}(\lambda), \quad \lambda \in \mathbb{R}. \tag{1.18}$$

In a forthcoming paper we give a rigorous derivation of the relations (1.17) which is called the Fermi coupling. With respect to the current continuity condition (1.16) the problem arises whether under the Fermi coupling for a given electrostatic potential φ the condition (1.16) can be always satisfied.

The arising compound system consisting of DD- and DS-systems is called a dissipative hybrid system, in short DH-system. If in addition the electrostatic potential φ satisfies the Poisson equation

$$-\frac{d}{dx}\epsilon\frac{d}{dx}\varphi(x) = C(x) + u^{+}(x) - u^{-}(x), \quad x \in \Delta, \tag{1.19}$$

with boundary conditions

$$\varphi(a_0) = \varphi_{a_0} \in \mathbb{R} \quad \text{and} \quad \varphi(b_0) = \varphi_{b_0} \in \mathbb{R}, \tag{1.20}$$

where the carrier densities $u^{\pm}$ are given by

$$u^{\pm}(x) := \begin{cases} u^{\pm}_{a}(x), & x \in \Sigma_a, \\ u^{\pm}_{Q}(x), & x \in \Omega, \\ u^{\pm}_{b}(x), & x \in \Sigma_b, \end{cases} \tag{1.21}$$

then the DH-system is called a dissipative hybrid model, in short DH-model. By ϵ and C the dielectric permittivity and the doping profile of the device are denoted, respectively. In fact, the Poisson equation for determining the electrostatic potential is non-linear. Notice that the quantum carrier densities depend non-locally on the potential.

A more advanced model is the so-called quantum transmitting hybrid model, in short QTH-model, which arises if one couples the drift-diffusion system to the quantum transmitting system, cf. Appendix B.1. The dissipative hybrid model is an approximation of QTH-model which one obtains replacing the quantum transmitting Schrödinger system (in short QTS-system) entering into the QTH-model in certain manner by a dissipative Schrödinger system, cf. Appendix B.3 and B.4. It has the advantage that a lot of quantities can be calculated in an explicit manner but nevertheless it preserves with an certain accuracy the mathematical problems of QTH-models. Finally, DH-models have an interest in its own. Indeed, the numerical treatment of QTH-models requires a discretization in the energy parameter λ which naturally leads to a finite collection of DH-models, see Appendix B.3.

The final aim of this paper is to show that the proposed DH-model admits a solution under natural assumptions for any choice of the approximation parameters $\mathfrak{A}$. The paper is organized as follows. In Section 2 we investigate the stationary drift-diffusion system on the disconnected set $\Sigma = \Sigma_a \cup \Sigma_b$ provided the current densities are given and equal on the different intervals Σ_a and Σ_b. This leads to certain restrictions on the current densities, cf. Lemma 2.2. Section 3 is devoted to the rigorous setup of the dissipative Schrödinger system used in the quantum zone. The dissipative hybrid model is defined in Section 4. In Section 4.1 the so-called Fermi coupling is explained. Using the Fermi coupling it is shown in Section 4.2 that the stationary DD-system and the DS-system admit a current coupling. This result is in fact non-trivial and is based on Proposition 4.1. Using the results of Section 4.2 in Section 4.3 the dissipative hybrid system is rigorously introduced. Finally, in Section 4.4 the dissipative hybrid system is coupled to the Poisson equation which yields the dissipative hybrid model. The problem to find a solution of the DH-model is reformulated in Section 4.4 as a fixed point problem. In Section 5 we show that the fixed point problem admits a solution. The existence proof is based on the Leray-Schauder fixed point theorem. Important for this step is that a certain balance condition for the distribution functions has to be satisfied, that means, the growth of the hole distribution function at minus infinity and the decay of electron distribution function at plus infinity and vice versa have to be related, cf. Assumption 5.6. The standard Boltzmann and Fermi distributions satisfy this balance condition. Uniqueness is not shown and not expected by physical reasons; however, it turns out that all solutions are uniformly bounded by a bound which is determined by the data of the problem but independent of the choice of the approximation parameters $\mathfrak{A}$. Moreover, the current densities are non-trivial in the non-equilibrium case. We end up with some comments in Section 6. In Appendix A we give an introduction to dissipative Schrödinger systems and prove some continuity results for the carrier and current density operators. The derivation of the DS-system used in the quantum zone from the QTS-model is exposed in the Appendix B, in particular, in Appendix B.3 and B.4 .

Notation: By $L^p(\mathcal{O}, X, \mathfrak{m})$ $1 \leq p < \infty$ we denote the space of $\mathfrak{m}$-measurable and p-integrable functions over Borel sets $\mathcal{O} \subseteq \mathbb{R}$ with values in a Banach space X where usually $\mathcal{O} = \Omega, \Sigma, \Delta$. By $L^\infty(\mathcal{O}, X, \mathfrak{m})$ the space of essentially bounded functions is denoted. If $\mathfrak{m}$ is the Lebesgue measure, then we write $L^p(\mathcal{O}) = L^p(\mathcal{O}, \mathbb{C}, \mathfrak{m})$ and $L^p_{\mathbb{R}}(\mathcal{O}) := L^p(\mathcal{O}, \mathbb{R}, \mathfrak{m})$, $1 \leq p \leq \infty$. For closed sets $\mathcal{O} \subseteq \mathbb{R}$ we denote by $C(\mathcal{O})$ and $C_{\mathbb{R}}(\mathcal{O})$ the spaces of continuous complex- or real-valued functions on $\mathcal{O}$ equipped with the supremum norm, respectively.

The norm of a Banach or Hilbert space X is indicated by $\|\cdot\|_X$ or simply by $\|\cdot\|$, the scalar product of a Hilbert space X by $(\cdot,\cdot)_X$ or simply by $(\cdot,\cdot)$ where the first argument is the linear one. The dual space is indicated by X^*. By $\mathcal{B}(X,Y)$ the space of all linear bounded operators from the Banach space X to the Banach space Y is denoted with norm $\|\cdot\|_{\mathcal{B}(X,Y)}$. If $X = Y$, then $\mathcal{B}(X,X) = \mathcal{B}(X)$ and $\|\cdot\|_{\mathcal{B}(X,Y)} = \|\cdot\|_{\mathcal{B}(X)}$. If X is a Hilbert spaces, then $\mathcal{B}_1(X)$ denotes the space of trace class operators. For a densely defined linear operator $A : X \longrightarrow Y$ we denote by A^*, $\mathrm{spec}(A)$ and $\mathrm{res}(A)$ its adjoint, spectrum and resolvent set, respectively.

Furthermore, for $\mathcal{O} = (a_0, b_0)$ or $\mathcal{O} = (a, b)$ we denote by $W^{1,2}(\mathcal{O})$ the usual Sobolev spaces of complex-valued functions on $\mathcal{O}$. The subspace of elements with homogeneous Dirichlet boundary conditions at the end points of the interval $\mathcal{O} \subseteq \mathbb{R}$ is denoted by $\overset{o}{W}{}^{1,2}(\mathcal{O})$. Its dual with respect to the L^2-pairing is denoted by $\overset{o}{W}{}^{-1,2}(\mathcal{O}) = \left(\overset{o}{W}{}^{1,2}(\mathcal{O})\right)^*$. If we have in mind only real-valued functions, then we write $W^{1,2}_{\mathbb{R}}(\mathcal{O})$ and $\overset{o}{W}{}^{1,2}_{\mathbb{R}}(\mathcal{O})$.

Moreover, in the following we distinguish between variable and parameter dependence using the convention: if we have in mind a variable dependence, then we put the variable into parentheses, if a parameter dependence, then the parameter is put into brackets, see above (1.7), (1.10), (1.12), (1.14). It happens, that a parameter dependence becomes a variable one what means the parameter is now included into parentheses. The superscripts "+" and "-" always indicate quantities related to holes and electrons, respectively.

2 Classical zone

In this section we consider the stationary drift-diffusion equations (1.4) and (1.5) on the disconnected set Σ with boundary conditions (1.6). The boundary conditions at a and b are replaced by the conditions that (i) the current densities at a and b are equal and (ii) these current densities are given. We show in this section that the DD-system is well-posed and admits solutions provided the given current densities are located in some interval around zero which depends on the fixed electrostatic potential φ. Later on the given current densities will be the quantum current densities for a fixed potential φ which is finally determined self-consistently by the Poisson equation.

We suppose that the carrier and current densities $u^\pm(\cdot)$ and $J^\pm_\nu$, $\nu = a, b$, are given by (1.4). We make the following assumptions.

Assumption 2.1

(C.1) The effective carrier mobilities $\mu^\pm_\nu$ are positive constants on Σ_ν, $\nu = a, b$.

(C.2) The effective density of states $N^\pm_\nu$ are positive constants on Σ_ν, $\nu = a, b$.

(C.3) The band-edge offsets $E^\pm_\nu$ are real constants on Σ_ν, $\nu = a, b$.

(C.4) Generation and recombination are absent.

By (C.4) we obtain the continuity equations (1.5) which implies that $J^\pm(x) := J^\pm_\nu(x)$ is the same current density on Σ_ν, $\nu = a, b$. In particular, one has

$$J^\pm(x) = J^\pm_a(a), \quad x \in \Sigma_a, \quad \text{and} \quad J^\pm(x) = J^\pm_b(b), \quad x \in \Sigma_b. \tag{2.1}$$

Therefore, one gets that

$$J^-_a(a) = \mu^-_a N^-_a \frac{e^{-\phi^-_{a_0}} - e^{-\phi^-_a(a)}}{\int_{a_0}^a dy\, e^{-\varphi(y)+E^-_a}} \tag{2.2}$$

and

$$J_b^-(b) = \mu_b^- N_b^- \frac{e^{-\phi_b^-(b)} - e^{-\phi_{b_0}^-}}{\int_b^{b_0} dy\, e^{-\varphi(y)+E_b^-}}. \tag{2.3}$$

In the same manner we verify that

$$J_a^+(a) = \mu_a^+ N_b^+ \frac{e^{\phi_{a_0}^+} - e^{\phi_a^+(a)}}{\int_{a_0}^a dy\, e^{\varphi(y)+E_a^+}} \tag{2.4}$$

and

$$J_b^+(b) = \mu_b^+ N_b^+ \frac{e^{\phi_b^+(b)} - e^{\phi_{b_0}^+}}{\int_b^{b_0} dy\, e^{\varphi(y)+E_b^+}}. \tag{2.5}$$

Lemma 2.2 *Let the electrostatic potential $\varphi \in C_{\mathbb{R}}(\Delta)$ be given. There are solutions $\phi_\nu^- \in C_{\mathbb{R}}^1(\Sigma_\nu)$, $\nu = a, b$, of (1.4) and (1.5) satisfying the boundary conditions* (1.6) *and $J_a^-(a) = J_b^-(b) = J^-$ if and only if $J^- \in (J_{min}^-[\varphi], J_{max}^-[\varphi])$ where*

$$J_{min}^-[\varphi] := -\mu_b^- N_b^- \frac{e^{-\phi_{b_0}^-}}{\int_b^{b_0} dy\, e^{-\varphi(y)+E_b^-}}, \quad J_{max}^-[\varphi] := \mu_a^- N_a^- \frac{e^{-\phi_{a_0}^-}}{\int_{a_0}^a dy\, e^{-\varphi(y)+E_a^-}}. \tag{2.6}$$

Similarly, there is a solution $\phi_\nu^+ \in C_{\mathbb{R}}^1(\Sigma_\nu)$, $\nu = a, b$, of (1.4) and (1.5) satisfying the boundary conditions (1.6) *and $J_a^+(a) = J_b^+(b) = J^+$ if and only if $J^+ \in (J_{min}^+[\varphi], J_{max}^+[\varphi])$ where*

$$J_{min}^+[\varphi] := -\mu_b^+ N_b^+ \frac{e^{\phi_{b_0}^+}}{\int_b^{b_0} dy\, e^{\varphi(y)+E_b^+}}, \quad J_{max}^+[\varphi] := \mu_a^+ N_a^+ \frac{e^{\phi_{a_0}^+}}{\int_{a_0}^a dy\, e^{\varphi(y)+E_a^+}}. \tag{2.7}$$

Proof. From (2.2) and (2.3) one gets

$$J_a^-(a) < \mu_a^- N_a^- \frac{e^{-\phi_{a_0}^-}}{\int_{a_0}^a dy\, e^{-\varphi(y)+E_a^-}} = J_{max}^-[\varphi] \tag{2.8}$$

and

$$J_b^-(b) < -\mu_b^- N_b^- \frac{e^{-\phi_{b_0}^-}}{\int_b^{b_0} dy\, e^{-\varphi(y)+E_b^-}} = J_{min}^-[\varphi]. \tag{2.9}$$

If we assume that $J_a^-(a) = J_b^-(b) = J^-$, then (2.8) and (2.9) imply $J^- \in (J_{min}^-[\varphi], J_{max}^-[\varphi])$. Conversely, if $J^- \in (J_{min}^-[\varphi], J_{max}^-[\varphi])$, then the definitions

$$\phi_a^-[J^-,\varphi](x) := -\ln\left(e^{-\phi_{a_0}^-} - \frac{J^-}{\mu_a^- N_a^-}\int_{a_0}^x dy\, e^{-\varphi(y)+E_a^-}\right), \quad x \in \Sigma_a, \tag{2.10}$$

and

$$\phi_b^-[J^-,\varphi](x) := -\ln\left(e^{-\phi_{b_0}^-} + \frac{J^-}{\mu_b^- N_b^-}\int_x^{b_0} dy\, e^{-\varphi(y)+E_b^-}\right), \quad x \in \Sigma_b, \tag{2.11}$$

make sense.

Similarly, we prove that $J^+ \in (J^+_{min}[\varphi], J^+_{max}[\varphi])$ has to be satisfied. Moreover, if $J^+ \in (J^+_{min}[\varphi], J^+_{max}[\varphi])$, then the definitions

$$\phi^+_a[J^+,\varphi](x) := \ln\left(e^{\phi^+_{a_0}} - \frac{J^+}{\mu^+_a N^+_a}\int_{a_0}^{x} dy\; e^{\varphi(y)+E^+_a}\right), \quad x \in \Sigma_a, \tag{2.12}$$

and

$$\phi^+_b[J^+,\varphi](x) := \ln\left(e^{\phi^+_{b_0}} + \frac{J^+}{\mu^+_b N^+_b}\int_{x}^{b_0} dy\; e^{\varphi(y)+E^+_b}\right), \quad x \in \Sigma_b, \tag{2.13}$$

are correct. If in accordance with (1.4) we set

$$u^\pm_\nu[J^\pm,\varphi](x) := N^\pm_\nu e^{\mp(\varphi(x)-\phi^\pm_\nu[J^\pm,\varphi](x)\pm E^\pm_\nu)}, \quad x \in \Sigma_\nu, \quad \nu = a,b, \tag{2.14}$$

then a straightforward computation shows that

$$J^\pm = \mp\mu^\pm_\nu u^\pm_\nu[J^\pm,\varphi](x)\frac{d}{dx}\phi^\pm_\nu[J^\pm,\varphi](x), \quad x \in \Sigma_\nu, \quad \nu = a,b, \tag{2.15}$$

which completes the proof. □

It is convenient to introduce sets of pairs $\{J^\pm,\varphi\}$

$$\mathcal{E}^- := \left\{ \{J^-,\varphi\} \in \mathbb{R}\times C_{\mathbb{R}}(\Delta) : \begin{array}{l} 0 < e^{-\phi^-_{a_0}} - \frac{J^-}{\mu^-_a N^-_a}\int_{a_0}^{a} dx\; e^{-\varphi(x)+E^-_a} \\ 0 < e^{-\phi^-_{b_0}} + \frac{J^-}{\mu^-_b N^-_b}\int_{b}^{b_0} dx\; e^{-\varphi(x)+E^-_b} \end{array} \right\} \tag{2.16}$$

and

$$\mathcal{E}^+ := \left\{ \{J^+,\varphi\} \in \mathbb{R}\times C_{\mathbb{R}}(\Delta) : \begin{array}{l} 0 < e^{\phi^+_{a_0}} - \frac{J^+}{\mu^+_a N^+_a}\int_{a_0}^{a} dx\; e^{\varphi(x)+E^+_a} \\ 0 < e^{\phi^+_{b_0}} + \frac{J^+}{\mu^+_b N^+_b}\int_{b}^{b_0} dx\; e^{\varphi(x)+E^+_b} \end{array} \right\}. \tag{2.17}$$

To prevent confusion we note that the curly brackets in (2.16) and (2.17) indicate pairs in the sense of set theory.

Notice that the definitions (2.10), (2.11), (2.12) and (2.13) make sense if $\{J^\pm,\varphi\} \in \mathcal{E}^\pm$. We note that $\phi^\pm_a[J^\pm,\varphi](a_0) = \phi^\pm_{a_0}$ and $\phi^\pm_b[J^\pm,\varphi](b_0) = \phi^\pm_{b_0}$ for $\{J^\pm,\varphi\} \in \mathcal{E}^\pm$. According to (1.4) and (2.14) we obtain

$$\begin{aligned} u^-_a[J^-,\varphi](x) &= N^-_a e^{\varphi(x)-E^-_a}\left\{e^{-\phi^-_{a_0}} - \frac{J^-}{\mu^-_a N^-_a}\int_{a_0}^{x} dy\; e^{-\varphi(y)+E^-_a}\right\}, \quad x \in \Sigma_a, \\ u^-_b[J^-,\varphi](x) &= N^-_b e^{\varphi(x)-E^-_b}\left\{e^{-\phi^-_{b_0}} + \frac{J^-}{\mu^-_b N^-_b}\int_{x}^{b_0} dy\; e^{-\varphi(y)+E^-_b}\right\}, \quad x \in \Sigma_b, \end{aligned} \tag{2.18}$$

for $\{J^\pm,\varphi\} \in \mathcal{E}^-$ and

$$\begin{aligned} u^+_a[J^+,\varphi](x) &= N^+_a e^{-(\varphi(x)+E^+_a)}\left\{e^{\phi^+_{a_0}} - \frac{J^+}{\mu^+_a N^+_a}\int_{a_0}^{x} dy\; e^{\varphi(y)+E^+_a}\right\}, \quad x \in \Sigma_a, \\ u^+_b[J^+,\varphi](x) &= N^+_b e^{-(\varphi(x)+E^+_b)}\left\{e^{\phi^+_{b_0}} + \frac{J^+}{\mu^+_b N^+_b}\int_{x}^{b_0} dy\; e^{\varphi(y)+E^+_b}\right\}, \quad x \in \Sigma_b, \end{aligned} \tag{2.19}$$

for $\{J^+,\varphi\} \in \mathcal{E}^+$ which clearly shows that the densities $u^\pm_\nu[J^\pm,\varphi]$, $\nu = a,b$, are positive if $\{J^\pm,\varphi\} \in \mathcal{E}^\pm$. The classical carrier density operators $\mathcal{D}^\pm : \mathcal{E}^\pm \longrightarrow L^1_{\mathbb{R}}(\Sigma)$ are defined by

$$\mathcal{D}^\pm[J^\pm,\varphi] := \begin{cases} u^\pm_a[J^\pm,\varphi], & x \in \Sigma_a, \\ u^\pm_b[J^\pm,\varphi], & x \in \Sigma_b, \end{cases} \tag{2.20}$$

where $\mathrm{dom}(\mathcal{D}^\pm) = \mathcal{E}^\pm$. Of course, the carrier densities are not only from L^1 but in fact continuous. However, in Section 3 we see that for the quantum densities the adequate function space is $L^1(\Omega)$. This suggests to demand here the same.

3 Quantum zone

In this section we rigorously define the dissipative Schrödinger system $\{h^\pm[\varkappa^\pm_a(\varphi),\varkappa^\pm_b(\varphi),\rho^\pm\}$ defined by (1.7)-(1.15) for $\varphi \in C_{\mathbb{R}}(\Delta)$ under the following general assumptions.

Assumption 3.1

(Q.1) The effective masses $m^\pm$ are positive and obey $m^\pm,\ \frac{1}{m^\pm} \in L^\infty_{\mathbb{R}}(\Omega)$.

(Q.2) The effective masses $m^\pm_a$ and $m^\pm_b$ outside the interval $[a,b]$ are positive and constant.

(Q.3) The band-edge offsets $w^\pm$ belong to $L^\infty_{\mathbb{R}}(\Omega)$.

(Q.4) The distribution functions $f^\pm : \mathbb{R} \longrightarrow \mathbb{R}_+$ are continuously differentiable and non-increasing, i.e $\frac{d}{dx}f^\pm(x) \le 0$ for $x \in \mathbb{R}$, such that

$$D^\pm(s) := \sup_{\lambda\in[s,\infty)} f^\pm(\lambda)\sqrt{1+\lambda^2} < \infty, \quad s \in \mathbb{R}, \tag{3.1}$$

$$F^\pm(s) := \int_s^\infty d\lambda\, f^\pm(\lambda) < \infty, \quad s \in \mathbb{R}, \tag{3.2}$$

A DS-system consists of two dissipative Schrödinger-type operators $h^\pm[\tau^\pm]$ on $\mathfrak{h} = L^2(\Omega)$,

$$\tau^\pm := \{\varkappa^\pm_a,\varkappa^\pm_b,v^\pm\} \in \mathcal{T}_+ := \mathbb{C}_+ \times \mathbb{C}_+ \times L^\infty_{\mathbb{R}}(\Omega), \tag{3.3}$$

and two density matrices $\rho^\pm \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ with values in the set of non-negative self-adjoint two-by-two matrices. We recall that the superscripts "+" or "-" corresponds to holes and electrons, respectively. The dissipative Schrödinger-type operator $h^\pm[\tau^\pm]$ are defined in the Hilbert space $\mathfrak{h} = L^2(\Omega)$ by

$$\mathrm{dom}(h[\tau^\pm]) = \left\{ g \in W^{1,2}(\Omega) : \begin{array}{l} \frac{1}{m^\pm}g' \in W^{1,2}(\Omega), \\ \frac{1}{2m^\pm(a)}g'(a) = -\varkappa^\pm_a g(a), \\ \frac{1}{2m^\pm(b)}g'(b) = \varkappa^\pm_b g(b) \end{array} \right\}, \tag{3.4}$$

and

$$(h^\pm[\tau^\pm]g)(x) = (l^\pm[v^\pm]g)(x), \quad g \in \mathrm{dom}(h[\tau]), \tag{3.5}$$

where

$$(l^{\pm}[v^{\pm}]g)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m^{\pm}(x)}\frac{d}{dx}g(x) + v^{\pm}(x)g(x). \tag{3.6}$$

The dissipative operators $h^{\pm}[\varphi]$ used in the following are defined by $h^{\pm}[\varphi] := h^{\pm}[\tau^{\pm}(\varphi)]$ where

$$\tau^{\pm}(\varphi) := \{\varkappa_a^{\pm}(\varphi), \varkappa_b^{\pm}(\varphi), w^{\pm} \pm \varphi\} \in \mathcal{T}_+, \quad \varphi \in C_{\mathbb{R}}(\Delta) \tag{3.7}$$

and $\varkappa_a^{\pm}(\varphi)$, $\varkappa_b^{\pm}(\varphi)$ are given by (1.10). Together with the density matrices

$$\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi](\lambda) := \begin{pmatrix} f^{\pm}(\lambda - \varepsilon_b^{\pm}) & 0 \\ 0 & f^{\pm}(\lambda - \varepsilon_a^{\pm}) \end{pmatrix} \chi_{\Lambda^{\pm}[\varphi]}(\lambda), \quad \lambda \in \mathbb{R}, \tag{3.8}$$

$\varphi \in C_{\mathbb{R}}(\Delta)$, cf. (1.15), this leads to the dissipative Schrödinger system $\{h^{\pm}[\varphi], \rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]\}$ where $\varepsilon_a^{\pm}, \varepsilon_b^{\pm}$ are called the Fermi energies of the reservoirs.

In accordance with Appendix A.2 and A.3 one associates with the dissipative Schrödinger system $\{h^{\pm}[\varphi], \rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}]\}$ carrier density operators $\mathcal{N}^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \cdot] : C_{\mathbb{R}}^{\infty}(\Delta) \longrightarrow L_{\mathbb{R}}^1(\Omega)$ and current density operators $j^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \cdot] : C_{\mathbb{R}}^{\infty}(\Delta) \longrightarrow \mathbb{R}$ defined by

$$\mathcal{N}^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] := \mathcal{N}^{\pm}_{\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]}[\tau^{\pm}(\varphi)], \quad \varphi \in C_{\mathbb{R}}(\Delta), \tag{3.9}$$

and

$$j^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] := j^{\pm}_{\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]}[\tau^{\pm}(\varphi)], \quad \varphi \in C_{\mathbb{R}}(\Delta), \tag{3.10}$$

see also [3, 32]. For us it is important that the carrier density operators admit the estimate

$$\begin{aligned} &\|\mathcal{N}^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]\|_{L^1(\Omega)} \leq \\ &\quad C_{\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]} \left(3 + \left[8 + 4\sqrt{\|m^{\pm}\|_{L^{\infty}(\Omega)}}(b-a)\right] \sqrt{1 + \|v_-^{\pm}\|_{L^{\infty}(\Omega)}}\right) \end{aligned} \tag{3.11}$$

where

$$v_-^{\pm}(x) := \max\{0, -v^{\pm}(x)\}, \quad x \in \Omega, \quad v^{\pm} := w^{\pm} \pm \varphi, \tag{3.12}$$

and

$$C_{\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]} := \sup_{\lambda \in \mathbb{R}} \|\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \sqrt{1 + \lambda^2}, \tag{3.13}$$

cf. Proposition A.2 of Appendix A.2. Further, it is crucial that the current density operators $j^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]$ have the representations

$$j^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] = \int_{\mathbb{R}} d\lambda \; \mathrm{tr}\big(\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi](\lambda) C^{\pm}[\varphi](\lambda)\big) \tag{3.14}$$

where $C^{\pm}[\varphi]$ are the so-called current density observables given by

$$C^{\pm}[\varphi](\lambda) := \frac{1}{2\pi}\big(P_a \Theta^{\pm}[\varphi](\lambda) P_b - P_b \Theta^{\pm}[\varphi](\lambda) P_a\big) \Theta^{\pm}[\varphi](\lambda)^*, \quad \lambda \in \mathbb{R}, \tag{3.15}$$

and $\Theta^{\pm}[\varphi] := \Theta^{\pm}[\tau^{\pm}(\varphi)]$ denote the so-called characteristic functions of the maximal dissipative operators $h^{\pm}[\varphi]$, see Appendix A.1. By P_a and P_b are indicated projections on the Hilbert space $\mathbb{C}^2$ given by

$$P_a := (\cdot, e_a)_{\mathbb{C}^2}\, e_a, \qquad P_b := (\cdot, e_b)_{\mathbb{C}^2}\, e_b, \tag{3.16}$$

where

$$e_b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad e_a = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.17}$$

and $(\cdot, \cdot)_{\mathbb{C}^2}$ is the scalar product in $\mathbb{C}^2$.

4 Hybrid model

Next we are going to couple the DS-system $\{h^{\pm}[\varphi], \rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi]\}$ to the DD-system. This coupling is done in two steps.

4.1 Fermi coupling

Fermi coupling means to choose the Fermi energies $\varepsilon_a^{\pm}$ and $\varepsilon_b^{\pm}$ in an appropriate manner. In the following we choose the Fermi energies in accordance with (1.17). In a forthcoming paper we legitimize this choice. Inserting the expressions (2.10)-(2.13) for the quasi Fermi potentials into (3.8) one gets the density matrices

$$\rho^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] = \rho^{\pm}[J^{\pm}, \varphi](\lambda) := \qquad (4.1)$$
$$\begin{pmatrix} f^{\pm}(\lambda \mp \phi_b^{\pm}[J^{\pm}, \varphi](b)) & 0 \\ 0 & f^{\pm}(\lambda \mp \phi_a^{\pm}[J^{\pm}, \varphi](a)) \end{pmatrix} \chi_{\Lambda^{\pm}[\varphi]}(\lambda),$$

$\lambda \in \mathbb{R}$. We note again explicitly that the density matrices $\rho^{\pm}[J^{\pm}, \varphi]$ are only well defined if $\{J^{\pm}, \varphi\} \in \mathcal{E}^{\pm}$, cf. (2.16) and (2.17). Inserting the expression (4.1) into equations (3.9) and (3.10) the carrier and current density operators of the dissipative Schrödinger system $\{h^{\pm}[\varphi], \rho^{\pm}[J^{\pm}, \varphi]\}$ transform into

$$\mathcal{N}^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] = \mathcal{N}^{\pm}[J^{\pm}, \varphi] := \mathcal{N}^{\pm}_{\rho^{\pm}[J^{\pm}, \varphi]}[\tau^{\pm}(\varphi)], \quad \varphi \in C_{\mathbb{R}}(\Delta), \qquad (4.2)$$

and

$$j^{\pm}[\varepsilon_a^{\pm}, \varepsilon_b^{\pm}, \varphi] = j^{\pm}[J^{\pm}, \varphi] := j^{\pm}_{\rho^{\pm}[J^{\pm}, \varphi]}[\tau^{\pm}(\varphi)], \quad \varphi \in C_{\mathbb{R}}(\Delta). \qquad (4.3)$$

4.2 Current coupling

The DS-system $\{h^{\pm}[\varphi], \rho^{\pm}[J^{\pm}, \varphi]\}$ includes the classical current densities $J^{\pm}$ as a free parameter provided $J^{\pm} \in (J^{\pm}_{min}[\varphi], J^{\pm}_{max}[\varphi])$, cf. (2.6) and (2.7). In following we are going to eliminate this free parameter by the current continuity condition (1.16) which takes the form

$$J^{\pm} = j^{\pm}[J^{\pm}, \varphi], \quad \{J^{\pm}, \varphi\} \in \mathcal{E}^{\pm}. \qquad (4.4)$$

We show that for each fixed electrostatic potential $\varphi \in C_{\mathbb{R}}(\Delta)$ the equations (4.4) admit unique solutions $J^{\pm} \in (J^{\pm}_{min}[\varphi], J^{\pm}_{max}[\varphi])$.

Proposition 4.1 *If the Assumptions 2.1 and 3.1 are satisfied, then for any $\varphi \in C_{\mathbb{R}}(\Delta)$ the equations (4.4) admit unique solutions $J^{\pm}[\varphi]$ such that $\{J^{\pm}[\varphi], \varphi\} \in \mathcal{E}^{\pm}$.*

Proof. Using (3.14), (3.15) and (4.1) we get

$$j^{\pm}[J^{\pm}, \varphi] = \frac{1}{2\pi} \int_{\mathbb{R}} d\lambda \, \mathrm{tr}\left(\rho^{\pm}[J^{\pm}, \varphi](\lambda)\left(P_a \Theta^{\pm}[\varphi](\lambda) P_b - P_b \Theta^{\pm}[\varphi](\lambda) P_a\right) \Theta^{\pm}[\varphi](\lambda)^*\right)$$

or

$$j^{\pm}[J^{\pm}, \varphi] = \frac{1}{2\pi} \int_{\Lambda^{\pm}[\varphi]} d\lambda \left(f^{\pm}(\lambda \mp \phi_a^{\pm}[J^{\pm}, \varphi](a)) |(e_b, \Theta^{\pm}[\varphi](\lambda) e_a)_{\mathbb{C}^2}|^2 - \right.$$
$$\left. f^{\pm}(\lambda \mp \phi_b^{\pm}[J^{\pm}, \varphi](b)) |(e_a, \Theta^{\pm}[\varphi](\lambda) e_b)_{\mathbb{C}^2}|^2 \right)$$

where e_a, e_b are given by (3.17). From [32, Section 3] we know that $(e_b, \Theta^{\pm}[\varphi](\lambda)e_a)_{\mathbb{C}^2} = (e_a, \Theta^{\pm}[\varphi](\lambda)e_b)_{\mathbb{C}^2}$. Introducing the transmission coefficients

$$t^{\pm}[\varphi](\lambda) := \left|(e_b, \Theta^{\pm}[\varphi](\lambda)e_a)_{\mathbb{C}^2}\right|^2, \quad \lambda \in \mathbb{R}, \quad \varphi \in C_{\mathbb{R}}(\Delta), \tag{4.5}$$

we obtain the representations

$$\begin{aligned} &j^{\pm}[J^{\pm}, \varphi] = \\ &\quad \frac{1}{2\pi}\int_{\Lambda^{\pm}[\varphi]} d\lambda\, t^{\pm}[\varphi](\lambda)\left(f^{\pm}(\lambda \mp \phi^{\pm}_a[J^{\pm},\varphi](a)) - f^{\pm}(\lambda \mp \phi^{\pm}_b[J^{\pm},\varphi](b))\right). \end{aligned} \tag{4.6}$$

Since the considerations for holes and electrons are the same we restrict ourselves in the following to holes. We consider only the current continuity equation $J^+ = j^+[J^+, \varphi]$, $\{J^+, \varphi\} \in \mathcal{E}^+$. The characteristic function $\Theta^+[\varphi](z)$ is holomorphic and contractive in $z \in \mathbb{C}_-$. Hence, the function $(e_b, \Theta^+[\varphi](z)e_a)_{\mathbb{C}^2}$ is holomorphic and bounded by one in $z \in \mathbb{C}_-$. We note that the limit $(e_b, \Theta^+[\varphi](\lambda)e_a)_{\mathbb{C}^2} = \lim_{\beta\uparrow 0}(e_b, \Theta^+[\varphi])](\lambda - i\beta)e_a)_{\mathbb{C}^2}$ exist for all $\lambda \in \mathbb{R}$ and is bounded by one. Using the uniqueness theorem for H^∞-function, cf. Corollary II.4.2 of [25], we find that this limit is different from zero for a.e $\lambda \in \mathbb{R}$. Hence the function $t^+[\varphi](\lambda)$ is different from zero and obeys the estimate

$$0 \le t^+[\varphi](\lambda) \le 1, \quad \varphi \in C_{\mathbb{R}}(\Delta), \tag{4.7}$$

for a.e. $\lambda \in \mathbb{R}$. Inserting (2.12) and (2.13) into (4.6) we find

$$\begin{aligned} &j^+[J^+, \varphi] = \\ &\quad \frac{1}{2\pi}\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+\left(\lambda - \ln\left(e^{\phi^+_{a_0}} - \frac{J^+}{\mu^+_a N^+_a}\int_{a_0}^{a} dy\, e^{\varphi(y)+E^+_a}\right)\right) - \\ &\quad \frac{1}{2\pi}\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+\left(\lambda - \ln\left(e^{\phi^+_{b_0}} + \frac{J^+}{\mu^+_b N^+_b}\int_{b}^{b_0} dy\, e^{\varphi(y)+E^+_b}\right)\right) \end{aligned}$$

Since $\frac{d}{dx} f^+ \le 0$ one gets $\frac{\partial}{\partial J^+} j^+[J^+, \varphi] \le 0$. Hence, if φ is fixed, then the function $j^+[J^+, \varphi]$ is non-increasing in J^+. By Lemma 2.2 one has $\{J^+, \varphi\} \in \mathcal{E}^+ \iff J^+ \in (J^+_{min}[\varphi], J^+_{max}[\varphi])$. If $J^+ \uparrow J^+_{max}[\varphi]$, then $\phi^+[J^+, \varphi](a) \to -\infty$. Using the estimate

$$\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+(\lambda - \phi^+_a[J^+, \varphi](a)) \le \int_{v^+_{max} - \phi^+_a[J^+,\varphi](a)}^{\infty} d\lambda\, f^+(\lambda),$$

we find

$$\lim_{J^+\uparrow J^+_{max}[\varphi]} \int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+(\lambda - \phi^+_a[J^+, \varphi](a)) = 0$$

which gives

$$\begin{aligned} &j^+[J^+_{max}[\varphi], \varphi] := \lim_{J^+\uparrow J^+_{max}[\varphi]} j^+[J^+, \varphi] = \\ &\quad -\frac{1}{2\pi}\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+\left(\lambda - \ln\left(e^{\phi^+_{b_0}} + \frac{J^+_{max}[\varphi]}{\mu^+_b N^+_b}\int_{b}^{b_0} dy\, e^{\varphi(y)+E^+_b}\right)\right). \end{aligned} \tag{4.8}$$

Similarly, if $J^+ \downarrow J^+_{min}[\varphi]$, then $\phi^+_b[J^+, \varphi](b) \to -\infty$. Hence

$$\lim_{J^+\downarrow J^+_{min}[\varphi]} \int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+(\lambda - \phi^+_b[J^+, \varphi](b)) = 0$$

which yields

$$j^+[J^+_{min}[\varphi],\varphi] := \lim_{J^+\downarrow J^+_{min}[\varphi]} j^+[J^+,\varphi] = \tag{4.9}$$
$$\frac{1}{2\pi}\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda) f^+\left(\lambda - \ln\left(e^{\phi^+_{a_0}} - \frac{J^+_{min}[\varphi]}{\mu^+_a N^+_a}\int_{a_0}^{a} dy\, e^{\varphi(y)+E^+_a}\right)\right).$$

Since $j^+[J^+,\varphi]$ is continuous and non-increasing in J^+ as well as $j^+[J^+_{min}[\varphi],\varphi] > 0$ and $j^+[J^+_{max}[\varphi],\varphi] < 0$ one immediately gets that the equation $J^+ = j^+[J^+,\varphi]$ admits a unique solution $J^+[\varphi]$ for each $\varphi \in C_{\mathbb{R}}(\Delta)$ which satisfies $\{J^+[\varphi],\varphi\} \in \mathcal{E}^+$. Similarly, one shows that the equation $J^- = j^-[J^-,\varphi]$ admits a unique solution $J^-[\varphi]$ for each $\varphi \in C_{\mathbb{R}}(\Delta)$ such that $\{J^-[\varphi],\varphi\} \in \mathcal{E}^-$. □

4.3 Dissipative hybrid system

If $J^\pm[\varphi]$ is the solution of Proposition 4.1 for given $\varphi \in C_{\mathbb{R}}(\Delta)$, then it makes sense to introduce the following quantities of the dissipative hybrid system (DH-system):

$$\begin{array}{lcll} \phi^\pm_\nu[\varphi] & := & \phi^\pm_\nu[J^\pm[\varphi],\varphi], \quad \nu = a,b, & \text{cf. (2.10), (2.11), (2.12), (2.13)}, \\ \rho^\pm[\varphi] & := & \rho^\pm[J^\pm[\varphi],\varphi], & \text{cf. (4.1)}, \\ \mathcal{N}^\pm[\varphi] & := & \mathcal{N}^\pm[J^\pm[\varphi],\varphi], & \text{cf. (4.2)}, \\ \mathcal{D}^\pm[\varphi] & := & \mathcal{D}^\pm[J^\pm[\varphi],\varphi], & \text{cf. (2.20)}. \end{array} \tag{4.10}$$

Moreover, it makes sense to introduce carrier density operators for the DH-system:

Definition 4.2 Let the Assumptions 2.1 and 3.1 be satisfied. The carrier density operator $\mathcal{U}^\pm[\cdot] : C_{\mathbb{R}}(\Delta) \longrightarrow L^1_{\mathbb{R}}(\Delta)$ of the dissipative hybrid system is defined by

$$\mathcal{U}^\pm[\varphi](x) := \begin{cases} \mathcal{D}^\pm[\varphi](x), & x \in \Sigma, \\ \mathcal{N}^\pm[\varphi](x), & x \in \Omega, \end{cases} \tag{4.11}$$

cf. (4.10).

In this section we verify certain properties of the quantities (4.10) which are needed later for the existence proof. In the following lemma we give an L^∞-estimate of the quasi Fermi potentials $\phi^\pm[\varphi]$ which is uniform in $\varphi \in C_{\mathbb{R}}(\Delta)$.

Lemma 4.3 *If the Assumptions 2.1 and 3.1 are satisfied, then for any $\varphi \in C_{\mathbb{R}}(\Delta)$ one has*

$$\max\{|\phi^\pm_a[\varphi](x)|, \phi^\pm_b[\varphi](x)|\} \le \eta^\pm, \quad x \in \Sigma, \tag{4.12}$$

where

$$\eta^\pm := \max\left\{\left|\phi^\pm_{a_0}\right|, \left|\phi^\pm_{b_0}\right|\right\} \tag{4.13}$$

Proof. Assume that $J^+[\varphi] \ge 0$. Since $J^+[\varphi]$ solves the equation (4.4) one gets from (4.6) that

$$f^+(\lambda - \phi^+_a[\varphi](a)) \ge f^+(\lambda - \phi^+_b[\varphi](b)), \quad \lambda \in \Lambda^+[\varphi].$$

Taking into account the monotonicity of f^+ we find that

$$-\phi_a^+[\varphi](a) \le -\phi_b^+[\varphi](b).$$

If $J^+[\varphi] \ge 0$, then $-\phi_\nu^+[\varphi](x)$, $x \in \Sigma_\nu$, $\nu = a, b$, is non-decreasing. That means we have

$$-\phi_a^+[\varphi](a_0) \le -\phi_a^+[\varphi](a) \quad \text{and} \quad -\phi_b^+[\varphi](b) \le -\phi_b^+[\varphi](b_0).$$

Hence

$$-\phi_a^+[\varphi](a_0) \le -\phi_a^+[\varphi](a) \le -\phi_b^+[\varphi](b) \le -\phi_b^+[\varphi](b_0).$$

which shows that

$$\max\{|\phi_a^+[\varphi](a)|, |\phi_b^+[\varphi](b)|\} \le \max\{|\phi_a^+[\varphi](a_0)|, |\phi_b^+[\varphi](b_0)|\}.$$

If $J^+[\varphi] \le 0$, then from equation (4.6) one gets

$$f^+(\lambda - \phi_a^+[\varphi](a)) \le f^+(\lambda - \phi_b^+[\varphi](b)), \quad \lambda \in \Lambda^+[\varphi],$$

which yields

$$\phi_a^+[\varphi](a) \le \phi_b^+[\varphi](b).$$

Since $\phi_\nu^+[\varphi](x)$ is non-decreasing on Σ_ν, $\nu = a, b$, we find

$$\phi_a^+[\varphi](a_0) \le \phi_a^+[\varphi](a) \le \phi_b^+[\varphi](b) \le \phi_b^+[\varphi](b_0)$$

which yields

$$\max\{|\phi_a^+[\varphi](a)|, |\phi_b^+[\varphi](b)|\} \le \max\{|\phi_a^+[\varphi](a_0)|, |\phi_a^+[\varphi](b_0)|\}.$$

Since $\phi_a^+[\varphi](a_0) = \phi_{a_0}^+$ and $\phi_b^+[\varphi](b_0) = \phi_{b_0}^+$ we obtain (4.12) for $x = a, b$. We complete the proof for holes by the remark that the quasi Fermi potentials $\phi_\nu^+[\varphi]$, $\nu = a, b$, are monotone. The proof for electrons is similar. □

We note that the constants $\eta^\pm$ are independent of the potential φ. With help of Lemma 4.3 we prove an estimate for the carrier density operators.

Lemma 4.4 *If the Assumptions 2.1 and 3.1 are satisfied, then for any $\varphi \in C_{\mathbb{R}}(\Delta)$ the carrier density operators $\mathcal{N}^\pm[\cdot]$ admit the estimates*

$$\|\mathcal{N}^\pm[\varphi]\|_{L^1(\Omega)} \le \tag{4.14}$$
$$C^\pm(v_{max}^\pm(\varphi))\left(3 + \left[8 + 4\sqrt{\|m^\pm\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|w^\pm\|_{L^\infty(\Omega)} + \|\varphi_\mp\|_{L^\infty(\Omega)}}\right)$$

where

$$\varphi_+(x) := \max\{0, \varphi(x)\}, \quad \textit{and} \quad \varphi_-(x) := \max\{0, -\varphi(x)\}, \quad x \in \Omega, \tag{4.15}$$

$v_{max}^\pm(\varphi)$ is defined by (1.13),

$$C^\pm(s) := D^\pm(s - \eta^\pm)(1 + \eta^\pm), \quad s \in \mathbb{R}, \tag{4.16}$$

$D^\pm(\cdot)$ and $\eta^\pm$ are given by (3.1) and (4.13), *respectively.*

Proof. From (3.11)-(3.13) we get

$$\|\mathcal{N}^{\pm}[\varphi]\|_{L^1(\Omega)} \le C_{\rho^{\pm}[\varphi]}\left(3 + \left[8 + 4\sqrt{\|m^{\pm}\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|v_-^{\pm}\|_{L^\infty(\Omega)}}\right)$$

where $C_{\rho^{\pm}[\varphi]} = \sup_{\lambda\in\mathbb{R}} \|\rho^{\pm}[\varphi](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)}\sqrt{1+\lambda^2}$. A simple calculation shows that

$$\|v_-^{\pm}\|_{L^\infty(\Omega)} \le \|w^{\pm}\|_{L^\infty(\Omega)} + \|\varphi_{\mp}\|_{L^\infty(\Omega)}.$$

Hence, we obtain

$$\begin{aligned}&\|\mathcal{N}^{\pm}[\varphi]\|_{L^1(\Omega)} \le \\ &\quad C_{\rho^{\pm}[\varphi]}\left(3 + \left[8 + 4\sqrt{\|m^{\pm}\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|w^{\pm}\|_{L^\infty(\Omega)} + \|\varphi_{\mp}\|_{L^\infty(\Omega)}}\right).\end{aligned}$$

The next step is to estimate the constant $C_{\rho^{\pm}[\varphi]}$ by $C^{\pm}(v^{\pm}_{max}(\varphi))$. Let us consider the case of holes. We find

$$\begin{aligned}&\sup_{\lambda\in\Lambda^+[\varphi]} \sqrt{1+\lambda^2} f^+(\lambda - \phi_b^+[\varphi](b)) \le \\ &\qquad D^+(v^+_{max}(\varphi) - \phi_b^+[\varphi](b)) \sup_{x\in\mathbb{R}}\left(\frac{1 + (x + \phi_b^+[\varphi](b))^2}{1+x^2}\right)^{1/2}\end{aligned}$$

Since

$$\sup_{x\in\mathbb{R}}\left(\frac{1 + (x + \phi_b^+[\varphi](b))^2}{1+x^2}\right)^{1/2} \le 1 + |\phi_b^+[\varphi](b)|$$

we get

$$\sup_{\lambda\in\Lambda^+[\varphi]} \sqrt{1+\lambda^2} f^+(\lambda - \phi_b^+[\varphi](b)) \le D^+(v^+_{max}(\varphi) - \phi_b^+[\varphi](b))(1 + |\phi_b^+[\varphi](b)|).$$

In the same manner we prove

$$\sup_{\lambda\in\Lambda^+[\varphi]} \sqrt{1+\lambda^2} f^+(\lambda - \phi_a^+[\varphi](a)) \le D^+(v^+_{max}(\varphi) - \phi_a^+[\varphi](a))(1 + |\phi_a^+[\varphi](a)|).$$

which yields

$$C_{\rho^+[\varphi]} \le \max_{\nu\in\{a,b\}}\left\{D^+(v^+_{max}(\varphi) - \phi_\nu^+[\varphi](\nu))(1 + |\phi_\nu^+[\varphi](\nu)|)\right\}. \tag{4.17}$$

Since $D^+(\cdot)$ is not increasing we complete the proof using Lemma 4.3. The proof for electrons is similar. □

Like the carrier densities $\mathcal{N}^{\pm}[\varphi]$ the current densities $J^{\pm}[\varphi]$ admit an estimation, too.

Lemma 4.5 *If the Assumptions 2.1 and 3.1 are satisfied, then for any $\varphi \in C_{\mathbb{R}}(\Delta)$ the estimates*

$$|J^{\pm}[\varphi]| \le \frac{1}{\pi} F^{\pm}(v^{\pm}_{max}(\varphi) - \eta^{\pm}) \tag{4.18}$$

are valid, where $v^{\pm}_{max}(\varphi)$ are defined by (1.13), *$\eta^{\pm}$ and the functions $F^{\pm}(\cdot)$ are given by (4.13) and by (3.2), respectively*

Proof. We consider the case of holes. Since $J^+[\varphi]$ is a solution of (4.4) one has $J^+[\varphi] = j^{\pm}[J^+[\varphi],\varphi]$ where $j^{\pm}[J^+[\varphi],\varphi]$ is defined by (4.3). From (4.6) and the fact that the transmission coefficient $t^+[\varphi](\lambda)$, cf. (4.5), is uniformly bounded by one, cf. (4.7), we obtain

$$|J^+[\varphi]| \le \frac{1}{2\pi}\left\{\int_{\Lambda^+[\varphi]} d\lambda\ f^+(\lambda - \phi_b^+[\varphi](b)) + f^+(\lambda - \phi_a^+[\varphi](a))\right\}$$

which yields

$$|J^+[\varphi]| \le \frac{1}{2\pi}\left\{F^+(v^+_{max}(\varphi) - \phi_b^+[\varphi](b)) + F^+(v^+_{max}(\varphi) - \phi_a^+[\varphi](a))\right\}.$$

By Lemma 4.3 we immediately get (4.18). Similarly, one handles the case of electrons. $\square$

We are going to show the continuity of the current density operator with respect to the electrostatic potential φ.

Lemma 4.6 *Let the Assumptions 2.1 and 3.1 be satisfied. If $\varphi, \varphi_n \in C_{\mathbb{R}}(\Delta)$, $n \in \mathbb{N}$, and $\lim_{n\to\infty} \|\varphi_n - \varphi\|_{L^\infty(\Delta)} = 0$, then $\lim_{n\to\infty} J^{\pm}[\varphi_n] = J^{\pm}[\varphi]$.*

Proof. We set $J^{\pm} := J^{\pm}[\varphi]$ and $J^{\pm}_n := J^{\pm}[\varphi_n]$, $n \in \mathbb{N}$. If $J^{\pm}_n \not\to J^{\pm}$ as $n \to \infty$, then there is a subsequence $\{J^{\pm}_{n_k}\}_{k\in\mathbb{N}}$ such that $\lim_{k\to\infty} J^{\pm}_{n_k} = J^{\pm}_{\infty} \ne J^{\pm}$. This results from Lemma 4.5 which shows the uniform boundedness of $\{J^{\pm}_n\}^{\infty}_{n\in\mathbb{N}}$.

Let us show that $\{J^{\pm}_\infty, \varphi\} \in \mathcal{E}^{\pm}$. Since $\{J^{\pm}_n, \varphi_n\} \in \mathcal{E}^{\pm}$, $n \in \mathbb{N}$, and

$$\lim_{n\to\infty} J^{\pm}_{min}[\varphi_n] = J^{\pm}_{min}[\varphi] \quad \text{and} \quad \lim_{n\to\infty} J^{\pm}_{max}[\varphi_n] = J^{\pm}_{max}[\varphi]$$

one has $\{J^{\pm}_\infty, \varphi\} \notin \mathcal{E}^{\pm}$ if and only if either $J^{\pm}_\infty = J^{\pm}_{max}[\varphi]$ or $J^{\pm}_\infty = J^{\pm}_{min}[\varphi]$. However, this is impossible: Namely, if $\lim_{k\to\infty} J^+_{n_k} = J^+_{max}[\varphi] > 0$, then $\lim_{k\to\infty} j^+[J^+_{n_k}, \varphi_{n_k}] = j^+[J^+_\infty, \varphi] \le 0$, cf. (4.8). Similarly, if $\lim_{k\to\infty} J^+_{n_k} = J^+_{min}[\varphi] < 0$, then $\lim_{k\to\infty} j^+[J^+_{n_k}, \varphi_{n_k}] = j^+[J^+_\infty, \varphi] \ge 0$, cf. (4.9) The proof for the electrons is similar.

Since $\{J^{\pm}_\infty, \varphi\} \in \mathcal{E}^{\pm}$ the quantities $\phi^{\pm}_\nu[J^{\pm}_\infty, \varphi]$, $\nu = a, b$, and $\rho^{\pm}[J^{\pm}_\infty, \varphi]$ are well-defined. One gets $\lim_{k\to\infty} \phi^{\pm}_b[J^{\pm}_{n_k}, \varphi_{n_k}](b) = \phi^{\pm}_b[J^{\pm}_\infty, \varphi](b)$ and $\lim_{k\to\infty} \phi^{\pm}_a[J^{\pm}_{n_k}, \varphi_{n_k}](a) = \phi^{\pm}_a[J^{\pm}_\infty, \varphi](a)$ which yields $\lim_{k\to\infty} \rho^{\pm}[J^{\pm}_{n_k}, \varphi_{n_k}](\lambda) = \rho^{\pm}[J^{\pm}_\infty, \varphi](\lambda)$ for a.e. $\lambda \in \mathbb{R}$ as well as $L_{\rho^{\pm}[J^{\pm}_{n_k}, \varphi_{n_k}]} < \infty$, $k \in \mathbb{R}$, and $L_{\rho^{\pm}[J^{\pm}_\infty, \varphi]} < \infty$, cf. (A.32), (3.2) and (4.1). Moreover, we find

$$\lim_{k\to\infty} \int_{\mathbb{R}} d\lambda\ \left(\rho^{\pm}[J^{\pm}_{n_k}, \varphi_{n_k}](\lambda)e, e\right)_{\mathbb{C}^2} = \int_{\mathbb{R}} d\lambda\ \left(\rho^{\pm}[J^{\pm}_\infty, \varphi](\lambda)e, e\right)_{\mathbb{C}^2}$$

for each $e \in \mathbb{C}^2$. By the assumption $\lim_{n\to\infty} \|\varphi_n - \varphi\|_{L^\infty(\Delta)} = 0$ we get $\tau^{\pm}[\varphi_n] \to \tau^{\pm}(\varphi)$ as $n \to \infty$, cf. (3.7). Applying Theorem A.6 we verify that

$$\lim_{k\to\infty} j^{\pm}[J^{\pm}_{n_k}, \varphi_{n_k}] = j^{\pm}[J^{\pm}_\infty, \varphi].$$

Since $J^{\pm}_{n_k} = j^{\pm}[J^{\pm}_{n_k}, \varphi_{n_k}]$ we find

$$J^{\pm}_\infty = \lim_{k\to\infty} J^{\pm}_{n_k} = j^{\pm}[J^{\pm}_\infty, \varphi].$$

Since the solutions of these equations are unique one gets $J^{\pm}_\infty = J^{\pm}[\varphi]$, which proves the continuity. $\square$

Next, let us show that the carrier density operators $\mathcal{U}^{\pm}[\cdot]$ are continuous. To this end we first prove the continuity of the dissipative carrier density operators $\mathcal{N}^{\pm}[\cdot]$.

Lemma 4.7 *Let the Assumptions 2.1 and 3.1 be satisfied. If* $\varphi, \varphi_n \in C_{\mathbb{R}}(\Delta)$, $n \in \mathbb{N}$, *and* $\lim_{n\to\infty} \|\varphi_n - \varphi\|_{L^\infty(\Delta)} = 0$, *then* $\lim_{n\to\infty} \|\mathcal{N}^\pm[\varphi_n] - \mathcal{N}^\pm[\varphi]\|_{L^1(\Omega)} = 0$.

Proof. We set $\tau^\pm := \tau^\pm(\varphi)$ and $\tau_n^\pm := \tau^\pm(\varphi_n)$, $n \in \mathbb{N}$, cf (3.7). Notice that $\lim_{n\to\infty} \tau_n^\pm = \tau^\pm$, cf. (A.1). Since $C_{\rho^\pm[\varphi]} \leq D^\pm(v^\pm_{max}(\varphi) - \eta^\pm)$ (cf. (A.23) for the definition of $C_{\rho^\pm[\varphi]}$) for any $\varphi \in C_{\mathbb{R}}(\Delta)$ we get $\sup_n C_{\rho^\pm[\varphi_n]} < \infty$, see proof of Lemma 4.4. Furthermore, by $\lim_{n\to\infty} \phi_\nu^\pm[\varphi_n](x) = \phi_\nu^\pm[\varphi](x)$, $x \in \Sigma_\nu$, $\nu = a, b$, we find $\lim_{n\to\infty} \rho^\pm[\varphi_n](\lambda) = \rho^\pm[\varphi](\lambda)$ for a.e. $\lambda \in \mathbb{R}$. Applying Theorem A.5 we complete the proof. $\square$

Proposition 4.8 *Let the Assumptions 2.1 and 3.1 be satisfied. If* $\varphi, \varphi_n \in C_{\mathbb{R}}(\Delta)$, $n \in \mathbb{N}$, *and* $\lim_{n\to\infty} \|\varphi_n - \varphi\|_{L^\infty(\Delta)} = 0$, *then* $\lim_{n\to\infty} \|\mathcal{U}^\pm[\varphi_n] - \mathcal{U}^\pm[\varphi]\|_{L^1(\Delta)} = 0$.

Proof. Taking into account Lemma 4.7 it remains to show that

$$\lim_{n\to\infty} \|\mathcal{D}^\pm[\varphi_n] - \mathcal{D}^\pm[\varphi]\|_{L^1(\Sigma)} = 0.$$

By Lemma 4.6 one gets $\lim_{n\to\infty} u_\nu^\pm[J^\pm[\varphi_n], \varphi_n] = u_\nu^\pm[J^\pm[\varphi], \varphi]$, $\nu = a, b$, cf. (2.18) and (2.19), which yields $\lim_{n\to\infty} \|\mathcal{D}[\varphi_n] - \mathcal{D}[\varphi]\|_{L^1(\Sigma)} = 0$. $\square$

4.4 Coupling to Poisson's equation: dissipative hybrid model

In order to have a meaningful model for semi-conductors, the electrostatic potential has to be self-consistently computed by a Poisson equation. In this section we pose the Poisson equation on the whole device domain Δ, where the right hand side depends on the densities of the DH-system. This leads to a non-linear equation for the electrostatic potential φ. Moreover, we will reformulate the problem as a fixed point problem.

Concerning the data for Poisson's equation we make the following assumptions:

Assumption 4.9

(P.1) The doping profile C belongs to $\overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta)$.

(P.2) The dielectric permittivity ϵ is positive and obeys ϵ, $\frac{1}{\epsilon} \in L^\infty_{\mathbb{R}}(\Delta)$. We set $\tilde{\epsilon} := \max\{1, \|\frac{1}{\epsilon}\|_{L^\infty(\Delta)}\}$.

By $\widehat{\varphi}$ we denote the function

$$\widehat{\varphi}(x) := \frac{1}{\int_{a_0}^{b_0} dt\, \frac{1}{\epsilon(t)}} \left\{ \varphi_{b_0} \int_{a_0}^{x} dt\, \frac{1}{\epsilon(t)} + \varphi_{a_0} \int_{x}^{b_0} dt\, \frac{1}{\epsilon(t)} \right\}, \quad x \in \Delta, \tag{4.19}$$

where φ_{a_0} and φ_{b_0} are the boundary values (1.20) of the Poisson equation. Notice that $\widehat{\varphi} \in W^{1,2}_{\mathbb{R}}(\Delta)$, $\epsilon \frac{d}{dx}\widehat{\varphi} \in W^{1,2}_{\mathbb{R}}(\Delta)$ and $\widehat{\varphi}(a_0) = \varphi_{a_0}$ and $\widehat{\varphi}(b_0) = \varphi_{b_0}$. Furthermore, one has

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}\widehat{\varphi}(x) = 0, \quad x \in \Delta.$$

Definition 4.10 We define the Poisson operator $\mathcal{P} : W^{1,2}_{\mathbb{R}}(\Delta) \longrightarrow \overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta)$ by

$$\langle \mathcal{P}v, \zeta \rangle := \int_a^b dx\, \epsilon(x) \frac{dv}{dx}\frac{d\zeta}{dx}, \qquad v \in W^{1,2}_{\mathbb{R}}(\Delta),\ \zeta \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta) \tag{4.20}$$

The restriction of $\mathcal{P}$ to the subspace $\overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ will be denoted by $\mathcal{P}_0$.

Definition 4.11 Assume $u^\pm \in L^1(\Delta)$. We say $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ satisfies Poisson's equation if $\zeta := \varphi - \widehat{\varphi} \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ and, additionally, satisfies

$$\mathcal{P}_0\zeta = C + E_1 u^+ - E_1 u^- \tag{4.21}$$

where E_1 denotes the embedding operator from $L^1(\Delta)$ into $\overset{o}{W}{}^{-1,2}(\Delta)$.

By E_∞ we denote further the embedding operator from $W^{1,2}(\Delta)$ into $C(\Delta)$.

Definition 4.12 Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. We say an element $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ is a solution of the dissipative hybrid model (DH-model) if

(i) the carrier densities $u^\pm \in L^1(\Delta)$ are given by the hybrid densities, i.e. $u^\pm = \mathcal{U}^\pm[E_\infty\varphi]$, cf. (4.11), and

(ii) the potential φ satisfies Poisson's equation.

We note that if $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ is a solution of the DH-model, then the current densities are given by $J^\pm[\varphi]$.

Let us introduce for each fixed $\varphi \in C_{\mathbb{R}}(\Delta)$ the operator $\mathcal{P}[\varphi] : \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta) \longrightarrow \overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta)$,

$$\mathcal{P}[\varphi](\zeta) := \mathcal{P}_0\zeta + E_1\left\{p^-[\varphi]e^{\zeta} - p^+[\varphi]e^{-\zeta}\right\}, \tag{4.22}$$

where

$$p^-[\varphi](x) := \begin{cases} N_a^- e^{\widehat{\varphi}(x)-E_a^-}\left(e^{-\phi^-_{a_0}} - \frac{J^-[\varphi]}{\mu_a^- N_a^-}\int_{a_0}^x dy\, e^{-\varphi(y)+E_a^-}\right), & x \in \Sigma_a, \\ 0, & x \in \Omega, \\ N_b^- e^{\widehat{\varphi}(x)-E_b^-}\left(e^{-\phi^-_{b_0}} + \frac{J^-[\varphi]}{\mu_b^- N_b^-}\int_x^{b_0} dy\, e^{-\varphi(y)+E_b^-}\right), & x \in \Sigma_b \end{cases} \tag{4.23}$$

and

$$p^+[\varphi](x) := \begin{cases} N_a^+ e^{-(\widehat{\varphi}(x)+E_a^+)}\left(e^{\phi^+_{a_0}} - \frac{J^+[\varphi]}{\mu_a^+ N_a^+}\int_{a_0}^x dy\, e^{\varphi(y)+E_a^+}\right), & x \in \Sigma_a, \\ 0, & x \in \Omega, \\ N_b^+ e^{-(\widehat{\varphi}(x)+E_b^+)}\left(e^{\phi^+_{b_0}} + \frac{J^+[\varphi]}{\mu_b^+ N_b^+}\int_x^{b_0} dy\, e^{\varphi(y)+E_b^+}\right), & x \in \Sigma_b, \end{cases} \tag{4.24}$$

$\varphi \in C_{\mathbb{R}}(\Delta)$. We note that $p^\pm[\varphi] \in L^\infty_{\mathbb{R}}(\Delta)$. Notice that drift-diffusion densities can be written as

$$u^\pm_\nu[J^\pm[\varphi], \varphi](x) = p^\pm[\varphi](x)e^{\mp\zeta(x)}, \quad x \in \Sigma_\nu, \quad \nu = a, b,$$

where $\varphi = \zeta + \widehat{\varphi}$ and $u_\nu^\pm[J^\pm[\varphi], \varphi]$ are given by (2.18) and (2.19).

Concerning the next Lemma and its proof we follow the terminology of [23], in particular, the notions of strong monotonicity and boundedly Lipschitz continuity are used in accordance with Definitions III.1.1 and III.1.2 of [23].

Lemma 4.13 *Let the Assumption 2.1 and 4.9 be satisfied. If $\varphi \in C_{\mathbb{R}}(\Delta)$, then the operator $\mathcal{P}[\varphi]$ is strongly monotone with monotonicity constant $m_{\mathcal{P}}$,*

$$m_{\mathcal{P}} := \frac{1}{\|1/\epsilon\|_{L^\infty(\Delta)}}, \tag{4.25}$$

and boundedly Lipschitz continuous.

Proof. We note that the operator $\mathcal{P}_0$ is linear, bounded and obeys

$$\langle \mathcal{P}_0 \zeta, \zeta \rangle \;\geq\; m_{\mathcal{P}} \|\zeta\|^2_{\overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)} \tag{4.26}$$

where the constant $m_{\mathcal{P}}$ is given by (4.25). Hence $\mathcal{P}_0$ is a strongly monotone operator with monotonicity constant $m_{\mathcal{P}}$ which maps $\overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ onto $\overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta)$.

By Proposition 4.1 one has $\{J^\pm[\varphi], \varphi\} \in \mathcal{E}^\pm$, hence, $p^\pm[\varphi](x) \geq 0$ for $x \in \Delta$. Using this one verifies that for each $\varphi \in C_{\mathbb{R}}(\Delta)$ the nonlinear operator $T[\varphi] : \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta) \longrightarrow \overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta)$,

$$T[\varphi](\zeta) := E_1 \left\{ p^-[\varphi] e^{\zeta} - p^+[\varphi] e^{-\zeta} \right\}, \tag{4.27}$$

is a monotone Nemytskij operator. Hence the sum $\mathcal{P}[\varphi] = \mathcal{P}_0 + T[\varphi]$ is a strongly monotone operator with the same monotonicity constant $m_{\mathcal{P}}$ as $\mathcal{P}_0$. Since $\mathcal{P}_0$ is bounded and linear it is obviously Lipschitz continuous. A straightforward computation shows that $T[\varphi]$ is boundedly Lipschitz continuous, too. Hence the sum $\mathcal{P}[\varphi]$ is also boundedly Lipschitz continuous. ☐

From Lemma 4.13 and Corollary III.2.3 of [23] we obtain that for $\varphi \in C_{\mathbb{R}}(\Delta)$ the operator $\mathcal{P}[\varphi]^{-1} : \overset{o}{W}{}^{-1,2}_{\mathbb{R}}(\Delta) \longrightarrow \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ exits, is bounded and Lipschitz continuous with a Lipschitz constant not bigger than $1/m_{\mathcal{P}}$. Let us introduce the mapping $\mathcal{Q} : C_{\mathbb{R}}(\Delta) \longrightarrow W^{1,2}_{\mathbb{R}}(\Delta)$ defined by

$$\mathcal{Q}(\varphi) := \widehat{\varphi} + \mathcal{P}[\varphi]^{-1}(C - E_1 Y \mathcal{N}^-[\varphi] + E_1 Y \mathcal{N}^+[\varphi]) \tag{4.28}$$

where $\varphi \in \operatorname{dom}(\mathcal{Q}) = C_{\mathbb{R}}(\Delta)$ and $Y : L^1(\Omega) \longrightarrow L^1(\Delta)$ is the extension operator

$$(Yf)(x) := \begin{cases} 0 & x \in \Sigma, \\ f(x) & x \in \Omega. \end{cases} \tag{4.29}$$

We set $\mathcal{Q}_\infty : C_{\mathbb{R}}(\Delta) \longrightarrow C_{\mathbb{R}}(\Delta)$,

$$\mathcal{Q}_\infty := E_\infty \mathcal{Q}, \quad \operatorname{dom}(\mathcal{Q}_\infty) := C_{\mathbb{R}}(\Delta). \tag{4.30}$$

Proposition 4.14 *Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. An element* $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *is a solution of the DH-model if* $\varphi_\infty := E_\infty\varphi \in C_{\mathbb{R}}(\Delta)$ *is a fixed point of the mapping* $\mathcal{Q}_\infty$. *Conversely, if* $\varphi_\infty \in C_{\mathbb{R}}(\Delta)$ *is a fixed point of* $\mathcal{Q}_\infty$, *then there is a* $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *such that* $\varphi_\infty = E_\infty\varphi$ *and* φ *is a solution of the DH-model.*

Proof. Let us assume that $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ is a solution of the DH-model. Then $\varphi_\infty := E_\infty\varphi \in C_{\mathbb{R}}(\Delta)$. Further, Definition 4.12 implies

$$\mathcal{P}_0\zeta = C - E_1\mathcal{U}^-[\varphi_\infty] + E_1\mathcal{U}^+[\varphi_\infty] \tag{4.31}$$

where $\varphi = \zeta + \widehat{\varphi}$. Since

$$-\mathcal{D}^-[\varphi_\infty] + \mathcal{D}^+[\varphi_\infty] = -p^-[\varphi_\infty]e^{\zeta} + p^+[\varphi_\infty]e^{-\zeta} \tag{4.32}$$

we find

$$\mathcal{P}_0\zeta + E_1\left(p^-[\varphi_\infty]e^{\zeta} - p^+[\varphi_\infty]e^{-\zeta}\right) = C - E_1Y\mathcal{N}^-[\varphi_\infty] + E_1Y\mathcal{N}^+[\varphi_\infty]. \tag{4.33}$$

which yields

$$\mathcal{P}[\varphi_\infty](\zeta) = C - E_1Y\mathcal{N}^-[\varphi_\infty] + E_1Y\mathcal{N}^+[\varphi_\infty]. \tag{4.34}$$

Therefore we obtain

$$\varphi = \widehat{\varphi} + \mathcal{P}[\varphi_\infty]^{-1}(C - E_1Y\mathcal{N}^-[\varphi_\infty] + E_1Y\mathcal{N}^+[\varphi_\infty]) \tag{4.35}$$

which implies $\varphi_\infty = \mathcal{Q}_\infty[\varphi_\infty]$.

Conversely, if φ_∞ is a fixed point of $\mathcal{Q}$, then $\varphi_\infty \in C_{\mathbb{R}}(\Delta)$ and

$$\varphi_\infty = E_\infty\left(\widehat{\varphi} + \mathcal{P}[\varphi_\infty]^{-1}\left(C - E_1Y\mathcal{N}^-[\varphi_\infty] + E_1Y\mathcal{N}^+[\varphi_\infty]\right)\right). \tag{4.36}$$

Setting

$$\varphi := \widehat{\varphi} + \mathcal{P}[\varphi_\infty]^{-1}\left(C - E_1Y\mathcal{N}^-[\varphi_\infty] + E_1Y\mathcal{N}^+[\varphi_\infty]\right) \tag{4.37}$$

one gets $\varphi_\infty = E_\infty\varphi$. Hence

$$\mathcal{P}_0\zeta + E_1\left(p^-[E_\infty\varphi]e^{\zeta} - p^+[E_\infty\varphi]e^{-\zeta}\right) = C - E_1Y\mathcal{N}^-[E_\infty\varphi] + E_1Y\mathcal{N}^+[E_\infty\varphi] \tag{4.38}$$

where $\zeta := \varphi - \widehat{\varphi}$. However, the last equality implies

$$\mathcal{P}_0\zeta = C - E_1\mathcal{U}^-[E_\infty\varphi] + E_1\mathcal{U}^+[E_\infty\varphi]. \tag{4.39}$$

Hence φ is a solution of the DH-model. □

5 Existence

5.1 Preliminaries

Our final aim is to show that the DH-model always admits a solution. By Proposition 4.14 this is equivalent to show that the non-linear mapping $\mathcal{Q}_\infty : C_{\mathbb{R}}(\Delta) \longrightarrow C_{\mathbb{R}}(\Delta)$ admits a fixed point. This will be done by applying the Leray-Schauder fixed point theorem [24, Theorem 11.3]. To this end we consider the non-linear equation

$$\vartheta = t\mathcal{Q}_\infty(\vartheta), \quad \vartheta \in C_{\mathbb{R}}(\Delta), \quad t \in [0,1]. \tag{5.1}$$

Let us introduce the modified carrier density operators $\mathcal{U}_t^\pm[\cdot] : C_{\mathbb{R}}(\Delta) \longrightarrow L^1(\Delta)$, $t \in [0,1]$,

$$\mathcal{U}_t^\pm[\varphi](x) := \begin{cases} \mathcal{D}^\pm[t\varphi](x)e^{\mp(1-t)\varphi(x)}, & x \in \Sigma, \\ \mathcal{N}^\pm[t\varphi](x), & x \in \Omega. \end{cases} \tag{5.2}$$

We note that $\mathcal{U}^\pm[\varphi] = \mathcal{U}_1^\pm[\varphi]$, $\varphi \in C_{\mathbb{R}}(\Delta)$, cf. (4.11).

Lemma 5.1 *Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. If $\vartheta \in C_{\mathbb{R}}(\Delta)$ satisfies the equation (5.1) for $t \in [0,1]$, then there is an element $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ such that $\vartheta = tE_\infty\varphi$ and $\zeta := \varphi - \widehat{\varphi} \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ satisfies the modified Poisson equation*

$$\mathcal{P}_0\zeta = C + E_1\mathcal{U}_t^+[E_\infty\varphi] - E_1\mathcal{U}_t^-[E_\infty\varphi] \tag{5.3}$$

for $t \in [0,1]$.

Proof. If ϑ satisfies (5.1), then $\vartheta \in C_{\mathbb{R}}(\Delta)$ and

$$\vartheta = tE_\infty\left(\widehat{\varphi} + \mathcal{P}[\vartheta]^{-1}\left(C - E_1Y\mathcal{N}^-[\vartheta] + E_1Y\mathcal{N}^+[\vartheta]\right)\right). \tag{5.4}$$

Setting

$$\varphi := \widehat{\varphi} + \mathcal{P}[\vartheta]^{-1}\left(C - E_1Y\mathcal{N}^-[\vartheta] + E_1Y\mathcal{N}^+[\vartheta]\right) \tag{5.5}$$

we find $\vartheta = tE_\infty\varphi$ and

$$\zeta := \varphi - \widehat{\varphi} = \mathcal{P}[tE_\infty\varphi]^{-1}\left(C - E_1Y\mathcal{N}^-[tE_\infty\varphi] + E_1Y\mathcal{N}^+[tE_\infty\varphi]\right) \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta). \tag{5.6}$$

Hence

$$\mathcal{P}[tE_\infty\varphi](\zeta) = C - E_1Y\mathcal{N}^-[tE_\infty\varphi] + E_1Y\mathcal{N}^+[tE_\infty\varphi], \tag{5.7}$$

which leads to

$$\mathcal{P}_0\zeta + E_1(p^-[tE_\infty\varphi]e^\zeta - p^+[tE_\infty\varphi]e^{-\zeta}) = C - E_1Y\mathcal{N}^-[tE_\infty\varphi] + E_1Y\mathcal{N}^+[tE_\infty\varphi] \tag{5.8}$$

By

$$p^-[tE_\infty\varphi]e^\zeta - p^+[tE_\infty\varphi]e^{-\zeta} = \mathcal{D}^-[tE_\infty\varphi]e^{(1-t)\varphi} - \mathcal{D}^+[tE_\infty\varphi]e^{-(1-t)\varphi} \tag{5.9}$$

one finally verifies (5.3). □

Having in mind an application of the Leray-Schauder fixed point theorem one has to show that the mapping $\mathcal{Q}_\infty$ is compact, i.e. continuous and maps every bounded set into a precompact one, cf. Section 11.3 of [24]. This will be shown by the following lemmas.

Lemma 5.2 *If the Assumptions 2.1, 3.1 and 4.9 are satisfied, then the mapping $\mathcal{Q}_\infty$ is continuous.*

Proof. Let $\varphi, \varphi_n \in C_{\mathbb{R}}(\Delta)$, $n \in \mathbb{N}$, such that $\lim_{n\to\infty} \|\varphi - \varphi_n\|_{L^\infty(\Delta)} = 0$. We set

$$\psi := C - E_1 Y \mathcal{N}^-[\varphi] + E_1 Y \mathcal{N}^+[\varphi]$$

and

$$\psi_n := C - E_1 Y \mathcal{N}^-[\varphi_n] + E_1 Y \mathcal{N}^+[\varphi_n], \quad n \in \mathbb{N}.$$

By Lemma 4.7 we find $\lim_{n\to\infty} \|\mathcal{N}^\pm[\varphi_n] - \mathcal{N}^\pm[\varphi]\|_{L^1(\Delta)} = 0$ which yields

$$\lim_{n\to\infty} \|\psi_n - \psi\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} = 0. \tag{5.10}$$

Let us show that

$$\lim_{n\to\infty} \|\mathcal{P}[\varphi_n]^{-1}(\psi_n) - \mathcal{P}[\varphi]^{-1}(\psi)\|_{\overset{\circ}{W}{}^{1,2}(\Delta)} = 0. \tag{5.11}$$

Obviously one has

$$\psi_n - \mathcal{P}[\varphi_n](P[\varphi]^{-1}(\psi)) = \psi_n - \psi - \left\{\mathcal{P}[\varphi_n](P[\varphi]^{-1}(\psi)) - \psi\right\}. \tag{5.12}$$

The sequence $\mathcal{P}[\varphi_n] : \overset{o}{W}{}^{1,2}(\Delta) \longrightarrow \overset{o}{W}{}^{-1,2}(\Delta)$ strongly converges to $\mathcal{P}[\varphi]$, i.e. for each $\zeta \in \overset{o}{W}{}^{1,2}(\Delta)$ one has $\mathcal{P}[\varphi_n](\zeta) \to \mathcal{P}[\varphi](\zeta)$ as $n \to \infty$. Hence

$$\lim_{n\to\infty} \|\mathcal{P}[\varphi_n](P[\varphi]^{-1}(\psi)) - \psi\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} = 0. \tag{5.13}$$

From (5.10), (5.12) and (5.13) we get

$$\lim_{n\to\infty} \|\psi_n - \mathcal{P}[\varphi_n](P[\varphi]^{-1}(\psi))\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} = 0. \tag{5.14}$$

Using the representation

$$\mathcal{P}[\varphi_n]^{-1}(\psi_n) - \mathcal{P}[\varphi]^{-1}(\psi) = \mathcal{P}[\varphi_n]^{-1}(\psi_n) - \mathcal{P}[\varphi_n]^{-1}(\mathcal{P}[\varphi_n](\mathcal{P}[\varphi]^{-1}(\psi)))$$

and (5.14) we obtain from Lemma 4.13 and Corollary III.2.3 of [23] the relation (5.11) which yields the continuity of $\mathcal{Q}_\infty$. □

To prove the compactness of the mapping let us introduce the following constants Γ_Σ^- and Γ_Σ^+,

$$\Gamma_\Sigma^\pm := e^{\eta^\pm}\left\{N_a^\pm e^{-E_a^\pm}\int_{\Sigma_a} dx\, e^{\mp\widehat{\varphi}(x)} + N_b^\pm e^{-E_b^\pm}\int_{\Sigma_b} dx\, e^{\mp\widehat{\varphi}(x)}\right\} \tag{5.15}$$

and

$$\Gamma_\Sigma := \Gamma_\Sigma^- + \Gamma_\Sigma^+ \tag{5.16}$$

where $\eta^\pm$ is given by (4.13). Further, we introduce the constants

$$\Gamma_\Omega^\pm := 3 + \left[8 + 4\sqrt{\|m^\pm\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|w^\pm\|_{L^\infty(\Omega)}}, \tag{5.17}$$

$$\Upsilon_\Omega^\pm := 8 + 4\sqrt{\|m^\pm\|_{L^\infty(\Omega)}}(b-a). \tag{5.18}$$

We set

$$\Gamma_\Omega(s) := C^-(s)\Gamma_\Omega^- + C^+(s)\Gamma_\Omega^+, \quad s \in \mathbb{R}, \tag{5.19}$$

$$\Upsilon_\Omega(s) := C^-(s)\Upsilon_\Omega^- + C^+(s)\Upsilon_\Omega^+, \quad s \in \mathbb{R}, \tag{5.20}$$

where the functions $C^{\pm}(\cdot)$ are defined by (4.16). Denoting by ε_1 the norm of the embedding operators $E_1 : L^1(\Delta) \longrightarrow \overset{o}{W}{}^{-1,2}(\Delta)$ we introduce the constants

$$\Gamma(s) := \|\widehat{\varphi}\|_{W^{1,2}(\Delta)} + \|1/\epsilon\|_{L^\infty(\Delta)}\|C\|_{\overset{o}{W}{}^{-1,2}(\Delta)} + \varepsilon_1\|1/\epsilon\|_{L^\infty(\Delta)}(\Gamma_\Sigma + \Gamma_\Omega(s)) \tag{5.21}$$

and

$$\Upsilon(s) := \varepsilon_1\|1/\epsilon\|_{L^\infty(\Delta)}\Upsilon_\Omega(s), \tag{5.22}$$

$s \in \mathbb{R}$. Finally, we set

$$E_{min} := \min\{E_a^-, E_b^-, E_a^+, E_b^+\}. \tag{5.23}$$

Lemma 5.3 *If the Assumptions 2.1, 3.1 and 4.9 are satisfied, then the mapping $\mathcal{Q}_\infty$ is compact.*

Proof. By Lemma 5.2 it remains to show that $\mathcal{Q}_\infty$ maps a bounded set into a precompact set. To this end we are going to verify that the mapping $\mathcal{Q} : C_{\mathbb{R}}(\Delta) \longrightarrow W^{1,2}(\Delta)$ defined by (4.28) maps bounded sets into bounded sets. Using the definition (4.28) we get the estimate

$$\|\mathcal{Q}(\varphi)\|_{W^{1,2}(\Delta)} \le \left\{\|\widehat{\varphi}\|_{W^{1,2}(\Delta)} + \|\mathcal{P}[\varphi]^{-1}(C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{1,2}(\Delta)}\right\}.$$

Since by Lemma 4.13 for each $\varphi \in C_{\mathbb{R}}(\Delta)$ the operator $\mathcal{P}[\varphi]$ is strongly monotone with monotonicity constant $m_{\mathcal{P}}$ we obtain from Theorem 2.17 of [35], see also [23], the estimate

$$\begin{aligned}
&\|\mathcal{P}[\varphi]^{-1}(C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{1,2}(\Delta)} \le \\
&\quad \le \frac{1}{m_{\mathcal{P}}}\|\mathcal{P}[\varphi](0) - (C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{-1,2}(\Delta)} \\
&\quad \le \|1/\epsilon\|_{L^\infty(\Delta)}\|\mathcal{P}[\varphi](0) - (C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{-1,2}(\Delta)},
\end{aligned} \tag{5.24}$$

where Lemma 4.13 was taken into account. By (4.22) one gets

$$\mathcal{P}[\varphi](0) = E_1\{p^-[\varphi] - p^+[\varphi]\}.$$

Hence

$$\begin{aligned}
&\|\mathcal{P}[\varphi]^{-1}(C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{1,2}(\Delta)} \le \\
&\|1/\epsilon\|_{L^\infty(\Delta)}\|E_1\{p^-[\varphi] - p^+[\varphi]\} - (C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{-1,2}(\Delta)}
\end{aligned}$$

which yields

$$\begin{aligned}
&\|\mathcal{P}[\varphi]^{-1}(C - E_1 Y\mathcal{N}^-[\varphi] + E_1 Y\mathcal{N}^+[\varphi])\|_{\overset{o}{W}{}^{1,2}(\Delta)} \le \\
&\quad \|1/\epsilon\|_{L^\infty(\Delta)}\|C\|_{\overset{o}{W}{}^{-1,2}(\Delta)} + \|1/\epsilon\|_{L^\infty(\Delta)}\sum_{s=\pm}\left\{\|p^s[\varphi]\|_{L^1(\Sigma)} + \|\mathcal{N}^s[\varphi]\|_{L^1(\Omega)}\right\}.
\end{aligned} \tag{5.25}$$

Using the definitions (2.10)–(2.13) as well as (4.23) and (4.24) we find the representations

$$p^{\pm}[\varphi](x) = \begin{cases} N_a^{\pm} e^{\mp(\widehat{\varphi}(x) \pm E_a^{\pm})} e^{\pm \phi_a^{\pm}[\varphi](x)}, & x \in \Sigma_a, \\ 0, & x \in \Omega, \\ N_b^{\pm} e^{\mp(\widehat{\varphi}(x) \pm E_b^{\pm})} e^{\pm \phi_a^{\pm}[\varphi](x)}, & x \in \Sigma_b, \end{cases}$$

and taking into account Lemma 4.3 we obtain the estimate

$$\|p^{\pm}[\varphi]\|_{L^1(\Sigma)} \leq \Gamma_{\Sigma}^{\pm},$$

which yields

$$\|p^{-}[\varphi]\|_{L^1(\Sigma)} + \|p^{+}[\varphi]\|_{L^1(\Sigma)} \leq \Gamma_{\Sigma}. \tag{5.26}$$

By Lemma 4.4 we find the estimate

$$\begin{aligned} &\|\mathcal{N}^{-}[\varphi]\|_{L^1(\Omega)} + \|\mathcal{N}^{+}[\varphi]\|_{L^1(\Omega)} \leq \\ &\quad C^{-}(v_{max}^{-}) \left(3 + \left[8 + 4\sqrt{\|m^{-}\|_{L^\infty(\Omega)}}(b-a)\right] \sqrt{1 + \|w^{-}\|_{L^\infty(\Omega)} + \|\varphi\|_{L^\infty(\Omega)}}\right) + \\ &\quad C^{+}(v_{max}^{+}) \left(3 + \left[8 + 4\sqrt{\|m^{+}\|_{L^\infty(\Omega)}}(b-a)\right] \sqrt{1 + \|w^{+}\|_{L^\infty(\Omega)} + \|\varphi\|_{L^\infty(\Omega)}}\right), \end{aligned} \tag{5.27}$$

where $v_{max}^{\pm}(\varphi)$ are given by (1.13). If $\varphi \in \mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r) := \{\varphi \in C_{\mathbb{R}}(\Delta) : \|\varphi\|_{L^\infty(\Delta)} \leq r\}$, then $v_{max}^{\pm}(\varphi) \geq -r + E_{min}$. Since the functions $C^{\pm}(\cdot)$ are non-increasing we find $C^{\pm}(v_{max}^{\pm}(\varphi)) \leq C^{\pm}(-r + E_{min})$ which yields

$$\begin{aligned} &\|\mathcal{N}^{-}[\varphi]\|_{L^1(\Omega)} + \|\mathcal{N}^{+}[\varphi]\|_{L^1(\Omega)} \leq \\ &\quad C^{-}(-r + E_{min}) \left(3 + [8 + 4\sqrt{\|m^{-}\|_{L^\infty(\Omega)}}(b-a)]\sqrt{1 + \|w^{-}\|_{L^\infty(\Omega)} + r}\right) + \\ &\quad C^{+}(-r + E_{min}) \left(3 + [8 + 4\sqrt{\|m^{+}\|_{L^\infty(\Omega)}}(b-a)]\sqrt{1 + \|w^{+}\|_{L^\infty(\Omega)} + r}\right). \end{aligned} \tag{5.28}$$

Using the notation (5.19) and (5.20) we obtain

$$\|\mathcal{N}^{-}[\varphi]\|_{L^1(\Omega)} + \|\mathcal{N}^{+}[\varphi])\|_{L^1(\Omega)} \leq \Gamma_{\Omega}(-r + E_{min}) + \Upsilon_{\Omega}(-r + E_{min}) r^{1/2}. \tag{5.29}$$

Finally, one gets the estimate

$$\|\mathcal{Q}(\varphi)\|_{W^{1,2}(\Delta)} \leq r_0 := \Gamma(-r + E_{min}) + \Upsilon(-r + E_{min}) r^{1/2}.$$

Hence $\mathcal{Q}(\mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r)) \subseteq \mathcal{B}_{W^{1,2}(\Delta)}(r_0)$, i.e. the mapping $\mathcal{Q}$ maps bounded sets into bounded sets of $W^{1,2}(\Delta)$. Since $\mathcal{Q}_\infty(\mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r)) = E_\infty \mathcal{Q}(\mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r)) \subseteq E_\infty \mathcal{B}_{W^{1,2}(\Delta)}(r_0)$ and E_∞ is compact one gets that the set $\mathcal{Q}_\infty(\mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r))$ is precompact. □

5.2 A priori estimates

Our next aim is to investigate solutions of (5.3) and to verify certain a priori estimates for them. By ε_∞ we denote the norm of the embedding operator $E_\infty : W^{1,2}(\Delta) \longrightarrow C(\Delta)$. We set

$$M_0^{\pm} := 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)} \|C\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} + \|\widehat{\varphi}\|_{L^\infty(\Omega)} + \|1/\epsilon\|_{L^1(\Delta)} \Gamma_{\Sigma}^{\pm}, \tag{5.30}$$

$$M_1^{\pm} := \|1/\epsilon\|_{L^1(\Delta)} \Gamma_{\Omega}^{\pm}, \tag{5.31}$$

$$M_2^{\pm} := \|1/\epsilon\|_{L^1(\Delta)} \Upsilon_{\Omega}^{\pm}, \tag{5.32}$$

where $\Gamma^{\pm}_{\Sigma}$, $\Gamma^{\pm}_{\Omega}$ and $\Upsilon^{\pm}_{\Omega}$ are defined by (5.15), (5.17) and (5.18), respectively. Further, we set

$$M := \max\{M_0^{\pm}, M_1^{\pm}, M_2^{\pm}\}. \tag{5.33}$$

Notice that M depends only on quantities entering into the Assumptions 2.1, 3.1 and 4.9.

Lemma 5.4 *Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. If* $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *and* $\zeta := \varphi - \widehat{\varphi} \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}$ *satisfies* (5.3) *for some* $t \in [0,1]$, *then*

$$\varphi(x) \quad \le \quad M\left\{1 + C^+(t\varphi_{max} + E^+_{min})\left(1 + \|E_\infty\varphi_-\|^{1/2}_{L^\infty(\Omega)}\right)\right\}, \tag{5.34}$$

$$-\varphi(x) \quad \le \quad M\left\{1 + C^-(-t\varphi_{min} + E^-_{min})\left(1 + \|E_\infty\varphi_+\|^{1/2}_{L^\infty(\Omega)}\right)\right\}, \tag{5.35}$$

$x \in \Delta$, *where*

$$\varphi_{max} := \max\{\varphi(a), \varphi(b)\} \qquad \textit{and} \qquad \varphi_{min} := \min\{\varphi(a), \varphi(b)\}, \tag{5.36}$$

$\varphi_\pm$ *are defined by* (4.15) *and* $E^{\pm}_{min} := \min\{E^{\pm}_a, E^{\pm}_b\}$.

Proof. Let $d := \mathcal{P}_0^{-1}C \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$. Since $\zeta := \varphi - \widehat{\varphi}$ is a solution of (5.3) one has

$$\mathcal{P}_0(\zeta - d) = E_1 u^+ - E_1 u^-$$

where $u^{\pm} = \mathcal{U}^{\pm}_t[E_\infty\varphi]$. Since $u^+ - u^- \in L^1(\Delta)$ one gets that $g := \zeta - d \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$, $\epsilon g' \in W^{1,1}_{\mathbb{R}}(\Delta)$ and

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}g(x) = u^+(x) - u^-(x)$$

for a.e. $x \in \Delta$. Notice that

$$\mathcal{P}_0(\zeta - d) = -E_1\frac{d}{dx}\epsilon(x)\frac{d}{dx}g.$$

Let $\Delta_0 = (x_0, x_1) \subseteq \Delta$ such that $\zeta(x_0) = \zeta(x_1) = 0$ and $\zeta(x) > 0$ for $x \in \Delta_0$. We set

$$g^+(x) = \int_{x_0}^{x} dy\,\frac{1}{\epsilon(y)}\int_{x_0}^{y} dz\; u^+(z), \quad x \in \Delta_0.$$

Obviously, one has

$$\frac{d}{dx}\epsilon(x)\frac{d}{dx}h(x) = u^-(x),$$

for a.e. $x \in \Delta_0$ where $h(x) := g(x) + g^+(x) = \zeta(x) - d(x) + g^+(x)$, $x \in \Delta_0$. Using the Maximum Principle [24, Theorem 8.1] we obtain that

$$\sup_{x\in\Delta_0} h(x) \le \max\{h(x_0), h(x_1)\}$$

which yields

$$\zeta(x) \le d(x) + \max\{-d(x_0), -d(x_1) + g^+(x_1)\}, \quad x \in \Delta_0.$$

Thus

$$\zeta(x) \leq 2\|E_\infty d\|_{L^\infty(\Delta)} + g^+(x_1), \quad x \in \Delta_0. \tag{5.37}$$

Using (5.2), (4.10), (2.20), (2.19) and (2.12), (2.13) one gets

$$u^+_\nu(x) = N^+_\nu e^{-E^+_\nu} e^{\phi^+_\nu[tE_\infty\varphi](x)} e^{-\widehat{\varphi}(x)} e^{-\zeta(x)}, \quad x \in \Delta_0 \cap \Sigma_\nu, \quad \nu = a, b.$$

By Lemma 4.3 and $\zeta(x) \geq 0$, $x \in \Delta_0$, we get

$$u^+_\nu(x) \leq N^+_\nu e^{-E^+_\nu} e^{\eta^+} e^{-\widehat{\varphi}(x)}, \quad x \in \Sigma_\nu \cap \Delta_0, \quad \nu = a, b,$$

which yields the estimate

$$\int_{\Delta_0\cap\Sigma_\nu} dz\; u^+_\nu(z) \leq N^+_\nu e^{-E^+_\nu} e^{\eta^+} \int_{\Delta_0\cap\Sigma_\nu} dz\; e^{-\widehat{\varphi}(z)}, \quad \nu = a, b.$$

Hence, we obtain the estimate

$$g^+(x_1) \leq \|1/\epsilon\|_{L^1(\Delta_0)} \int_{\Delta_0} dz\; u^+(z) \leq \|1/\epsilon\|_{L^1(\Delta_0)} \int_{\Delta_0\cap\Omega} dz\; u^+(z) +$$
$$\|1/\epsilon\|_{L^1(\Delta_0)} e^{\eta^+} \left\{ N^+_a e^{-E^+_a} \int_{\Delta_0\cap\Sigma_a} dz\; e^{-\widehat{\varphi}(z)} + N^+_b e^{-E^+_b} \int_{\Delta_0\cap\Sigma_b} dz\; e^{-\widehat{\varphi}(z)}. \right\}$$

Inserting this estimate into (5.37) we find

$$\zeta(x) \leq 2\|E_\infty d\|_{L^\infty(\Delta)} + \|1/\epsilon\|_{L^1(\Delta_0)} \Gamma^+_\Sigma + \|1/\epsilon\|_{L^1(\Delta_0)} \int_{\Delta_0\cap\Omega} dz\; u^+(z), \quad x \in \Delta_0.$$

Using the estimate

$$\|E_\infty d\|_{L^\infty(\Delta)} \leq \varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)} \|C\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)}$$

one gets that

$$\zeta(x) \leq 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)} \|C\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} + \|1/\epsilon\|_{L^1(\Delta)} \Gamma^+_\Sigma + \|1/\epsilon\|_{L^1(\Delta)} \int_\Omega dz\; u^+(z)$$

holds for $x \in \Delta^+ := \{x \in \Delta : \zeta(x) > 0\}$.

Further, let $\Delta_0 = (x_0, x_1)$ be an interval such that $\zeta(x_0) = \zeta(x_1) = 0$ and $\zeta(x) < 0$ for $x \in \Delta_0$. Setting

$$g^-(x) = \int_{x_0}^x dy\; \frac{1}{\epsilon(y)} \int_{x_0}^y dz\; u^-(z)$$

yields the equation

$$\frac{d}{dx}\epsilon(x)\frac{d}{dx}\left\{-g(x) + g^-(x)\right\} = u^+(x)$$

for a.e. $x \in \Delta_0$. Using again Theorem 8.1 of [24] we obtain the estimate

$$-\zeta(x) \leq 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)} \|C\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} + g^-(x_1), \quad x \in \Delta_0.$$

Following the reasoning above we finally obtain the estimate

$$-\zeta(x) \leq 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)} \|C\|_{\overset{\circ}{W}{}^{-1,2}(\Delta)} + \|1/\epsilon\|_{L^1(\Delta)} \Gamma^-_\Sigma + \|1/\epsilon\|_{L^1(\Delta)} \int_\Omega dz\; u^-(z)$$

for $x \in \Delta^- := \{x \in \Delta : \zeta(x) < 0\}$.

Since $u^\pm \restriction \Omega = \mathcal{N}^\pm[tE_\infty\varphi]$ we obtain from Lemma 4.4

$$\begin{aligned}\zeta(x) \quad &\le \quad 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)}\|C\|_{\overset{\circ}{W}^{-1,2}(\Delta)} + \\ &\|1/\epsilon\|_{L^1(\Delta)}\Gamma^+_\Sigma + C^+(v^+_{max}(t\varphi))\left(M^+_1 + t^{1/2}M^+_2\|E_\infty\varphi_-\|^{1/2}_{L^\infty(\Omega)}\right),\end{aligned} \tag{5.38}$$

$x \in \Delta^+$, $v^+_{max}(t\varphi) := t\varphi_{max} + E^+_{min}$, $E^+_{min} = \min\{E^+_a, E^+_b\}$, and

$$\begin{aligned}-\zeta(x) \quad &\le \quad 2\varepsilon_\infty \|1/\epsilon\|_{L^\infty(\Delta)}\|C\|_{\overset{\circ}{W}^{-1,2}(\Delta)} + \\ &\|1/\epsilon\|_{L^1(\Delta)}\Gamma^-_\Sigma + C^-(v^-_{max}(t\varphi))\left(M^-_1 + t^{1/2}M^-_2\|E_\infty\varphi_+\|^{1/2}_{L^\infty(\Omega)}\right),\end{aligned} \tag{5.39}$$

$x \in \Delta^-$, $v^-_{max}(t\varphi) := -t\varphi_{min} + E^-_{min}$, $E^-_{min} = \min\{E^-_a, E^-_b\}$, where the constants $M^\pm_1$ and $M^\pm_2$ are given by (5.31) and (5.32). Since $\zeta(x) \le 0$ for $x \in \Delta \setminus \Delta^+$ and $-\zeta(x) \le 0$ for $x \in \Delta \setminus \Delta^-$ we obtain from (5.38) and (5.39) that in fact these relations are valid for each $x \in \Delta$.

Finally, using the estimates $\pm\varphi(x) \le \pm\zeta(x) + \|E_\infty\widehat{\varphi}\|_{L^\infty(\Delta)}$, $x \in \Delta$, and $t \in [0,1]$, we immediately obtain from (5.38) and (5.39) the estimates

$$\varphi(x) \le M^+_0 + C^+(t\varphi_{max} + E^+_{min})\left(M^+_1 + M^+_2\|E_\infty\varphi_-\|^{1/2}_{L^\infty(\Omega)}\right),$$

and

$$-\varphi(x) \le M^-_0 + C^-(-t\varphi_{min} + E^-_{min})\left(M^-_1 + M^-_2\|E_\infty\varphi_+\|^{1/2}_{L^\infty(\Omega)}\right),$$

for $x \in \Delta$. Using the notation (5.33) we obtain the estimates (5.34) and (5.35). □

Corollary 5.5 *Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. If $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ and $\zeta := \varphi - \widehat{\varphi} \in \overset{o}{W}{}^{1,2}_{\mathbb{R}}(\Delta)$ satisfies the equation (5.3) for some $t \in [0,1]$, then*

$$\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \le M\left(1 + C^+(t\varphi_{max} + E^+_{min})\left(1 + \|E_\infty\varphi_-\|^{1/2}_{L^\infty(\Omega)}\right)\right) \tag{5.40}$$

and

$$\|E_\infty\varphi_-\|_{L^\infty(\Omega)} \le M\left(1 + C^-(-t\varphi_{max} + E^-_{min})\left(1 + \|E_\infty\varphi_+\|^{1/2}_{L^\infty(\Omega)}\right)\right). \tag{5.41}$$

Proof. From (5.34) and (5.35) we obtain the estimates

$$\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \le M\left(1 + C^+(t\varphi_{max} + E^+_{min})\left(1 + \|E_\infty\varphi_-\|^{1/2}_{L^\infty(\Omega)}\right)\right)$$

and

$$\|E_\infty\varphi_-\|_{L^\infty(\Omega)} \le M\left(1 + C^-(-t\varphi_{min} + E^-_{min})\left(1 + \|E_\infty\varphi_+\|^{1/2}_{L^\infty(\Omega)}\right)\right).$$

Since $\varphi_{min} \le \varphi_{max}$ one has $-t\varphi_{max} \le -t\varphi_{min}$, $t \in [0,1]$. Taking into account the fact that the functions $C^\pm(\cdot)$ are non-increasing we obtain the estimates (5.40) and (5.41). □

5.3 Main theorem

Using Corollary 5.5 our aim is to show that all solutions of (5.3) are included in an uniform ball, that is, there is a $r_0 > 0$ such that

$$\mathfrak{L} := \{\vartheta \in C_{\mathbb{R}}(\Delta) : \vartheta = t\mathcal{Q}_\infty(\vartheta), \quad t \in [0,1]\} \subseteq \mathcal{B}_{C_{\mathbb{R}}(\Delta)}(r_0). \tag{5.42}$$

For this last step we need the additional balance condition.

Assumption 5.6 (balance condition) Let the distribution functions $f^\pm$ satisfy the assumption (Q.4). We say the distributions functions $f^\pm$ obeys the balance condition if

$$G(x,y) := \sup_{s \geq 0} \left\{ D^+(s+x)D^-(-s+y)^{1/2} + D^+(-s+x)^{1/2}D^-(s+y) \right\} < \infty$$

for $x, y \in \mathbb{R}$ where $D^\pm(\cdot)$ are defined by (3.1).

Theorem 5.7 *Let the Assumptions 2.1, 3.1 and 4.9 be satisfied. If the balance condition, i.e. Assumption 5.6, is valid, then for any choice of the approximation parameters* $\{\delta_0^\pm, \delta^\pm\}$, $0 < \delta_0^\pm < \delta^\pm$,

(i) a solution $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *of DH-model in the sense of Definition 4.12 exists and*

(ii) there is a $r_0 \in (0, \infty)$ *independent of the approximation parameters* $\{\delta_0^\pm, \delta^\pm\}$ *such that any solution* $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *of the DH-model obeys* $\|E_\infty \varphi\|_{L^\infty(\Delta)} \leq r_0$.

The corresponding current densities $J^\pm[E_\infty\varphi]$ *of a solution* $\varphi \in W^{1,2}_{\mathbb{R}}(\Delta)$ *of the DH-model are different from zero if and only if the boundary values of the quasi Fermi potentials are different, i.e.* $\phi^\pm_{a_0} \neq \phi^\pm_{b_0}$ *provided the distribution functions* $f^\pm(\cdot)$ *are strictly decreasing.*

Proof. To prove (i) it is enough to show that $\mathcal{Q}_\infty$ has fixed point, see Proposition 4.14. To prove this we use the Leray-Schauder fixed point theorem. Since by Lemma 5.2 and Lemma 5.3 the mapping $\mathcal{Q}_\infty$ is continuous and compact it remains to show that the set $\mathfrak{L}$ defined by (5.42) is uniformly bounded in $t \in [0,1]$. If $\varphi \in \mathfrak{L}$, then by Lemma 5.1 it satisfies the equation (5.3). If φ satisfies the equation (5.3), then the estimates of Corollary 5.5 hold.

Let us assume that $\varphi_{max} \geq 0$. Using the estimate $1 + \|E_\infty\varphi_\pm\|^{1/2}_{L^\infty(\Omega)} \leq \sqrt{2}\left(1 + \|E_\infty\varphi_\pm\|_{L^\infty(\Omega)}\right)^{1/2}$ and setting $x_\pm := 1 + \|E_\infty\varphi_\pm\|_{L^\infty(\Omega)}$ we obtain from Corollary 5.5 the estimates

$$x_+ \leq 1 + M + \sqrt{2}MC^+x_-^{1/2}, \tag{5.43}$$

$$x_- \leq 1 + M + \sqrt{2}MC^-x_+^{1/2}, \tag{5.44}$$

where the abbreviations $C^\pm := C^\pm(\pm t\varphi_{max} + E^\pm_{min})$ are used. Inserting (5.44) into (5.43) we get

$$x_+ \leq 1 + M + \sqrt{2}MC^+\left(1 + M + \sqrt{2}MC^-x_+^{1/2}\right)^{1/2}$$

which yields

$$x_+ \le 1 + M + \sqrt{2}M(1+M)^{1/2}C^+ + 2^{3/4}M^{3/2}C^+\sqrt{C^-}x_+^{1/4}.$$

Dividing by $x_+^{1/4}$ we obtain

$$x_+^{3/4} \le \frac{1 + M + \sqrt{2}M(1+M)^{1/2}C^+}{x_+^{1/4}} + 2^{3/4}M^{3/2}C^+\sqrt{C^-}.$$

Using the fact that $x_+ \ge 1$ we find

$$x_+ \le \left(1 + M + \sqrt{2}M(1+M)^{1/2}C^+ + 2^{3/4}M^{3/2}C^+\sqrt{C^-}\right)^{4/3}.$$

Hence

$$\begin{aligned}
\|E_\infty\varphi_+\|_{L^\infty(\Omega)} &\le \left(1 + M + \sqrt{2}M(1+M)^{1/2}C^+ + 2^{3/4}M^{3/2}C^+\sqrt{C^-}\right)^{4/3} - 1 \\
&\le \left(M + \sqrt{2}M(1+M)^{1/2}C^+ + 2^{3/4}M^{3/2}C^+\sqrt{C^-}\right)^{4/3}.
\end{aligned}$$

By the assumption $\varphi_{max} \ge 0$ and the monotonicity of the function $C^+(\cdot)$ defined by (4.16) we get $C^+ = C^+(t\varphi_{max} + E^+_{min}) \le C^+(E^+_{min})$, $t \in [0,1]$. Thus we find the estimate

$$\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \le \left(M + \sqrt{2}M(1+M)^{1/2}C^+(E^+_{min}) + 2^{3/4}M^{3/2}C^+\sqrt{C^-}\right)^{4/3}.$$

Further by the definition (4.16) we get

$$\begin{aligned}
C^+\sqrt{C^-} &= C^+(t\varphi_{max} + E^+_{min})\sqrt{C^-(-t\varphi_{max} + E^-_{min})} \\
&= (1+\eta^+)\sqrt{1+\eta^-}D^+(t\varphi_{max} + E^+_{min} - \eta^+)D^-(-t\varphi_{max} + E^-_{min} - \eta^-)^{1/2}.
\end{aligned}$$

Taking into account the balance condition (Assumption 5.6) and $\varphi_{max} \ge 0$ we get

$$C^+\sqrt{C^-} \le (1+\eta^+)\sqrt{1+\eta^-}G(E^+_{min} - \eta^+, E^-_{min} - \eta^-)$$

which leads to the estimate

$$\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \le r_1,$$

where

$$\begin{aligned}
r_1 := \Big(&M + \sqrt{2}M(1+M)^{1/2}C^+(E^+_{min}) + \\
&2^{3/4}M^{3/2}(1+\eta^+)\sqrt{1+\eta^-}G(E^+_{min} - \eta^+, E^-_{min} - \eta^-)\Big)^{4/3}.
\end{aligned}$$

Since $0 \le \varphi_{max} \le \|E_\infty\varphi_+\|_{L^\infty(\Omega)}$ we have $-t\varphi_{max} \ge -t\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \ge -\|E_\infty\varphi_+\|_{L^\infty(\Omega)} \ge -r_1$, $t \in [0,1]$. By the monotonicity of $C^-(\cdot)$ we obtain $C^-(-t\varphi_{max} + E^-_{min}) \le C^-(-r_1)$. Using Corollary 5.5 we finally get

$$\|E_\infty\varphi_-\|_{L^\infty(\Omega)} \le r_2$$

where

$$r_2 := M\left(1 + C^-(-r_1 + E^-_{min})\left(1 + r_1^{1/2}\right)\right).$$

Hence $\|E_\infty \varphi\|_{L^\infty(\Omega)} \leq \max\{r_1, r_2\}$ which shows that the $\mathfrak{L}_\Omega := \{\varphi \restriction \Omega : \varphi \in \mathfrak{L}\} \subseteq \mathcal{B}_{C_\mathbb{R}(\Omega)}(\max\{r_1, r_2\})$ provided $\varphi_{max} \geq 0$.

Let $\varphi_{max} \leq 0$. In this case we insert (5.43) into (5.44) and get

$$x_- \leq 1 + M + \sqrt{2}MC^-\left(1 + M + \sqrt{2}MC^+ x_-^{1/2}\right)^{1/2}.$$

Similarly as above we obtain

$$\|E_\infty \varphi_-\|_{L^\infty(\Omega)} \leq \left(M + \sqrt{2}M(1+M)^{1/2}C^- + 2^{3/4}M^{3/2}C^-\sqrt{C^+}\right)^{4/3}.$$

Sine $\varphi_{max} \leq 0$ we get $-t\varphi_{max} + E^-_{min} \geq E^-_{min}$, $t \in [0,1]$, which yields the estimate $C^- = C^-(-t\varphi_{max} + E^-_{min}) \leq C^-(E^-_{min})$. Hence

$$\|E_\infty \varphi_-\|_{L^\infty(\Omega)} \leq \left(M + \sqrt{2}M(1+M)^{1/2}C^-(E^-_{min}) + 2^{3/4}M^{3/2}C^-\sqrt{C^+}\right)^{4/3}.$$

By the definition (4.16) we get

$$\begin{aligned} C^-\sqrt{C^+} &= C^-(-t\varphi_{max} + E^-_{min})\sqrt{C^+(t\varphi_{max} + E^+_{min})} \\ &= (1+\eta^-)\sqrt{1+\eta^+}D^-(-t\varphi_{max} + E^-_{min} - \eta^-)D^+(t\varphi_{max} + E^+_{min} - \eta^+)^{1/2}. \end{aligned}$$

Using again the Assumption 5.6 (balance condition) and $\varphi_{max} \leq 0$ we obtain

$$C^-\sqrt{C^+} \leq (1+\eta^-)\sqrt{1+\eta^+}G(E^+_{min} - \eta^+, E^-_{min} - \eta^-)$$

which gives the estimate

$$\|E_\infty \varphi_-\|_{L^\infty(\Omega)} \leq r_3,$$

where

$$\begin{aligned} r_3 \;:=\; &\Big(M + \sqrt{2}M(1+M)^{1/2}C^-(E^-_{min}) + \\ & 2^{3/4}M^{3/2}(1+\eta^-)\sqrt{1+\eta^+}G(E^+_{min} - \eta^+, E^-_{min} - \eta^-)\Big)^{4/3}. \end{aligned}$$

Since $\varphi_{max} \geq \varphi_{min} \geq -\|E_\infty \varphi_-\|_{L^\infty(\Omega)}$ we have $t\varphi_{max} + E^+_{min} \geq -t\|E_\infty \varphi_-\|_{L^\infty(\Omega)} + E^+_{min} - \geq -\|E_\infty \varphi_-\|_{L^\infty(\Omega)} + E^+_{min} \geq -r_3 + E^+_{min}$ which implies $C^+(t\varphi_{max} + E^+_{min}) \leq C^+(-r_3 + E^+_{min})$. Using the estimate (5.40) we get

$$\|E_\infty \varphi_+\|_{L^\infty(\Omega)} \leq r_4,$$

where

$$r_4 := M\left(1 + C^+(-r_3 + E^+_{min})\left(1 + r_3^{1/2}\right)\right).$$

Obviously, we have $\|E_\infty \varphi\|_{L^\infty(\Omega)} \leq \max\{r_3, r_4\}$ which yields that the restricted set $\mathfrak{L}_\Omega \subseteq \mathcal{B}_{C_\mathbb{R}(\Omega)}(\max\{r_3, r_4\})$ provided $\varphi_{max} \leq 0$.

Summing up we finally get $\mathfrak{L}_\Omega \subseteq \mathcal{B}_{C_{\mathbb{R}}(\Omega)}(r_{max})$, $r_{max} := \max\{r_1, r_2, r_3, r_4\}$. In particular, we have $-r_{max} \leq \varphi_{min} \leq \varphi_{max} \leq r_{max}$. Using Lemma 4.20 we find

$$\varphi(x) \leq r_6 := M\left(1 + C^+(-r_{max} + E^+_{min})\left(1 + r^{1/2}_{max}\right)\right)$$

and

$$-\varphi(x) \leq r_7 := M\left(1 + C^-(-r_{max} + E^-_{min})\left(1 + r^{1/2}_{max}\right)\right)$$

for $x \in \Delta$. Setting $r_0 = \max\{r_6, r_7\}$ we conclude that $\|E_\infty \varphi\|_{L^\infty(\Delta)} \leq r_0$. Hence, $\mathfrak{L} \subseteq B_{C_{\mathbb{R}}(\Delta)}(r_0)$. Since r_0 depends only on quantities entering into the Assumptions 2.1, 3.1, 4.9 and 5.6 but is independent of $t \in [0,1]$ the uniform boundedness of the set $\mathfrak{L}$ is verified. Hence the Leray-Schauder fixed point theorem implies the existence of a solution of DH-model. By the way the assertion (ii) was verified.

To prove the last assertion we note that in accordance with (4.6) the current density for holes $J^+[\varphi]$ satisfies the equation

$$J^+[\varphi] = \frac{1}{2\pi}\int_{\Lambda^+[\varphi]} d\lambda\, t^+[\varphi](\lambda)\left\{f^+(\lambda - \phi^+_a[\varphi](a)) - f^+(\lambda - \phi^+_b[\varphi](b))\right\}$$

where $t^+[\varphi](\lambda)$ is the transmission coefficient, cf. (4.5). Notice that $t^+[\varphi](\lambda) \geq 0$ for a.e. $\lambda \in \mathbb{R}$. If $J^+[\varphi] \geq 0$, then $-\phi^+_\nu[\varphi](x)$, $x \in \Sigma_\nu$, $\nu = a, b$, is non-decreasing such that $-\phi^+_a[\varphi](a) \leq -\phi^+_b[\varphi](b)$. Hence

$$f^+(\lambda - \phi^+_a[\varphi](a)) - f^+(\lambda - \phi^+_b[\varphi](b)) \geq 0.$$

If $J^+[\varphi] = 0$, then

$$f^+(\lambda - \phi^+_a[\varphi](a)) - f^+(\lambda - \phi^+_b[\varphi](b)) = 0$$

for a.e. $\lambda \in \Lambda^+[\varphi]$. Since the distribution functions $f^\pm(\cdot)$ are strictly decreasing one gets $\phi^+_a[\varphi](a) = \phi^+_b[\varphi](b)$. If $J^+[\varphi] = 0$, then $\phi^+_a[\varphi](a_0) = \phi^+_a[\varphi](a)$ and $\phi^+_b[\varphi](b) = \phi^+_b[\varphi](b_0)$ which yields $\phi^+_{a_0} = \phi^+[\varphi](a_0) = \phi^+[\varphi](b_0) = \phi^+_{b_0}$. Similarly we proceed if $J^+[\varphi] \leq 0$. Conversely, if $\phi^+_{a_0} = \phi^+_{b_0}$ and $J^+[\varphi] \geq 0$, then $-\phi^+_{a_0} = -\phi^+_a[\varphi](a_0) \leq -\phi^+_a[\varphi](a) \leq -\phi^+_b[\varphi](b) \leq -\phi^+[\varphi](b_0) = -\phi^+_{b_0} = -\phi^+_{a_0}$ which yields $J^+[\varphi] = 0$. Similarly we act if $J^+[\varphi] \leq 0$. The proof for electrons can be done in a similar manner. □

6 Comments

Let us denote by $\mathfrak{C} := \{\mu^\pm_a, \mu^\pm_b N^\pm_a, N^\pm_b, E^\pm_a, E^\pm_b, \phi^\pm_{a_0}, \phi^\pm_{b_0}\}$ the data of the stationary drift-diffusion system, by $\mathfrak{Q} := \{m^\pm, m^\pm_a, m^\pm_b, w^\pm, f^\pm\}$ the data of the Schrödinger system and by $\mathfrak{P} := \{C, \epsilon, \varphi_{a_0}, \varphi_{b_0}\}$ the data of the Poisson equation which respectively satisfy the Assumptions 2.1, 3.1 and 4.9.

1. For the sake of technical simplicity the Assumptions 2.1 for $\mathfrak{C}$ are taken rather restrictive. Usually, the mobilities $\mu^\pm_\nu$, the band-edge offsets $E^\pm_a$, $E^\pm_b$ and the densities of states $N^\pm_n u$ are not independent of x as assumed. Moreover, one has in general to take into account generation and recombination effects which are neglected here. In the classical zone a Boltzmann statistics is assumed which is widely used for drift-diffusion models. In principal, it is possible to consider the Fermi-Dirac case, i.e.

the classical densities and currents are given by (1.1), where $f^\pm_\nu$ are the Fermi-Dirac statistics given by

$$f^\pm_\nu(s) = N^\pm_\nu \mathfrak{F}_{1/2}(s/k_BT), \quad s \in \mathbb{R}, \quad \nu = a, b,$$

where

$$\mathfrak{F}_{1/2}(x) := \frac{2}{\sqrt{\pi}} \int_0^\infty d\xi \, \frac{\sqrt{\xi}}{1 + e^{\xi - x}}, \quad x \in \mathbb{R},$$

and $N^\pm_\nu$ are the density of states. However, in this case one loses the explicit expression for the carrier densities (2.18), (2.19). This is the reason why we prefer the Boltzmann statistics.

2. The Assumptions 3.1 for $\mathfrak{Q}$ are standard and used in many papers on Schrödinger-Poisson systems. We note that the Schrödinger system describes the purely ballistic charge transport in the quantum zone. Collisions in the quantum system could be taken into account by considering in addition a Pauli master equation, cf. [2, 18, 19], which is not done here. However, if the quantum zone can be chosen sufficiently small, then collisions can be neglected which makes the assumptions on ballistic transport quite reasonable.

   Typical distribution functions entering into the density matrices $\rho^\pm(\lambda)$, $\lambda \in \mathbb{R}$, (1.15) are the Boltzmann distribution

$$f^\pm(\lambda) = n^\pm e^{-\lambda/k_BT}, \quad \lambda \in \mathbb{R},$$

   or the Fermi-Dirac distribution

$$f^\pm(\lambda) = n^\pm \ln\left(1 + e^{-\lambda/k_BT}\right), \quad \lambda \in \mathbb{R},$$

   where $n^\pm$, are the integrated density of states.

3. The Boltzmann and the Fermi-Dirac distribution satisfy the Assumption 3.1, in particular (Q.4), and the balance condition (Assumption 5.6).

   Indeed, let $f^\pm(\cdot)$ be the Boltzmann distribution function, i.e., $f^\pm(s) = e^{-s}$, $s \in \mathbb{R}$. Using the definition (3.1) we get that $D^\pm(s) = e^{-s}\sqrt{1+s^2}$, $s \in \mathbb{R}$. A straightforward computations shows that

$$G(x, y) = \sup_{s \geq 0} \left\{ e^{-\frac{s}{2} - x - y} g(x, y, s) \right\},$$

   $x, y \in \mathbb{R}$, where

$$g(x, y, s) := \left(\sqrt{1 + (s+x)^2}\sqrt{1 + (s-y)^2} + \sqrt{1 + (s-x)^2}\sqrt{1 + (s+y)^2}\right).$$

   Obviously, one has $G(x, y) < \infty$ for $x, y \in \mathbb{R}$.

   The verification of the balance condition for Fermi-Dirac distribution functions is easier than for Boltzmann distributions since their growth at minus infinity is linear and not exponential as for Boltzmann distributions.

4. The Assumptions 2.1, 3.1, 4.9 and 5.6 are valid for a large class of semi-conductor devices which gives the possibility to compare numerical and experimental results. However, numerical calculations carried out in [2, 16] for resonant tunneling diodes show that they are very sensitive to the position and size of the quantum zone. Results, which are in a good agreement with the experiment, are only achievable if the quantum zone is chosen properly. Notice, however, that the existence of a solution for the dissipative hybrid model does not depend on the position and size of the quantum zone.

5. The dissipative hybrid model is a phenomenological 1D bipolar stationary model for charge transport in semi-conductors. It is interesting to note that for any data obeying the Assumptions 2.1, 3.1 and 4.9 and 5.6 a solution exists. The electrostatic potential φ is contained in a ball of $C_{\mathbb{R}}(\Delta)$ whose radius is determined by the data of $\mathfrak{C}$, $\mathfrak{Q}$ and $\mathfrak{P}$. The approximation parameters $\mathfrak{A} := \{\delta^\pm, \delta_0^\pm\}$ do not enter in this bound. In the unipolar case the balance condition (Assumption 5.6) is redundant.

6. The current densities are constant over the whole device Δ and bounded by constants which are – similar to the electrostatic potential – determined by the data $\mathfrak{C}$, $\mathfrak{Q}$ and $\mathfrak{P}$. The current densities are zero if and only if the boundary values of the quasi Fermi potentials at a_0 and b_0 are equal, that is, in the case of thermo-dynamical equilibrium.

7. The solution of the DH-model is in general not unique. However, one expects that for the thermo-dynamical equilibrium, i.e $\phi^\pm_{a_0} = \phi^\pm_{b_0}$, and in a neighbourhood of it, i.e. $\phi^\pm_{a_0} - \phi^\pm_{b_0}$ is small, the solution is unique.

8. The DH-model presented here takes into account only carrier densities above the current thresholds $v^\pm_{max}(\varphi)$. This a certain disadvantage of the model since usually carrier densities below the current threshold have an influence on the system, too. In a forthcoming paper we shall overcome this disadvantage.

Appendix

A Dissipative Schrödinger systems

Let us give a short introduction into the theory of dissipative Schrödinger systems, in short DS-systems, for details see [3, 5, 32, 30]. We start with some facts on Schrödinger-type operators.

A.1 Schrödinger-type operators

Let the conditions $0 < m \in L^\infty_{\mathbb{R}}(\Omega)$, $\frac{1}{m} \in L^\infty_{\mathbb{R}}(\Omega)$, $0 < m_a, m_b \in \mathbb{R}$, be satisfied and let $\tau := \{\varkappa_a, \varkappa_b, v\} \in \mathcal{T}_+ := \mathbb{C}_+ \times \mathbb{C}_+ \times L^\infty(\Omega)$, where $\mathbb{C}_+ := \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$. The Schrödinger-type operator $h[\tau]$ is defined by

$$(h[\tau]g)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}g(x) + v(x)g(x), \quad x \in \Omega, \quad g \in \mathrm{dom}(h[\tau]),$$

where its domain is given by

$$\mathrm{dom}(h[\tau]) := \left\{ g \in W^{1,2}(\Omega) : \begin{array}{c} \frac{1}{m} g' \in W^{1,2}(\Omega), \\ \frac{1}{2m_a} g'(a) = -\varkappa_a g(a), \\ \frac{1}{2m_b} g'(b) = \varkappa_b g(b) \end{array} \right\}.$$

The operator is maximal dissipative and completely non-selfadjoint on the Hilbert space $\mathfrak{h} = L^2(\omega)$, that is, the operator does not possess self-adjoint parts. Its spectrum consists only of discrete eigenvalues in the lower half plane. In the following we are interested in sequences $h[\tau_n]$, $\tau_n = \{\varkappa_{a,n}, \varkappa_{b,n}, v_n\} \in \mathcal{T}_+$, $n \in \mathbb{N}$. We write $\lim_{n\to\infty} \tau_n = \tau$ if we have in mind

$$\lim_{n\to\infty} \big(|\varkappa_{a,n} - \varkappa_a| + |\varkappa_{b,n} - \varkappa_b| + \|v_n - v\|_{L^\infty(\Omega)}\big) = 0. \tag{A.1}$$

A.2 Dilation and Lax-Phillips scattering

Let the boundary coefficients $\varkappa_a, \varkappa_b \in \mathbb{C}_+$ be represented by

$$\varkappa_a = q_a + i\frac{\alpha_a^2}{2} \quad \text{and} \quad \varkappa_b = q_b + i\frac{\alpha_b^2}{2} \tag{A.2}$$

where $\alpha_a, \alpha_b > 0$. Since $h[\tau]$ is maximal dissipative it admits a minimal self-adjoint dilation $K[\tau]$ on some dilation space $\mathfrak{K}$, see [20]. We choose the dilation space $\mathfrak{K}$,

$$\mathfrak{K} := L^2(\mathbb{R}_-, \mathbb{C}^2) \oplus \mathfrak{h} \oplus L^2(\mathbb{R}_+, \mathbb{C}^2). \tag{A.3}$$

To describe the minimal dilation $K[\tau]$ in $\mathfrak{K}$ we set

$$\vec{g} := g_- \oplus g \oplus g_+ \tag{A.4}$$

where $g \in \mathfrak{h}$,

$$g_-(x) := \begin{pmatrix} g_-^b(x) \\ g_-^a(x) \end{pmatrix} \in L^2(\mathbb{R}_-, \mathbb{C}^2) \quad \text{and} \quad g_+(x) := \begin{pmatrix} g_+^b(x) \\ g_+^a(x) \end{pmatrix} \in L^2(\mathbb{R}_+, \mathbb{C}^2) \tag{A.5}$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively.

Theorem A.1 *Let $\tau = \{\varkappa_a, \varkappa_b, v\} \in \mathcal{T}_+$. Then the operator $K[\tau]$ defined by*

$$\mathrm{dom}(K[\tau]) := \left\{ \vec{g} \in K : \begin{array}{c} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2),\ g, \frac{1}{m} g' \in W^{1,2}([a,b]) \\ \frac{1}{2m(b)} g'(b) - q_b g(b) = \alpha_b \frac{g_-^b(0) + g_+^b(0)}{2} \\ i\alpha_b g(b) = g_+^b(0) - g_-^b(0) \\ \frac{1}{2m(a)} g'(a) + q_a g(a) = \alpha_a \frac{g_-^a(0) + g_+^a(0)}{2} \\ i\alpha_a g(a) = g_-^a(0) - g_+^a(0) \end{array} \right\} \tag{A.6}$$

and

$$K[\tau]\vec{g} := -i\frac{d}{dx} g_- \oplus l[v](g) \oplus -i\frac{d}{dx} g_+, \qquad \vec{g} \in \mathrm{dom}(K), \tag{A.7}$$

is self-adjoint.

Proof. The proof is given in [32, Theorem 4.1]. □

The operator $K[\tau]$ is a minimal self-adjoint dilation of $h[\tau]$, i.e.

$$(h[\tau] - z)^{-1} = P^{\mathfrak{K}}_{\mathfrak{h}}(K[\tau] - z)^{-1}|\mathfrak{h}, \quad z \in \mathbb{C}_+ \tag{A.8}$$

and

$$\mathfrak{K} = \bigvee_{z\in\mathbb{C}\setminus\mathbb{R}} (K[\tau] - z)^{-1}\mathfrak{h} \tag{A.9}$$

where $P^{\mathfrak{K}}_{\mathfrak{h}}$ is the orthogonal projection from the dilation space $\mathfrak{K}$ onto the subspace $\mathfrak{h}$. Setting

$$\mathcal{D}_- := L^2(\mathbb{R}_-, \mathbb{C}^2) \quad \text{and} \quad \mathcal{D}_+ := L^2(\mathbb{R}_+, \mathbb{C}^2) \tag{A.10}$$

we introduce the identification operators $J^{\pm}_0 : \mathfrak{K}_0 \longrightarrow \mathfrak{K}$, $\mathfrak{K}_0 = \mathcal{D}_- \oplus \mathcal{D}_+ = L^2(\mathbb{R}, \mathbb{C}^2)$,

$$\begin{aligned} J_-\vec{f} &:= P^{\mathfrak{K}_0}_{\mathcal{D}_-}\vec{f} \oplus 0 \oplus 0, \\ J_+\vec{f} &:= 0 \oplus 0 \oplus P^{\mathfrak{K}_0}_{\mathcal{D}+}\vec{f}, \end{aligned} \qquad \vec{f} \in \mathfrak{K}_0. \tag{A.11}$$

Let K_0 be the differentiation operator $K_0 = -i\frac{d}{dx}$ defined on $\mathfrak{K}_0$. The Lax-Phillips wave operators

$$W_\pm[\tau] := s - \lim_{t\to\pm\infty} e^{itK[\tau]} J_\pm e^{-itK_0}, \quad \tau \in \mathcal{T}_+, \tag{A.12}$$

always exist, see [3, 30], and are unitary.

By $\mathcal{F} : \mathfrak{K}_0 \longrightarrow \widehat{\mathfrak{K}}_0 = L^2(\mathbb{R}, \mathbb{C}^2)$ we denote the Fourier transform

$$(\mathcal{F}\vec{f})(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx\, e^{-ix\lambda} \vec{f}(x), \quad \vec{f} \in \mathfrak{K}_0, \quad \lambda \in \mathbb{R}. \tag{A.13}$$

The incoming Fourier transform of $K[\tau]$, see [3, 32, 30], is defined by

$$\Phi_-[\tau] := \mathcal{F}W_-[\tau]^* : \mathfrak{K} \longrightarrow \widehat{\mathfrak{K}}_0, \quad \tau \in \mathcal{T}_+. \tag{A.14}$$

It establishes a unitary equivalence between the dilation $K[\tau]$ and the multiplication operator M with the independent variable λ.

The Lax-Phillips scattering operator $S[\tau] : \mathfrak{K}_0 \longrightarrow \mathfrak{K}_0$ is defined by

$$S[\tau] := W_+[\tau]^* W_-[\tau], \quad \tau \in \mathcal{T}_+. \tag{A.15}$$

The scattering operator commutes with K_0 which yields that the operator $\widehat{S}[\tau] : \widehat{\mathfrak{K}}_0 \longrightarrow \widehat{\mathfrak{K}}_0$,

$$\widehat{S}[\tau] := \mathcal{F}S[\tau]\mathcal{F}^* \tag{A.16}$$

commutes with M. Hence the operator $\widehat{S}[\tau]$ can be represented as a multiplication operator with a two-by-two matrix-valued function $\{\widehat{S}[\tau](\lambda)\}_{\lambda\in\mathbb{R}}$ which is called the scattering matrix, in particular, the Lax-Phillips scattering matrix. It turns out that the scattering matrix can be computed directly from the operator $h[\tau]$. To this end let us introduce the unclosed operator $\alpha : \mathfrak{h} \to \mathbb{C}^2$,

$$\alpha f = \begin{pmatrix} \alpha_b f(b) \\ -\alpha_a f(a) \end{pmatrix}, \qquad f \in \mathrm{dom}(\alpha) = W^{1,2}(\Omega) \tag{A.17}$$

and the boundary operator $T[\tau] : \mathrm{res}(h[\tau]) \longrightarrow \mathcal{B}(\mathfrak{h}, \mathbb{C}^2)$, $\tau \in \mathcal{T}_+$, defined by

$$T[\tau](z)g := \alpha(h[\tau] - z)^{-1}g, \quad g \in \mathfrak{H}, \tag{A.18}$$

where $\mathrm{res}(\cdot)$ denotes the resolvent set of an operator. The two-by-two matrix-valued function $\Theta[\tau] : \mathrm{res}(h[\tau]^*) \longrightarrow \mathcal{B}(\mathbb{C}^2)$ defined by

$$\Theta[\tau](z) = I_{\mathbb{C}^2} - i\alpha T[\tau](\overline{z})^*, \tag{A.19}$$

is holomorphic, contractive on $\mathbb{C}_-$ and unitary on $\mathbb{R}$. Moreover, it satisfies the relation

$$S[\tau](\lambda) = \Theta[\tau](\lambda)^* \tag{A.20}$$

for a.e. $\lambda \in \mathbb{R}$. The matrix-valued function $\Theta[\tau]$ is called the characteristic function of $h[\tau]$, for definition and importance see [20, 32].

A.3 Carrier density operator

For a given maximal dissipative Schrödinger-type operator $h[\tau]$ and a so-called density matrix ρ it is possible to associate a carrier density operator $\mathcal{N}_\rho : \mathcal{T}_+ \longrightarrow L^1_{\mathbb{R}}(\Omega)$. A density matrix is an element of the Banach space $L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that it values are self-adjoint and non-negative two-by-two matrices for a.e. $\lambda \in \mathbb{R}$. With ρ one associates a bounded multiplication operator $\widehat{\rho} : \widehat{\mathfrak{K}}_0 \longrightarrow \widehat{\mathfrak{K}}_0$ on the Hilbert space $\mathfrak{K}_0 = L^2(\mathbb{R}, \mathbb{C}^2)$ defined

$$(\widehat{\rho}\vec{f})(\lambda) := \rho(\lambda)\vec{f}(\lambda). \tag{A.21}$$

Using the transformation (A.14) one defines by

$$\varrho[\tau] := \Phi_-[\tau]^*\widehat{\rho}\Phi_-[\tau], \quad \tau \in \mathcal{T}_+, \tag{A.22}$$

an operator on the dilation space $\mathfrak{K}$ which is self-adjoint, non-negative and commutes with the dilation $K[\tau]$. The operator $\varrho[\tau]$ is called a density operator or a steady state albeit that $\varrho[\tau]$ is not a trace class operator. However, it turns out that if the additional condition

$$C_\rho := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2 + 1}\|\rho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty \tag{A.23}$$

is satisfied, then the product $\varrho[\tau]P^{\mathfrak{K}}_{\mathfrak{h}}$ always belongs to the trace class, cf. [30]. Using this observation in [3, 32] for a fixed density matrix satisfying (A.23) the carrier density operator $\mathcal{N}_\rho : \mathcal{T}_+ \longrightarrow L^1(\Omega)$ is defined by the L^∞-L^1 pairing

$$\mathrm{tr}(\varrho[\tau]M(h)) = \int_\Omega dx\, \mathcal{N}_\rho[\tau](x)h(x), \quad \tau \in \mathcal{T}_+, \quad h \in L^\infty_{\mathbb{R}}(\Omega), \tag{A.24}$$

where $M(h)$ is the multiplication operator defined by

$$M(h)\vec{g} := 0 \oplus hg \oplus 0, \quad \vec{g} = g_- \oplus g \oplus g_+ \in \mathfrak{K}, \quad (hg)(x) = h(x)g(x), \quad x \in \Omega,$$

see [32]. We note that condition (A.23) implies $\varrho[\tau]M(h) \in \mathcal{B}_1(\mathfrak{K})$ for each $h \in L^\infty_{\mathbb{R}}(\Omega)$.

Proposition A.2 *Let $\tau = \{\varkappa_a, \varkappa_b, v\} \in \mathcal{T}_+$. If the density matrix $\rho \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ satisfies the condition (A.23) and the boundary coefficients obey $\mathrm{Re}(\varkappa_a) \le 0$ and $\mathrm{Re}(\varkappa_b) \le 0$, then*

$$\|\mathcal{N}_\rho[\tau]\|_{L^1(\Omega)} \le C_\rho \left(3 + \left[8 + 4\sqrt{\|m\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|v_-\|_{L^\infty(\Omega)}}\right), \tag{A.25}$$

where $v_-(x) := \max\{0, -v(x)\}$, $x \in \Omega$, and C_ρ is given by (A.23).

Proof. In [4, Lemma 6.2] the estimate

$$\|\mathcal{N}_\rho[\tau]\|_{L^1(\Omega)} \le C_\rho \left(3 + \left[8 + 4\sqrt{\|m\|_{L^\infty(\Omega)}}(b-a)\right]\sqrt{1 + \|v\|_{L^\infty(\Omega)}}\right)$$

was proved. The improved estimate (A.25) can be obtained checking carefully the proof of Lemma 6.2 of [4]. Indeed, doing so one obtains that the non-negative part of the potential v moves the spectrum of the operator $h[\tau]$ to the right hand side which yields that it can be neglected. □

We are going to verify the continuity of the carrier density operator in its dependence of τ. To this end we need the following

Proposition A.3 *Let $\tau, \tau_n \in \mathcal{T}_+$, $n \in \mathbb{N}$. If $\tau_n \to \tau$ as $n \to \infty$, then*

$$\lim_{n\to\infty} \|(K[\tau_n] - z)^{-1} - (K[\tau] - z)^{-1}\|_{\mathcal{B}_1(\mathfrak{K})} = 0 \tag{A.26}$$

for $z \in \mathbb{C} \setminus \mathbb{R}$.

Proof. At first we show that for each $\vec{g} \in \mathrm{dom}(K[\tau])$ there is a sequence $\{\vec{g}_n\}_{n\in\mathbb{N}}$ such that $\vec{g}_n \in \mathrm{dom}(K[\varkappa_{a,n}, \varkappa_{b,n}, v])$, $\lim_{n\to\infty} \vec{g}_n = \vec{g}$ and $\lim_{n\to\infty} K[\varkappa_{a,n}, \varkappa_{b,n}, v]\vec{g}_n = K[\tau]\vec{g}$ in the sense of $\mathfrak{K}$. Let

$$\vec{g}_n = \vec{g} + \vec{h}_n, \quad n \in \mathbb{N},$$

where

$$\vec{h}_n := 0 \oplus h_n \oplus h_{+,n}, \quad n \in \mathbb{N}.$$

Furthermore, let $\theta(\cdot) : \mathbb{R} \longrightarrow [0,1]$ be a smooth function which is equal to one in a neighbourhood of zero and zero in neighbourhood of $y_0 := 2\int_a^b dt\, m(t)$. We set

$$h_n(x) := \theta\left(2\int_a^x dt\, m(t)\right) h_{a,n}(x) + \theta\left(2\int_x^b dt\, m(t)\right) h_{b,n}(x), \quad x \in \Omega, \quad n \in \mathbb{N}.$$

where

$$\begin{aligned} h_{a,n}(x) &:= 2C_{a,n}\int_a^x m(t)dt, \quad x \in [a,b], \\ h_{b,n}(x) &:= -2C_{b,n}\int_x^b m(t)dt, \quad x \in [a,b] \end{aligned}$$

and

$$\begin{aligned} C_{a,n} &:= (\alpha_{a,n} - \alpha_a)g_-^a(0) - (\varkappa_{a,n} - \varkappa_a)g(a) \\ C_{b,n} &:= (\alpha_{b,n} - \alpha_b)g_-^b(0) + (\varkappa_{b,n} - \varkappa_b)g(b). \end{aligned}$$

Notice that $\lim_{n\to\infty} C_{a,n} = \lim_{n\to\infty} C_{b,n} = 0$. Further we set

$$h^a_{+,n}(x) := h^a_{+,n}(0)e^{-x}, \quad x \in \mathbb{R}_+, \quad \text{and} \quad h^b_{+,n}(x) := h^b_{+,n}(0)e^{-x}, \quad x \in \mathbb{R}_+.$$

where

$$h^a_{+,n}(0) := -i(\alpha_{a,n} - \alpha_a)g(a), \quad \text{and} \quad h^b_{+,n}(0) := i(\alpha_{b,n} - \alpha_b)g(b), \quad n \in \mathbb{N}.$$

A straightforward computation shows that $\vec{g}_n \in \mathrm{dom}(K[\varkappa_{a,n}, \varkappa_{b,n}, v])$, $\lim_{n\to\infty} \vec{g}_n = \vec{g}$ and $\lim_{n\to\infty} K[\varkappa_{a,n}, \varkappa_{b,n}, v]\vec{g}_n = K[\tau]\vec{g}$.

Since the sequence $\{\vec{g}_n\}_{n\in\mathbb{N}}$ exists for each $\vec{g} \in \mathrm{dom}(K[\tau])$ one gets by [37, Theorem 2.1] that

$$s - \lim_{n\to\infty} (K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} = (K[\tau] - z)^{-1}. \tag{A.27}$$

The operators $K[\varkappa_{a,n}, \varkappa_{b,n}, v]$, $n \in \mathbb{N}$, and $K[\tau]$ are self-adjoint extensions of the symmetric operator $K_\bullet[v]$ given by

$$\mathrm{dom}(K_\bullet[v]) := \left\{ \vec{g} \in \mathfrak{K} : \begin{array}{c} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2) \quad g, \frac{1}{m}g' \in W^{1,2}(\Omega), \\ g(a) = g(b) = 0, \\ \frac{1}{m(a)}g'(a) = \frac{1}{m(b)}g'(b) = 0, \\ g_-(0) = g_+(0) = 0 \end{array} \right\}$$

and

$$K_\bullet[v]\vec{g} := -i\frac{d}{dx}g_- \oplus l[v](g) \oplus -i\frac{d}{dx}g_+, \quad \vec{g} \in \mathrm{dom}(K_\bullet[v])$$

which has the deficiency indices $\{4, 4\}$. This fact immediately improves the strong convergence (A.27) to the trace class convergence, i.e.

$$\lim_{n\to\infty} \|(K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} - (K[\tau] - z)^{-1}\|_{\mathcal{B}_1(\mathfrak{K})} = 0.$$

Since $P^{\mathfrak{K}}_{\mathfrak{h}}(K[\tau] - z)^{-1} \in \mathcal{B}_1(\mathfrak{H})$ one gets

$$\lim_{n\to\infty} \|(K[\tau_n] - z)^{-1}(v - v_n)P^{\mathfrak{K}}_{\mathfrak{h}}(K[\tau] - z)^{-1}\|_{\mathcal{B}_1(\mathfrak{K})} = 0.$$

Using the representation

$$\begin{aligned} &(K[\tau_n] - z)^{-1} - (K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} = \\ &\qquad (K[\tau_n] - z)^{-1}(v - v_n)P^{\mathfrak{K}}_{\mathfrak{h}}(K[\tau] - z)^{-1} + \\ &\qquad (K[\tau_n] - z)^{-1}(v - v_n)P^{\mathfrak{K}}_{\mathfrak{h}}\left((K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} - (K[\tau] - z)^{-1}\right) \end{aligned}$$

we find

$$\lim_{n\to\infty} \|(K[\tau_n] - z)^{-1} - (K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1}\|_{\mathcal{B}_1(\mathfrak{H})} = 0.$$

Finally, taking into account the representation

$$\begin{aligned} &(K[\tau_n] - z)^{-1} - (K[\tau] - z)^{-1} = \\ &\qquad (K[\tau_n] - z)^{-1} - (K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} + (K[\varkappa_{a,n}, \varkappa_{b,n}, v] - z)^{-1} - (K[\tau] - z)^{-1} \end{aligned}$$

we complete the proof. □

Proposition A.3 immediately implies the continuity of the incoming Fourier transform:

Proposition A.4 *Let $\tau, \tau_n \in \mathcal{T}_+$, $n \in \mathbb{N}$. If $\tau_n \longrightarrow \tau$ as $n \to \infty$, then*

$$s - \lim_{n\to\infty} \Phi_-[\tau_n] = \Phi_-[\tau]. \tag{A.28}$$

Proof. Let

$$W_-[\tau_n, \tau] := s - \lim_{t\to-\infty} e^{itK[\tau_n]}e^{-itK[\tau]}.$$

From Proposition A.3 we obtain that

$$s - \lim_{n\to\infty} W_-[\tau_n, \tau] = I_{\mathfrak{K}}$$

which yields

$$w - \lim_{n\to\infty} W_-[\tau_n, \tau]^* = I_{\mathfrak{K}}.$$

Since $W_-[\tau_n, \tau]$ is unitary for each $n \in \mathbb{N}$ we find

$$s - \lim_{n\to\infty} W_-[\tau_n, \tau]^* = I_{\mathfrak{K}}.$$

By the chain rule for wave operators we obtain

$$W_-[\tau_n] = W_-[\tau_n, \tau]W_-[\tau], \quad n \in \mathbb{N},$$

what gives

$$s - \lim_{n\to\infty} W_-[\tau_n]^* = W_-[\tau]^*. \tag{A.29}$$

Taking into account the representation (A.14) we complete the proof. □

Using Proposition A.4 we will now verify the continuity of the carrier density operator.

Theorem A.5 *Let $\tau, \tau_n \in \mathcal{T}_+$, $n \in \mathbb{N}$. Further, suppose that there is a density matrix $\rho \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that $C_\rho < \infty$ and a sequence of density matrices $\{\rho_n\}_{n\in\mathbb{N}}$, $\rho_n \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$, such that $\sup_{n\in\mathbb{N}} C_{\rho_n} < \infty$. If $\tau_n \to \tau$ as $n \to \infty$ and*

$$\lim_{n\to\infty} \rho_n(\lambda) = \rho(\lambda) \tag{A.30}$$

for a.e. $\lambda \in \mathbb{R}$, then

$$\lim_{n\to\infty} \|\mathcal{N}_{\rho_n}[\tau_n] - \mathcal{N}_\rho[\tau]\|_{L^1(\Omega)} = 0. \tag{A.31}$$

Proof. We set $\Phi_n := \Phi_-[\tau_n]$ and $\Phi := \Phi_-[\tau]$ as well as

$$\iota_n(\lambda) := (\lambda - i)\rho_n(\lambda) \quad \text{and} \quad \iota(\lambda) := (\lambda - i)\rho(\lambda), \quad \lambda \in \mathbb{R}, \quad n \in \mathbb{N}.$$

From (A.22) we find the representation

$$\varrho_n[\tau_n] - \varrho[\tau] = \Phi_n^* \widehat{\iota}_n \, \Phi_n (K_n - i)^{-1} - \Phi^* \widehat{\iota} \Phi (K - i)^{-1}, \quad n \in \mathbb{N},$$

where $K_n := K[\tau_n]$ and $K := K[\tau]$. Notice that $(K - i)^{-1} P_{\mathfrak{h}}^{\mathfrak{K}} \in \mathcal{B}_1(\mathfrak{K})$. Hence we find the estimate

$$\begin{aligned}
&\left\|(\varrho_n[\tau_n] - \varrho[\tau]) P_{\mathfrak{h}}^{\mathfrak{K}}\right\|_{\mathcal{B}_1(\mathfrak{K})} \leq \\
&\quad C_{\rho_n} \left\|(K_n - i)^{-1} - (K - i)^{-1}\right\|_{\mathcal{B}_1(\mathfrak{K})} + C_{\rho_n} \left\|(\Phi_n - \Phi)(K - i)^{-1} P_{\mathfrak{H}}^{\mathfrak{K}}\right\|_{\mathcal{B}_1(\mathfrak{K}, \mathfrak{K}_0)} + \\
&\quad \left\|(\widehat{\iota}_n - \widehat{\iota}) \Phi (K - i)^{-1} P_{\mathfrak{h}}^{\mathfrak{K}}\right\|_{\mathcal{B}_1(\mathfrak{K}, \mathfrak{K}_0)} + \left\|(\Phi_n^* - \Phi^*) \, \widehat{\iota} \, \Phi (K - i)^{-1} P_{\mathfrak{h}}^{\mathfrak{K}}\right\|_{\mathcal{B}_1(\mathfrak{K})}.
\end{aligned}$$

The first term of the r.h.s. goes to zero by Proposition A.3. The second term tends to zero by Proposition A.4 and $(K-i)^{-1}P^{\mathfrak{K}}_{\mathfrak{H}} \in \mathcal{B}_1(\mathfrak{K})$. By $s-\lim_{n\to\infty}\widehat{\iota}_n = \widehat{\iota}$ and $(K-i)^{-1}P^{\mathfrak{K}}_{\mathfrak{H}} \in \mathcal{B}_1(\mathfrak{K})$ the third term goes to zero. Finally, from Proposition A.4 and the isometry of the incoming Fourier transform we get $s-\lim_{n\to\infty}\Phi_n = \Phi$ which yields that the fourth term converges to zero. Hence we find

$$\lim_{n\to\infty}\left\|(\varrho_n[\tau_n]-\varrho[\tau])P^{\mathfrak{K}}_{\mathfrak{H}}\right\|_{\mathcal{B}_1(\mathfrak{K})} = 0.$$

Taking into account (A.24), this proves (A.31). □

A.4 Current density operator

Similar to the carrier density operator it is possible to introduce a current density operator $j_\rho : \mathcal{T}_+ \longrightarrow \mathbb{R}$ for a given maximal dissipative operator $h[\tau]$ and a density matrix $\rho \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ provided the density matrix satisfies the additional condition

$$L_\rho := \int_{\mathbb{R}} d\lambda\ \mathrm{tr}(\rho(\lambda)) < \infty. \tag{A.32}$$

cf. [3, 5, 32, 30]. In [30] it was shown that the current density operator admits a representation by the so-called current density observable $C[\tau](\lambda)$ at energy $\lambda \in \mathbb{R}$ which is defined by

$$C[\tau](\lambda) := \frac{1}{2\pi}\left(P_a\Theta[\tau](\lambda)P_b - P_b\Theta[\tau](\lambda)P_a\right)\Theta[\tau](\lambda)^*, \quad \tau \in \mathcal{T}_+, \tag{A.33}$$

where $\Theta[\tau]$ is the characteristic function of the maximal dissipative operator $h[\tau]$, cf. (A.19) and [5, 30], and the projections P_a, P_b are given by (3.16). Indeed, if the density matrix ρ satisfies the condition (A.32), then the current density operator $j_\rho[\cdot] : \mathcal{T}_+ \longrightarrow \mathbb{R}$ admits the representation

$$j_\rho[\tau] := \int_{\mathbb{R}} d\lambda\ \mathrm{tr}(\rho(\lambda)C[\tau](\lambda)). \tag{A.34}$$

Since $\|C[\tau](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \le \frac{1}{2\pi}$ one gets the estimate

$$|j_\rho[\tau]| \le \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \mathrm{tr}(\rho(\lambda)). \tag{A.35}$$

Theorem A.6 *Let $\tau, \tau_n \in \mathcal{T}_+$, $n \in \mathbb{N}$. Further, suppose that there is a density matrix $\rho \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ such that $L_\rho < \infty$, cf. (A.32), and a sequence of density matrices $\{\rho_n\}_{n\in\mathbb{N}}$, $\rho_n \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$, such that $\sup_{n\in\mathbb{N}} L_{\rho_n} < \infty$. If $\tau_n \longrightarrow \tau$ as $n \to \infty$, $\lim_{n\to\infty}\rho_n(\lambda) = \rho(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and*

$$\lim_{n\to\infty}\int_{\mathbb{R}} d\lambda\ (\rho_n(\lambda)e,e)_{\mathbb{C}^2} = \int_{\mathbb{R}} d\lambda\ (\rho(\lambda)e,e)_{\mathbb{C}^2}, \tag{A.36}$$

for each $e \in \mathbb{C}^2$, then $\lim_{n\to\infty} j_{\rho_n}[\tau_n] = j_\rho[\tau]$.

Proof. By Proposition A.3 we obtain that $s-\lim_{n\to\infty} S[\tau_n] = S[\tau]$. This yields

$$\lim_{n\to\infty}\int_{\mathbb{R}} d\lambda\ \left\|(S[\tau_n](\lambda)-S[\tau](\lambda))\vec{f}(\lambda)\right\|^2_{\mathbb{C}^2} = 0$$

for each $\vec{f} \in \widehat{\mathfrak{K}}_0 = L^2(\mathbb{R}, \mathbb{C}^2)$. Taking into account (A.20) we obtain

$$\lim_{n\to\infty} \int_{\mathbb{R}} d\lambda \, \left\|(\Theta[\tau_n](\lambda) - \Theta[\tau](\lambda))\vec{f}(\lambda)\right\|^2_{\mathbb{C}^2} = 0$$

for each $\vec{f} \in \widehat{\mathfrak{K}}_0$. Hence

$$\lim_{n\to\infty} \int_{\mathbb{R}} d\lambda \, \left\|(C[\tau_n](\lambda) - C[\tau](\lambda))\vec{f}(\lambda)\right\|^2_{\mathbb{C}^2} = 0 \tag{A.37}$$

for each $\vec{f} \in \widehat{\mathfrak{K}}_0$. Further, we have

$$\begin{aligned}
&\operatorname{tr}(\rho_n(\lambda)C[\tau_n](\lambda)) - \operatorname{tr}(\rho(\lambda)C[\tau](\lambda)) = \\
&\quad \operatorname{tr}(\rho_n(\lambda)^{1/2}C[\tau_n]\rho_n(\lambda)^{1/2})_{\mathbb{C}^2} - \operatorname{tr}(\rho^{1/2}(\lambda)C[\tau_n]\rho^{1/2}(\lambda))_{\mathbb{C}^2} = \\
&\quad \sum_{\nu=a,b} \left\{(C[\tau_n](\lambda)\rho_n(\lambda)^{1/2}e_\nu, \rho_n(\lambda)^{1/2}e_\nu)_{\mathbb{C}^2} - (C[\tau](\lambda)\rho(\lambda)^{1/2}e_\nu, \rho(\lambda)^{1/2}e_\nu)_{\mathbb{C}^2}\right\},
\end{aligned}$$

$\lambda \in \mathbb{R}$. Setting $\vec{f}_{\nu,n}(\lambda) := \rho_n(\lambda)^{1/2}e_\nu$ and $\vec{f}_\nu(\lambda) := \rho(\lambda)^{1/2}e_\nu$, $\nu = a, b$, we get $\vec{f}_{\nu,n}, \vec{f}_\nu \in \mathfrak{K}_0$ using $\|C[\tau](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \le \frac{1}{2\pi}$, $\lambda \in \mathbb{R}$, we obtain the estimate

$$\begin{aligned}
&|\operatorname{tr}(\rho_n(\lambda)C[\tau_n](\lambda)) - \operatorname{tr}(\rho(\lambda)C[\tau](\lambda))| \le \\
&\quad \sum_{i=a,b} \frac{1}{2\pi}\left\{\|\vec{f}_{\nu,n}(\lambda)\|_{\mathbb{C}^2} + \|\vec{f}_\nu(\lambda)\|_{\mathbb{C}^2}\right\}\|\vec{f}_{\nu,n}(\lambda) - \vec{f}_\nu(\lambda)\|_{\mathbb{C}^2} + \\
&\quad \sum_{i=a,b} \|\vec{f}_\nu(\lambda)\|_{\mathbb{C}^2}\|(C[\tau_n](\lambda) - C[\tau](\lambda))\vec{f}_\nu(\lambda)\|_{\mathbb{C}^2}.
\end{aligned}$$

We note that $\vec{f}_{\nu,n}, \vec{f}_\nu \in \widehat{\mathfrak{K}}_0$, $\nu = a, b$, $n \in \mathbb{N}$. Hence

$$\begin{aligned}
&|j_{\rho_n}[\tau_n] - j_\rho[\tau]| \le \int_{\mathbb{R}} d\lambda \, |\operatorname{tr}(C[\tau_n](\lambda)\rho_n(\lambda)) - \operatorname{tr}(C[\tau](\lambda)\rho(\lambda))| \le \\
&\left\{\left(\sum_{\nu=a,b}\|\vec{f}_{\nu,n}\|^2_{\widehat{\mathfrak{K}}_0}\right)^{1/2} + \left(\sum_{\nu=a,b}\|\vec{f}_\nu\|^2_{\widehat{\mathfrak{K}}_0}\right)^{1/2}\right\}\left(\sum_{\nu=a,b}\|\vec{f}_{\nu,n} - \vec{f}_\nu\|^2_{\widehat{\mathfrak{K}}_0}\right)^{1/2} + \\
&\left(\sum_{\nu=a,b}\|\vec{f}_\nu\|^2_{\widehat{\mathfrak{K}}_0}\right)^{1/2}\left(\sum_{\nu=a,b}\int_{\mathbb{R}} d\lambda \, \|(C[\tau_n](\lambda) - C[\tau](\lambda))\vec{f}_\nu(\lambda)\|^2_{\mathbb{C}^2}\right)^{1/2}
\end{aligned}$$

which yields

$$\begin{aligned}
|j_{\rho_n}[\tau_n] - j_\rho[\tau]| \le \left\{L^{1/2}_{\rho_n} + L^{1/2}_\rho\right\}\left(\sum_{\nu=a,b}\|\vec{f}_{\nu,n} - \vec{f}_\nu\|^2_{\widehat{\mathfrak{K}}_0}\right)^{1/2} + \\
L^{1/2}_\rho\left(\sum_{\nu=a,b}\int_{\mathbb{R}} d\lambda \, \|(C[\tau_n](\lambda) - C[\tau](\lambda))\vec{f}_\nu(\lambda)\|^2_{\mathbb{C}^2}\right)^{1/2}.
\end{aligned} \tag{A.38}$$

Since $\rho_n(\lambda) \to \rho(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ as $n \to \infty$ we find $\vec{f}_{\nu,n}(\lambda) \to \vec{f}_\nu(\lambda)$ for a.e $\lambda \in \mathbb{R}$ as $n \to \infty$. From (A.36) we get that $\lim_{n\to\infty} \|\vec{f}_{\nu,n}\|_{\widehat{\mathfrak{K}}_0} = \|\vec{f}_\nu\|_{\widehat{\mathfrak{K}}_0}$, $\nu = a, b$. Hence $\lim_{n\to\infty} \|\vec{f}_{\nu,n} - \vec{f}_\nu\|_{\widehat{\mathfrak{K}}_0} = 0$, $\nu = a, b$, which yields that the first term of the r.h.s. tends to zero as $n \to \infty$. Taking into account (A.37) we show that the second term of the r.h.s. goes to zero as $n \to \infty$. □

A.5 DS-systems

A dissipative Schrödinger system, in short DS-system, arises if the conditions (Q.1) and (Q.2) of Assumption 3.1 are satisfied which allows to define two maximal dissipative operators $h^\pm[\tau^\pm]$ for $\tau^\pm = \{\varkappa_a^\pm, \varkappa_b^\pm, v^\pm\} \in \mathcal{T}_+ = \mathbb{C}_+ \times \mathbb{C}_+ \times L^\infty_{\mathbb{R}}(\Omega)$ on the Hilbert space $\mathfrak{h}$. If further there are two density matrices $\rho^\pm \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ obeying both the condition (A.23) and (A.32), then the quadrouble $\{h^\pm[\tau^\pm], \rho^\pm\} = \{h^+[\tau^+], h^-[\tau^-], \rho^+, \rho^-\}$ is called a dissipative Schrödinger system. With a DS-system one associates two carrier density operators $\mathcal{N}^\pm_{\rho^\pm}[\cdot] : \mathcal{T}_+ \longrightarrow L^1_{\mathbb{R}}(\Omega)$ and two current density operators $j^\pm_{\rho^\pm}[\cdot] : \mathcal{T}_+ \longrightarrow \mathbb{R}$, [3]. One obtains a dissipative Schrödinger-Poisson system if the DS-system is coupled to the Poisson equation, cf. [3].

B Approximation

In the following we are going to derive the dissipative Schrödinger system, in short DS-system, from the quantum transmitting Schrödinger system, in short QTS-system. To this end let us briefly explain the quantum transmitting Schrödinger system, for more details we refer to [4, 8].

B.1 Quantum transmitting Schrödinger systems

For electrons (-) and holes (+) one considers the Buslaev-Fomin operators $H^\pm[V^\pm]$, cf. [11],

$$H^\pm[V^\pm] = -\frac{1}{2}\frac{d}{dx}\frac{1}{M^\pm}\frac{d}{dx} + V^\pm, \tag{B.1}$$

where

$$M^\pm(x) := \begin{cases} m_a^\pm & x \in (-\infty, a] \\ m^\pm(x) & x \in (a, b) \\ m_b^\pm & x \in [b, \infty) \end{cases} \tag{B.2}$$

are the effective masses of the electrons (-)and holes (+) and $V^\pm$ their potential energies defined by

$$V^\pm(x) := \begin{cases} v_a^\pm & x \in (-\infty, a] \\ v^\pm(x) & x \in (a, b) \\ v_b^\pm & x \in [b, \infty) \end{cases} \tag{B.3}$$

with

$$v^\pm(x) := w^\pm(x) \pm \varphi(x), \quad x \in \Omega \tag{B.4}$$

and

$$v_a^\pm := \pm\varphi(a) + E_a^\pm \quad \text{and} \quad v_b^\pm := \pm\varphi(b) + E_b^\pm. \tag{B.5}$$

where $E_a^\pm$, $w^\pm$ and $E_b^\pm$ are given band-edges offsets in the regions $(-\infty, a)$, $\Omega = [a, b]$ and (b, ∞), respectively. The band-edge offsets on $(-\infty, a)$ and (b, ∞) are assumed to be constant. The operator $H^\pm[V^\pm]$ can be rigorously defined in the Hilbert space $\mathfrak{H} := L^2(\mathbb{R})$.

The Buslaev-Fomin operator $H^\pm[V^\pm]$ decomposes into a purely discrete part $H_p^\pm[V^\pm]$ and an absolutely continuous part $H_{ac}^\pm[V^\pm]$, i.e.

$$H^\pm[V^\pm] = H_p^\pm[V^\pm] \oplus H_{ac}^\pm[V^\pm]. \tag{B.6}$$

In the following we are only interested into the absolutely continuous part which is legitimated by the fact that in applications like tunneling diodes the point spectrum is absent. The absolutely continuous spectrum is given by $\sigma_{ac}(H^\pm[V^\pm]) = [v_{min}^\pm, \infty)$ where

$$v_{min}^\pm := \min\{v_a^\pm, v_b^\pm\} \tag{B.7}$$

are called the thresholds of the continuous spectrum. On $[v_{min}^\pm, v_{max}^\pm)$,

$$v_{max}^\pm := \max\{v_a^\pm, v_b^\pm\}. \tag{B.8}$$

the absolutely continuous spectrum is simple while on $[v_{max}^\pm, \infty)$ the spectrum has the multiplicity two, cf. [4]. Since only energies above this thresholds $v_{max}^\pm$ contribute to the current densities we call them the current thresholds, cf. [4].

The absolutely continuous part $H_{ac}^\pm[V^\pm]$ can be realized as a multiplication operator in the Hilbert space $\widehat{\mathfrak{H}} := L^2(\mathbb{R}, \mathbb{C}^2)$. Indeed, let us denote by M the multiplication operator with the independent variable λ and let us introduce the projection-valued function

$$P[v_a^\pm, v_b^\pm](\lambda) := \begin{pmatrix} \chi_{[v_b^\pm,\infty)}(\lambda) & 0 \\ 0 & \chi_{[v_a^\pm,\infty)}(\lambda) \end{pmatrix}, \quad \lambda \in \mathbb{R}. \tag{B.9}$$

If $\widehat{P}[v_a^\pm, v_b^\pm]$ denotes the multiplication operator with the function $P[v_a^\pm, v_b^\pm]$ which is a projection commuting with M, then $M\widehat{P}[v_a^\pm, v_b^\pm] = \widehat{P}[v_a^\pm, v_b^\pm]M$ is unitarily equivalent to $H_{ac}^\pm[V^\pm]$.

The setup of a quantum transmitting Schrödinger-Poisson system is complete if one indicates density operators $\varrho_{QT}^\pm[V^\pm]$. As mentioned above the density operators are non-negative self-adjoint operators commuting with the Buslaev-Fomin operators $H^\pm[V^\pm]$. In accordance with the spectral decompositions

$$H^\pm[V^\pm] = H_p^\pm[V^\pm] \oplus H_{ac}^\pm[V^\pm] \tag{B.10}$$

the density operators decompose into

$$\varrho_{QT}^\pm[V^\pm] := \varrho_p^\pm[V^\pm] \oplus \varrho_{ac}^\pm[V^\pm]. \tag{B.11}$$

Since we are only interested in the absolutely continuous part we neglect the bounded states and set $\varrho_{QT}^\pm[V^\pm] = \varrho_{ac}^\pm[V^\pm]$. In the spectral representation of $H_{ac}^\pm[V^\pm]$ the operators $\varrho_{QT}^\pm[V^\pm]$ are unitarily equivalent to multiplication operators $\widehat{\rho}_{QT}^\pm$ arising from the density matrices $\rho_{QT}^\pm$ which are chosen by

$$\rho_{QT}^\pm(\lambda) = \begin{pmatrix} f^\pm(\lambda - \varepsilon_b^\pm)\chi_{[v_b^\pm,\infty)}(\lambda) & 0 \\ 0 & f^\pm(\lambda - \varepsilon_a^\pm)\chi_{[v_a^\pm,\infty)}(\lambda) \end{pmatrix}, \quad \lambda \in \mathbb{R}, \tag{B.12}$$

cf. [4, Example 5.6]. Here $f^{\pm}(\cdot)$ are non-negative distribution functions, for example Boltzmann or Fermi distribution functions, and $\varepsilon_b^{\pm}$, $\varepsilon_a^{\pm}$ are so-called Fermi energies.

In the following we call the quadrouble $\{H^{\pm}[V^{\pm}], \rho_{QT}^{\pm}\} = \{H^{+}[V^{+}], H^{-}[V^{-}], \rho_{QT}^{+}, \rho_{QT}^{-}\}$ the quantum transmitting Schrödinger system, in short QTS-system. With each QTS-system one associates carrier density operators $\mathcal{N}^{\pm}_{\rho_{QT}^{\pm}}[\cdot] : L^{\infty}(\mathbb{R}) \longrightarrow L^1(\Omega)$ and current density operators $j^{\pm}_{\rho_{QT}^{\pm}}[\cdot] : L^{\infty}(\mathbb{R}) \longrightarrow \mathbb{R}$ which assign to the potentials $V^{\pm} \in L^{\infty}(\Omega)$ carrier densities from $L^1(\Omega)$ and current densities from $\mathbb{R}$ for electrons "$-$" and holes "$+$", respectively. Putting these carrier densities into the Poisson equation supplemented by boundary conditions one gets the so-called quantum transmitting Schrödinger-Poisson system, in short QTSP-system, cf. [4].

The quantum transmitting hybrid system, in short QTH-system, arises if one unites the QTS-system living on Ω and the drift-diffusion system (DD-system) on Σ by a Fermi and current coupling. For the QTH-system one introduces in a natural way carrier density operators defining them equal to the carrier density operators of the drift-diffusion system on Σ and of the quantum transmitting system on Ω. If the electrostatic potential of QTH-system satisfies the Poisson equations on the whole interval Δ, where the carrier densities are given by the carrier density operators of QTH-system, then the arising compound system is called the quantum transmitting hybrid model, in short QTH-model. The problem is unsolved whether the QTH-model admits a solution for arbitrary data. However, a numerical treatment of the model carried out in [2] shows that the model is appropriate for modelling resonant tunneling diodes.

B.2 Equivalence of QTS- and DS-systems

The QTS-system can be simplified by using its equivalence to a uncountable sequence of DS-systems. In [4] it was shown that both systems are closely related. Indeed, let us consider the families $\{h^{\pm}[\varkappa_a^{\pm}(\mu), \varkappa_b^{\pm}(\mu), v^{\pm}]\}_{\mu\in\mathbb{R}}$ with boundary coefficients

$$\varkappa_a^{\pm}(z) = iq_a^{\pm}(z) \quad \text{and} \quad \varkappa_b^{\pm}(z) = iq_b^{\pm}(z), \quad z \in \mathbb{C}, \tag{B.13}$$

where

$$q_a^{\pm}(z) := \sqrt{\frac{z - v_a^{\pm}}{2m_a^{\pm}}} \quad \text{and} \quad q_b^{\pm}(z) := \sqrt{\frac{z - v_b^{\pm}}{2m_b^{\pm}}}. \tag{B.14}$$

The families consist either of self-adjoint or maximal dissipative operators. It turns out that the Buslaev-Fomin operators $H^{\pm}[V^{\pm}]$ and the families of maximal dissipative operators $h^{\pm}[\varkappa_a^{\pm}(z), \varkappa_b^{\pm}(z), v^{\pm}]$ are related by

$$P^{\mathfrak{H}}_{\mathfrak{h}}(H^{\pm}[V^{\pm}] - z)^{-1} \upharpoonright \mathfrak{h} = (h^{\pm}[\varkappa_a^{\pm}(z), \varkappa_b^{\pm}(z), v^{\pm}] - z)^{-1}, \quad z \in \mathbb{C}_{+}. \tag{B.15}$$

The families $\{h^{\pm}[\varkappa_a^{\pm}(s), \varkappa_b^{\pm}(s), v^{\pm}]\}_{s\in[v^{\pm}_{min},\infty)}$ are called the quantum transmitting boundary families, in short QTB-families. Moreover, let $\rho_{QT}^{\pm}$ be density matrices of the QTS-system. Introducing the density matrices $\rho_s^{\pm} \in L^{\infty}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$,

$$\rho_s^{\pm}(\lambda) := \rho_{QT}^{\pm}(\lambda)\delta(s - \lambda), \quad s \in [v^{\pm}_{min}, \infty), \quad \lambda \in \mathbb{R}, \tag{B.16}$$

where $\delta(\cdot)$ denotes the Dirac distribution. For each $s \in [v^{\pm}_{min}, \infty)$ the quadrouble $\{h^{\pm}[\varkappa_a^{\pm}(s), \varkappa_b^{\pm}(s), v^{\pm}], \rho_s^{\pm}\}$ performs a dissipative Schrödinger system. In [4] it was shown that to handle the QTS-system $\{H^\pm[V^\pm], \rho^\pm_{QT}\}$ or the uncountable family $\{h^\pm[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm], \rho^\pm_s\}_{s\in[v^\pm_{min},\infty)}$ of DS-systems is the same, see Remarks 5.4 and 5.10 of [4]. Denoting the carrier and current density operators of the DS-systems $\{h^\pm[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm], \rho^\pm_s\}_{s\in\mathbb{R}}$, $s \in [v^\pm_{min}, \infty)$, by $\mathcal{N}^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm]$ and $j^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm]$ this means that

$$\mathcal{N}^\pm_{\rho^\pm_{QT}}[V^\pm] = \int_{v^\pm_{min}}^\infty ds\, \mathcal{N}^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm]$$

and

$$j^\pm_{\rho^\pm_{QT}}[V^\pm] = \int_{v^\pm_{min}}^\infty ds\, j^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm].$$

Formally, one has

$$\{H^\pm[V^\pm], \rho^\pm_{QT}\} = \int_{v^\pm_{min}}^\infty ds\, \{h^\pm[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm], \rho^\pm_s\}.$$

B.3 Approximation of QTS-systems

This last observation gives rise to a natural approximation of a QTS-system by a finite number of DS-systems which is similar to the approximation of an improper Riemannian integral by a finite integral sum. Let $\Lambda^\pm \subseteq [v^\pm_{min}, \infty)$ be semi-intervals and let $\{\Lambda^\pm_j\}^N_{j=1}$, $\Lambda^\pm_j = [\lambda^\pm_{j-1}, \lambda^\pm_j)$, be finite partitions of $\Lambda^\pm$. Further, let us choose sequences of real numbers $\{s^\pm_j\}^N_{j=1}$, $s^\pm_j \in (\lambda^\pm_{j-1}, \lambda^\pm_j)$. With respect to a QTS-system $\{H^\pm[V^\pm], \rho^\pm_{QT}\}$ we set

$$\tilde{\varkappa}^\pm_a(s) := \sum_{j=1}^N \varkappa^\pm_a(s_j)\chi_{\Lambda^\pm_j}(s), \quad \text{and} \quad \tilde{\varkappa}^\pm_b(s) := \sum_{j=1}^N \varkappa^\pm_b(s_j)\chi_{\Lambda^\pm_j}(s).$$

The functions $\tilde{\varkappa}^\pm_a(s)$ and $\tilde{\varkappa}^\pm_b(s)$ are step functions with a finite number of values approximating $\varkappa^\pm_a(s)$ and $\varkappa^\pm_b(s)$ on $\Lambda^\pm$, respectively. The families $\{h^\pm[\tilde{\varkappa}^\pm_a(s), \tilde{\varkappa}^\pm_b(s), v^\pm]\}_{s\in\Lambda^\pm}$ are called approximate QTB-families, i.e.

$$h^\pm[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm] \approx h^\pm[\tilde{\varkappa}^\pm_a(s), \tilde{\varkappa}^\pm_b(s), v^\pm] = \sum_{j=1}^N h^\pm[\varkappa^\pm_a(s_j), \varkappa^\pm_b(s_j), v^\pm]\chi_{\Lambda^\pm_j}(s).$$

Notice that for $s \in \Lambda^\pm$ the approximate QTB-families consists only of a finite number of dissipative operators. Replacing in $\{h^\pm[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm], \rho^\pm_s\}_{s\in\Lambda^\pm}$ the QTB-families by the approximate QTB-families we obtain the modified family $\{h^\pm[\tilde{\varkappa}^\pm_a(s), \tilde{\varkappa}^\pm_b(s), v^\pm], \rho^\pm_s\}_{s\in\Lambda^\pm}$ of DS-systems which is called an approximate QTS-system. Since the boundary conditions of the approximate QTB-families are close to those of the QTB-families one can hope that the carrier and current densities are also close to each other, i.e.

$$\mathcal{N}^\pm_{\rho^\pm_{QT}}[V^\pm] = \int_{v^\pm_{min}}^\infty ds\, \mathcal{N}^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm] \approx$$
$$\int_{\Lambda^\pm} ds\, \mathcal{N}^\pm_{\rho^\pm_s}[\varkappa^\pm_a(s), \varkappa^\pm_b(s), v^\pm] \approx \int_{\Lambda^\pm} ds\, \mathcal{N}^\pm_{\rho^\pm_s}[\tilde{\varkappa}^\pm_a(s), \tilde{\varkappa}^\pm_b(s), v^\pm]$$

and

$$j^{\pm}_{\rho^{\pm}_{QT}}[V^{\pm}] = \int_{v^{\pm}_{min}}^{\infty} ds\, j^{\pm}_{\rho^{\pm}_s}[\varkappa^{\pm}_a(s), \varkappa^{\pm}_b(s), v^{\pm}] \approx$$
$$\int_{\Lambda^{\pm}} ds\, j^{\pm}_{\rho^{\pm}_s}[\varkappa^{\pm}_a(s), \varkappa^{\pm}_b(s), v^{\pm}] \approx \int_{\Lambda^{\pm}} ds\, j^{\pm}_{\rho^{\pm}_s}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}].$$

Since the approximate QTB-families $h^{\pm}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}]$ are constant on $\Lambda^{\pm}_j$ one easily verifies that the expectation values of carrier and current densities for the approximate QTS-system remain unchanged on $\Lambda^{\pm}$ if we replace the density matrices $\rho^{\pm}_s$ by $\tilde{\rho}^{\pm}_s$,

$$\tilde{\rho}^{\pm}_s(\lambda) := \sum_{j=1}^{N} \chi_{\Lambda^{\pm}_j}(s)\rho^{\pm}_{\Lambda^{\pm}_j}(\lambda), \quad s \in \Lambda^{\pm}, \quad \lambda \in \mathbb{R},$$

where

$$\rho^{\pm}_{\Lambda^{\pm}_j}(\lambda) := \int_{\Lambda^{\pm}_j} ds\, \rho^{\pm}_s(\lambda), \quad \lambda \in \mathbb{R}, \quad j = 1, 2, \ldots, N.$$

That means, we have

$$\int_{\Lambda\pm} ds\, \mathcal{N}^{\pm}_{\rho^{\pm}_s}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}] =$$
$$\int_{\Lambda\pm} ds\, \mathcal{N}^{\pm}_{\tilde{\rho}^{\pm}_s}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}] = \sum_{j=1}^{N} \mathcal{N}^{\pm}_{\rho^{\pm}_{\Lambda^{\pm}_j}}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}]$$

and

$$\int_{\Lambda\pm} ds\, j^{\pm}_{\rho^{\pm}_s}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}] =$$
$$\int_{\Lambda\pm} ds\, j^{\pm}_{\tilde{\rho}^{\pm}_s}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}] = \sum_{j=1}^{N} j^{\pm}_{\rho^{\pm}_{\Lambda^{\pm}_j}}[\tilde{\varkappa}^{\pm}_a(s), \tilde{\varkappa}^{\pm}_b(s), v^{\pm}].$$

The second equality relies on the fact that the density matrices $\tilde{\rho}^{\pm}_s[v^{\pm}]$ do not depend on $s \in \Lambda^{\pm}_j$, $j = 1, 2, 3, \ldots$. Hence, the approximate QTS-system decomposes into a finite sequence of associated DS-systems $\{h^{\pm}[\varkappa^{\pm}_a(s_j), \varkappa^{\pm}_b(s_j), v^{\pm}], \rho^{\pm}_{\Lambda^{\pm}_j}[v^{\pm}]\}_{j=1}^{N}$ on $\Lambda^{\pm}$. Taking into account (B.16) we obtain

$$\rho^{\pm}_{\Lambda^{\pm}_j}(\lambda) = \rho^{\pm}_{QT}(\lambda)\chi_{\Lambda^{\pm}_j}(\lambda), \quad \lambda \in \mathbb{R}, \quad j = 1, 2, \ldots, N,$$

which shows that the approximate QTS-system is equivalent to a finite sequence of DS-systems $\{h^{\pm}[\varkappa^{\pm}_a(s_j), \varkappa^{\pm}_b(s_j), v^{\pm}], \rho^{\pm}_{QT}\chi_{\Lambda^{\pm}_j}\}_{j=1}^{N}$.

Similar to the QTS-system the approximate QTS-system can be coupled to the drift-diffusion system. The arising compound system is called an approximate quantum transmitting hybrid system, in short approximate QTH-system. If we consider in addition the Poisson equation, then the arising system is called the approximate quantum transmitting hybrid model, in short approximate QTH-model.

B.4 Dissipative hybrid model

If we consider the degenerated partitions $\{\Lambda_j^\pm\}_{j=1}^1$, $\Lambda_1^\pm = \Lambda^\pm$, and the degenerated sequences $\{s_j^\pm\}_{j=1}^1$, $s_1^\pm = s^\pm \in (\lambda_0^\pm, \lambda_1^\pm)$, then we obtain a degenerate approximate QTS-system and approximate quantum transmitting hybrid system. In this case the finite sequence of associated DS-systems reduces to a single associated DS-system $\{h^\pm[\varkappa_a^\pm(s^\pm), \varkappa_b^\pm(s^\pm), v^\pm], \rho_{\Lambda^\pm}^\pm\}$,

$$\rho_{\Lambda^\pm}^\pm(\lambda) = \rho_{QT}^\pm(\lambda)\chi_{\Lambda^\pm}(\lambda). \quad \lambda \in \mathbb{R}. \tag{B.17}$$

Hence, the approximate QTH-system reduces to the coupling of one associated dissipative Schrödinger system on Ω with drift-diffusion systems on Σ_a and Σ_b which is nothing else as a dissipative hybrid system. Considering a Poisson equation in addition one gets that approximate QTH-model reduces to the dissipative hybrid model, in short DH-model.

Thus we get the dissipative hybrid model of the introduction if we make the special choices $\Lambda^\pm = [v_{max}^\pm, v_{max}^\pm + \delta^\pm)$, $\delta^\pm > 0$, and $s^\pm = v_{max}^\pm + \delta_0^\pm$, $0 < \delta_0^\pm < \delta^\pm$. The interest to the semi-intervals $\Lambda^\pm = [v_{max}^\pm, v_{max}^\pm + \delta^\pm)$ is due to the fact that only energies above the current thresholds $v_{max}^\pm$ contribute to the current densities in which we are interested in. From the view point of approximation the dissipative hybrid model is, of course, far from the quantum transmitting hybrid model. However, from the mathematical point of view this is not so because all main mathematical problems one meets already solving the dissipative hybrid model.

Furthermore, the results for dissipative hybrid models admit an immediate generalization to the approximate hybrid model since it is a finite family of dissipative hybrid models. However, approximate hybrid models have an interest in its own since they naturally appear by the numerical treatment of hybrid models.

Acknowledgements

The authors thank N. Ben Abdallah, P. Degond and H.-Chr. Kaiser for fruitful discussions and the Institute "Mathematiques pour l'Industrie et la Physique" in Toulouse for hospitality and financial support. The financial support of DFG, Grant RE 1480/2, of the DFG Research Center "Mathematics for key technologies" (FTZ 86) in Berlin and of DAAD, Grant D/0205756, is gratefully acknowledged.

References

[1] Arnold, A.; Nier, F.: The two-dimensional Wigner-Poisson problem for an electron gas in the charge neutral case. Math. Methods Appl. Sci. **14** (1991), no. 9, 595–613.

[2] Baro, M.; Ben Abdallah, N.; Degond, P.; El Ayyadi, A.: A 1-D coupled Schrödinger drift-diffusion model including collisions. Submitted. WIAS-Preprint No. 923 (2004).

[3] Baro, M.; Kaiser, H-Ch.; Neidhardt, H.; Rehberg, J.: Dissipative Schrödinger-Poisson systems. J. Math. Phys. **45** (2004), no. 1, 21-43.

[4] Baro, M.; Kaiser, H-Ch.; Neidhardt, H.; Rehberg, J.: A quantum transmitting Schrödinger-Poisson system. Rev. Math. Phys. **16** (2004) , no. 3, 281-330.

[5] Baro, M.; Neidhardt, H.: Dissipative Schrödinger-type operators as a model for generation and recombination. J. Math. Phys. **44** (2003) , no. 6, 2373-2401.

[6] Ben Abdallah, N.: A hybrid kinetic-quantum model for stationary electron transport. J. Statist. Phys. **90** (1998), no. 3-4, 627-662.

[7] Ben Abdallah, N.; Degond, P.; Gamba, I.: Coupling one-dimensional time-dependent classical and quantum transport models. J. Math. Phys. **43** (2002), no. 1, 1-24.

[8] Ben Abdallah, N.; Degond, P.; Markowich, P.: On a one-dimensional Schrödinger-Poisson scattering model. Z. Angew. Math. Phys. **48** (1997), no. 1, 135–155.

[9] Ben Abdallah, N.; Pinaud, O.: A mathematical model for the transient evolution of a resonant tunneling diode. C. R. Math. Acad. Sci Paris **334** (2002), no. 4, 283-288.

[10] Brezzi, F.; Markowich, P.A.: The three-dimensional Wigner-Poisson problem: existence, uniqueness and approximation. Math. Methods Appl. Sci **14** (1991). no. 1, 35-61.

[11] Buslaev, V.; Fomin, V.: On the inverse scattering problem for the one dimensional Schrödinger operator on whole real line. Vestnik of Leningrad. Univ. **17** (1962), no. 1, 56-64.

[12] Castella, F.: L^2-solutions to the Schrödinger-Poisson system: existence, uniqueness, time behaviour, and smoothing effects. Math. Models Methods Appl. Sci **7** (1997), no. 8, 1051-1083.

[13] Caussignac, Ph.; Descloux, J.; Yamnahakki: Simulation of some quantum models for semiconductors. Math. Models Methods Appl. Sci. **12** (2002), no. 8, 1049–1074.

[14] Chevoir, F.; Vinter, B.: Scattering-assisted tunneling in double-barrier diodes: scattering rates and valley current. Phys. Rev. B **47** (1993), no. 12, 7260-7274.

[15] Davies, J.H.: *The physics of low dimensional semi-conductors.* Cambridge Univ. Press, 1998.

[16] Degond, P.; El Ayyadi, A.: A coupled Schrödinger drift-diffusion model for quantum semiconductor device simulations. J. Comput. Phys. **181** (2002), no. 1, 222–259.

[17] Ferry, D.K., Goodnick, S.M.: *Transport in nanostructures.* Cambridge Univ. Press, 1997.

[18] Fischetti, M.V.: Theory of electron transport in small semiconductor devices using the Pauli master equation. J. Appl. Phys. **83** (1998), no. 1, 270-291.

[19] Fischetti, M.V.: Master-equation approach to the study of electronic transport in small semiconductor devices. Phys. Rev. B **59** (1999), no. 7, 4901.4917.

[20] Foias, C.; Sz.-Nagy, B.: *Harmonic analysis of operators on Hilbert space.* Akadémia Kiadó, Budapest, North-Holland Publishing Company, Amsterdam-London, 1970.

[21] Frensley, W. R.: Boundary conditions for open quantum systems driven far from equilibrium. Reviews of Modern Physics **62**, (1990) no. 3, 745-791.

[22] Gajewski, H.: Analysis and numerics of carrier transport in semiconductors. Mitt. Ges. Angew. Math. Mech. **16** (1993), no. 1, 35–57.

[23] Gajewski, H.; Gröger, K.; Zacharias, K.: *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen.* Mathematische Lehrbücher und Monographien. II. Abteilung, Band 38, Akademie-Verlag, Berlin 1974.

[24] Gilbarg, D.; Trudinger, N. S.: *Elliptic partial differential equations of second order.* Reprint of the 1998 ed. Classics in Mathematics. Springer-Verlag, Berlin 2001.

[25] Garnett, J. B.: *Bounded analytic functions.* Pure and Applied Mathematics, 96. Academic Press, New York-London 1981.

[26] Gummel, H. K.: A self-consistent iterative scheme for one-dimensional steady state transistor calculations. IEEE Trans. ED **11** (1964), 455-465.

[27] Illner, R.: The Wigner-Poisson and Schrödinger-Poisson systems. Transp. Theory Stat. Phys. **21** (1992), no. 4-6, 753-767.

[28] Illner, R.: Existence, uniqueness and asymptotic behavior of Wigner-Poisson and Vlasov-Poisson systems: a survey. Transp. Theory Stat. Phys. **26** (1997), no. 1-2, 195–207.

[29] Illner, R.; Zweifel, P.F.; Lange, H.: Global existence, uniqueness and asymptotic behaviour of solutions of the Wigner-Poisson and Schrödinger-Poisson systems. Math. Methods Appl. Sci. **17** (1994), no. 5, 349–376.

[30] Kaiser, H-Ch.; Neidhardt, H.; Rehberg, J.: Density and current of a dissipative Schrödinger operator. J. Math. Phys. **43** (2002), no. 11, 5325-5350.

[31] Kaiser, H-Ch.; Neidhardt, H.; Rehberg, J.: Macroscopic current induced boundary conditions for Schrödinger-type operators. Integr. Equa. Oper. Theory **45** (2003), 39-63.

[32] Kaiser, H-Ch.; Neidhardt, H.; Rehberg, J.: On 1-dimensional dissipative Schrödinger-type operators, their dilations and eigenfunction expansions. Math. Nachr. **252** (2003), 51-69.

[33] Kaiser, H.-Chr.; Rehberg, J.: On stationary Schrödinger-Poisson equations. Z. Angew. Math. Mech. **75** (1995), Suppl. 2, S467-S468.

[34] Kaiser, H.-Chr.; Rehberg, J.: On stationary Schrödinger-Poisson equations modelling an electron gas with reduced dimension. Math. Methods Appl. Sci. **20** (1997), no. 15, 1283-1312.

[35] Kaiser, H.-Chr.; Rehberg, J.: About a one-dimensional stationary Schrödinger-Poisson system with Kohn-Sham potential. Z. Angew. Math. Phys. **50** (1999), no. 3, 423-458.

[36] Kaiser, H.-Chr.; Rehberg, J.: About a stationary Schrödinger-Poisson system with Kohn-Sham potential in a bounded two- or three-dimensional domain. Nonlinear Anal., Theory Methods Appl. **41A** (2000), no. 1-2, 33-72.

[37] Kurtz, Th. G.: Extensions of Trotter's operator semigroup approximation theorems. J. Functional Analysis **3** (1969), 354–375.

[38] Lange, H.; Toomire, B,; Zweifel, P.F.: An overview of Schrödinger-Poisson problems. Rep. Math. Phys. **36** (1995), no. 2-3, 331–345.

[39] Markowich, P.A.: Boltzmann distributed quantum steady states and their classical limit. Forum Math. **6** (1994), no. 1, 1-33.

[40] Markowich, P. A.: *The stationary semi-conductor device equations.* Springer-Verlag, Vienna, 1986.

[41] Mock, M. S.: *Analysis of mathematical models of semi-conductor devices.* Boole-Press, Dublin 1983.

[42] Mounaix, P.; Vanbesien, O.; Lippens, D.: Effect of cathode space layer on the current-voltage characteristic of resonant tunneling diodes. Appl. Phys. Lett. **57** (1990), no. 8, 1517-1519.

[43] Nier, F.: A stationary Schrödinger-Poisson system arising from the modelling of electronic devices. Forum Math. **2** (1990), no. 5, 489-510.

[44] Nier, F.: A variational formulation of Schrödinger-Poisson systems in dimension $d \leq 3$. Commun. Partial Differ. Equations **18** (1993), no. 7-8, 1125-1147.

[45] Nier, F.: Schrödinger-Poisson systems in dimension $d \leqq 3$: The whole-space case. Proc. R. Soc. Edinb., Sect. A **123** (1993), no.6, 1179-1201.

[46] van Roosbroeck, W.: Theory of flow electrons and holes in germanium and other semi-conductors. Bell Systems Tech. J. **29** (1950), 560-607.

[47] Selberherr, S.: *Analysis and simulation of semi-conductor devices.* Springer-Verlag, Vienna, 1984.

[48] Steinrück, H.: The one-dimensional Wigner-Poisson problem and its relation to the Schrödinger-Poisson problem. SIAM J. Math. Anal. **22** (1991), no. 4, 957-972.

[49] Weissbuch, C.; Vinter, B.: *Quantum Semi-conductor Strucutres.* Academic Press, 1991.