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Uniqueness for Dissipative Schrödinger-Poisson Systems

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Abstract

The paper is devoted to the dissipative Schrödinger-Poisson system. We indicate conditions in terms of the Schrödinger-Poisson data which guarantee the uniqueness of the solution. Moreover, it is shown that if the system is sufficiently small shrunken, then it always admits a unique solution.

Contents

1 Introduction

Let us first consider a closed quantum system on the bounded domain Ω consisting of positively and negatively charged carriers which are called holes and electrons in the following. These systems can be described by one-electron Hamiltonians in effective mass approximation (Ben-Daniel-Duke form)

$$H^{\pm}[V]\psi = -\frac{1}{2}\nabla \cdot \left(\frac{1}{m^{\pm}}\nabla\psi\right) + V\psi, \tag{1.1}$$

supplemented by self-adjoint boundary conditions where "+" indicates holes and "−" stands for electrons. By $m^{\pm}$ the position dependent effective masses of holes and electrons are denoted. The potential V is different for holes and electrons:

$$V^{\pm} = V_0^{\pm} \pm \varphi$$

where $V_0^{\pm}$ are potentials which are fixed for a given device, for instance, a double barrier. The Planck constant $\hbar$ and the elementary charge q are scaled to 1 for simplicity.

The collective behaviour of holes and electrons is described by density operators $\varrho^{\pm}[V]$. If the system is closed, then it is assumed that the density operators are equilibrium states, i.e non-negative trace class operators of the form by

$$\varrho^{\pm}[V] = f^{\pm}\Big(H^{\pm}[V]\Big)$$

where $f^{\pm}$ are equilibrium distribution functions. The trace class property is satisfied if the distribution functions $f^{\pm}$ decay sufficiently fast. In this case they admit the definition of carrier density operators $\mathcal{N}^{\pm}_{f^{\pm}}(\cdot) : L^{\infty}_{\mathbb{R}}(\Omega) \longrightarrow L^{1}_{\mathbb{R}}(\Omega)$, cf. [16, 17], which assign for bounded electrostatic potentials $V \in L^{\infty}_{\mathbb{R}}(\Omega)$ a L^1-function which is called the carrier densities such that the relations

$$\mathrm{tr}(\varrho^{\pm}[V]\chi_{\omega}) = \mathrm{tr}(f^{\pm}(H^{\pm}[V])\chi_{\omega}) = \int_{\omega} dx\, \mathcal{N}^{\pm}_{f^{\pm}}(V)(x)$$

are satisfied for all Borel subsets ω of Ω. The subindex $\mathbb{R}$ indicates real functions. If to the quadrouble $\{H^{+}[V_0^{+} + \varphi], H^{-}[V_0^{-} - \varphi], f^{+}, f^{-}\}$ we add the Poisson equation

$$-\nabla \cdot (\epsilon \nabla \varphi) = C + \mathcal{N}^{+}_{f^{+}}(V_0^{+} + \varphi) - \mathcal{N}^{-}_{f^{-}}(V_0^{-} - \varphi) \tag{1.2}$$

with boundary conditions

$$\varphi(a) = \varphi_a \quad \text{and} \quad \varphi(b) = \varphi_b, \tag{1.3}$$

then we get the so-called (closed) Schrödinger-Poisson system. By ϵ and C the dielectric permittivity and the doping profile are denoted. It turns out that if the functions $f^{\pm}$ are strictly monotone, then the carrier density operators $\mathcal{N}^{\pm}_{f^{\pm}}(\cdot)$ are anti-monotone, cf. [8, 21]. Using this anti-monotonicity one gets that the (closed) Schrödinger-Poisson system admits a unique solution, [8, 27, 28], even for heterogeneous material compositions and mixed Dirichlet and Neumann boundary conditions for Schrödinger's operator, see [16, 17].

Up to now the quantum system was supposed to be closed. Hence, there is no interaction with the environment, in particular, no exchange of carriers, i.e. the carrier currents vanish.

In view of modelling semiconductor devices the operating principle of which is the flow of electrons and holes this is not justified. That is why we pass to open quantum systems, see also [10, 29]. In [16] non-selfadjoint boundary conditions for the Schrödinger operators (1.1) were proposed which are induced by a potential flow acting on the boundary $\partial\Omega$ of the quantum system. The spectral theory for the associated non self-adjoint Schrödinger-type operators has been developed in [18]. For a one dimensional device this ansatz was analyzed in detail in [2, 18, 19, 20]. The arising model was called a dissipative Schrödinger-Poisson system.

More precisely, on the Hilbert space $\mathfrak{H} := L^2(\Omega)$, $\Omega := (a,b) \subseteq \mathbb{R}^1$, the self-adjoint operators $H^{\pm}[V]$ are now replaced by dissipative Schrödinger-type operators which arise from the same differential expressions (1.1), however, supplemented by dissipative boundary conditions of the form

$$\frac{1}{2m^{\pm}(a)}\psi'(a) = -\kappa_a^{\pm}\psi(a) \quad \text{and} \quad \frac{1}{2m^{\pm}(b)}\psi'(b) = \kappa_b^{\pm}\psi(b) \tag{1.4}$$

$\kappa_a^{\pm}, \kappa_b^{\pm} \in \mathbb{C}_+ := \{z \in \mathbb{C} : \Im\mathrm{m}(z) > 0\}$. The equilibrium distribution functions $f^{\pm}$ are substituted by density matrices $\rho^{\pm} \in L^{\infty}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ obeying

$$\rho^{\pm}(\lambda) = \rho^{\pm}(\lambda)^* \quad \text{and} \quad \rho^{\pm}(\lambda) \geq 0$$

for a.e $\lambda \in \mathbb{R}$ with respect to the Lebesgue measure. The density matrices $\rho^{\pm}$ define density operators $\varrho^{\pm}[V]$ on the so-called dilation space $\mathfrak{K} \supseteq \mathfrak{H}$ which are non-negative self-adjoint but not trace class operators commuting with the minimal self-adjoint dilation $K^{\pm}[V]$ of $H^{\pm}[V]$, see [19]. However, under certain decaying assumptions on the density matrices $\rho^{\pm}$ the reduced density operators $\varrho_{\mathfrak{H}}^{\pm}[V^{\pm}] := P_{\mathfrak{H}}^{\mathfrak{K}}\varrho^{\pm}[V^{\pm}] \restriction \mathfrak{H}$ are always of trace class. Using this property one can introduce carrier density operators $\mathcal{N}_{\rho^{\pm}}^{\pm}(\cdot) : L_{\mathbb{R}}^{\infty}(\Omega) \longrightarrow L_{\mathbb{R}}^{1}(\Omega)$, cf. [20], which like above assign to each electrostatic $V \in L_{\mathbb{R}}^{\infty}(\Omega)$ carrier densities from $L_{\mathbb{R}}^{1}(\Omega)$ such that

$$\mathrm{tr}(\varrho_{\mathfrak{H}}^{\pm}[V]\chi_{\omega}) = \int_{\omega} dx\, \mathcal{N}_{\rho^{\pm}}^{\pm}(V)(x)$$

holds for all Borel subsets ω of Ω. Again, if to the quadrouble $\{H^+[V_0^+ + \varphi], H^-[V_0^- - \varphi], \rho^+, \rho^-\}$ we add the Poisson equation (1.2), where $\mathcal{N}_{f^{\pm}}^{\pm}(\cdot)$ is replaced by $\mathcal{N}_{\rho^{\pm}}^{\pm}(\cdot)$, and the boundary conditions (1.3), then we get the so-called open or dissipative Schrödinger-Poisson system, see [2, 3, 20]. In contrast to the closed case the monotonicity property of the carrier density operators is lost now. This has the consequence that one can prove the existence of a solution of the dissipative Schrödinger-Poisson system but not its uniqueness, see [3].

In the following we are going to fill this gap. The main technical tool for this business is to show that the carrier density operators are in fact locally Lipschitz continuous and not only continuous as proven in [3]. The proof of this property relies on the theory of Kato-smooth operators, see [22, 23]. We show that the orthogonal projection $P_{\mathfrak{H}}^{\mathfrak{K}}$ from the dilation space $\mathfrak{K}$ onto the original space $\mathfrak{H}$ is Kato-smooth with respect to the minimal self-adjoint dilations $K^{\pm}[V]$ and we calculate their smoothness constants which allows us to compute the local Lipschitz constants for the carrier density operators. For this purpose we have to strengthen the assumptions on the effective masses $m^{\pm}$. In [3] it was assumed that $m^{\pm} + \frac{1}{m^{\pm}} \in L_{\mathbb{R}}^{\infty}(\Omega)$. In addition we demand that now that $m^{\pm}$ has a finite total variation. This admits countably many discontinuities, what is sufficient for applications to heterogeneous material compositions. The solutions becomes unique if the local Lipschitz constants of the carrier density operators are small enough. This result should be interpreted as follows: it is known that uniqueness cannot be expected in general because there are physical situations where the existence of several solutions explain well observed hysteresis phenomena [14, 30]. Thus, our uniqueness result can physically be seen as a filtering instrument in the following sense: if the parameters of the system obey our conditions, then the above hysteresis phenomena are definitely absent.

It turns out that uniqueness takes always place if we shrink the dissipative Schrödinger-Poisson system to a sufficiently small subdevice $\Omega' \subseteq \Omega$. That means, we consider the same boundary conditions (1.4) and (1.3), the same density matrices $\rho^{\pm}$ but replace the mass functions $m^{\pm}$ by $m^{\pm} \restriction \Omega'$, the potentials $V_0^{\pm}$ by $V_0^{\pm} \restriction \Omega'$, the dielectric permittivity ϵ by $\epsilon \restriction \Omega'$ and the doping profile C by $C \restriction \Omega'$. If Ω' will be sufficiently small, then the shrunken Schrödinger-Poisson systems admits a unique solution.

This has implications for dissipative hybrid models considered in [4] which use a mixed description by a drift-diffusion model and a dissipative Schrödinger-Poisson system. In more detail, one divides the device $\Delta = [a_0, b_0]$ into two regions $\Omega_c = (a_0, a) \cup (b, b_0)$ and $\Omega_q = (a, b)$, which are called "classical zone" and "quantum zone", respectively. On the "classical zone" Ω_c, which is disconnected, one uses a classical drift diffusion description, cf. [11, 25, 31], while on the "quantum zone" Ω_q a dissipative Schrödinger-Poisson system is considered. The length $|\Omega_q|$ of the quantum zone Ω_q is crucial for the hybrid model. Indeed, if Ω is very large, then we have nearly a quantum description of the device which increases the costs of the numerical treatment of the model. If the quantum zone Ω is very small, then by the above result it can happen that the hybrid model has only one solution in contradiction to a pure classical description which usually allows several solutions. This shows us that one has very carefully to choose the quantum zone in hybrid models.

The paper is organized as follows. In Section 2 we introduce a series of constants repeatedly used in the following. If the Schrödinger-Poisson data are fixed, then the constants are fixed.The dissipative Schrödinger-type operator is introduced and in detail investigated in Section 3. Crucial are the notions of the characteristic function, see subsection 3.3, and the phase shift, see subsection 3.4. The self-adjoint dilations and Lax-Phillips scattering theory are recalled in subsection 3.6 and 3.7. The carrier density operator is defined in Section 4. Its local Lipschitz continuity is verified in subsection 4.2. The dissipative Schrödinger-Poisson system is considered in Section 5. The existence proof is sketched in subsection 5.2, the uniqueness is proven in subsection 5.3, the uniqueness for a sufficiently small shrunken Schrödinger-Poisson system is established in subsection 5.4. We end with some remarks in Section 6.

2 Notation, Assumptions and Constants

By $L^p(\Omega, X, \mathfrak{m})$ $1 \leq p < \infty$, $\Omega = (a,b)$, we denote the space of $\mathfrak{m}$-measurable and p-integrable functions over Ω with values in a Banach space X. By $L^\infty(\Omega, X, \mathfrak{m})$ the space of essentially bounded functions is denoted. If $\mathfrak{m}$ is the Lebesgue measure, then we write $L^p(\Omega) = L^p(\Omega, \mathbb{C}, \mathfrak{m})$ and $L^p_{\mathbb{R}}(\Omega) := L^p(\Omega, \mathbb{R}, \mathfrak{m})$, $1 \leq p \leq \infty$. The Lebesgue measure of a set is denoted by $|\cdot|$.

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 $\mathcal{B}_1(X)$ and $\mathcal{B}_2(X)$ denote the spaces of trace class and Hilbert-Schmidt operators, respectively. 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. We write $X[V]$ if we have in mind a parameter dependence on V and $X(V)$ if a functional dependence on V is considered. Of course, it is quite possible that a parameter dependence becomes a functional one and vice versa.

Furthermore, we denote by $W^{1,2}(\Omega)$ the usual Sobolev spaces of complex-valued functions on Ω. The subspace of elements with homogeneous Dirichlet boundary conditions at the end points of the interval $\Omega \subseteq \mathbb{R}$ is denoted by $W^{1,2}_0(\Omega)$. Its dual with respect to the L^2-pairing is denoted by $W^{-1,2}_0(\Omega) = (W^{1,2}_0(\Omega))^*$. If we have in mind only real-valued functions, then we write $W^{1,2}_{\mathbb{R}}(\Omega)$ and $W^{1,2}_{0,\mathbb{R}}(\Omega)$.

With respect to the Schrödinger-type operators we made the following

Assumptions 2.1 (Schrödinger assumptions)

(Q_1) There are constants $\underline{m}^{\pm} > 0$ and $\overline{m}^{\pm} > 0$ such that $\underline{m}^{\pm} \le m^{\pm}(x) \le \overline{m}^{\pm}$ for $x \in \Omega$.

(Q_2) $\kappa^{\pm}_a, \kappa^{\pm}_b \in \mathbb{C}_+ = \{z \in \mathbb{C} : \Im\mathrm{m}(z) > 0\}$

(Q_3) $V^{\pm}_0 \in L^{\infty}_{\mathbb{R}}(\Omega)$

(Q_4) The matrix valued-functions $\rho^{\pm}(\cdot) \in L^{\infty}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ obey $0 \le \rho^{\pm}(\lambda) = \rho^{\pm}(\lambda)^*$. There are real, continuous differentiable, even functions $g^{\pm}(\cdot) : \mathbb{R} \longrightarrow \mathbb{R}_+$ such that

$$0 \le \rho^{\pm}(\lambda) \le g^{\pm}(\lambda) I_{\mathbb{C}^2}, \quad \lambda \in \mathbb{R}, \tag{2.1}$$

$$\mathrm{sign}(\lambda) \frac{d}{d\lambda} g^{\pm}(\lambda) \le 0, \quad \lambda \in \mathbb{R}, \tag{2.2}$$

$$\int_0^{\infty} d\lambda\, \frac{g^{\pm}(\lambda)}{\sqrt{\lambda}} < \infty \tag{2.3}$$

and

$$\left| \frac{d}{d\lambda} g^{\pm}(\lambda) \right| \le \mathfrak{c}^{\pm} g^{\pm}(\lambda), \quad \lambda \in \mathbb{R}, \tag{2.4}$$

where $\mathfrak{c}^{\pm}$ are given real constants.

In particular, the functions

$$g^{\pm}(\lambda) = \mathfrak{c}^{\pm}_0 (1+\lambda^2)^{-1/2}, \quad \lambda \in \mathbb{R},$$

used in [2] satisfy the assumptions (2.2)-(2.4) with $\mathfrak{c}^{\pm} = \mathfrak{c}^{\pm}_0$.

The parameter set $\mathfrak{Q} := \{m^{\pm}, \kappa^{\pm}_a, \kappa^{\pm}_b, V^{\pm}_0, \rho^{\pm}\}$ is called the Schrödinger data of the device Ω. The Schrödinger data are fixed in the following.

With respect to the Poisson equation we made the following

Assumptions 2.2 (Poisson assumptions)

(P_1) The doping profile C is from $W_0^{-1,2}(\Omega)$.

(P_2) The dielectric permittivity ϵ is positive and satisfies $\epsilon + \frac{1}{\epsilon} \in L^\infty_{\mathbb{R}}(\Omega)$.

The quadrouble $\mathfrak{P} := \{C, \epsilon, \varphi_a, \varphi_b\}$ is called the Poisson data of the device Ω which are also fixed through the paper. The union $\mathfrak{D} := \mathfrak{Q} \cup \mathfrak{P}$ is called the Schrödinger-Poisson data of the device Ω.

For the convenience of the reader we collect here important constants which are composed of the Schrödinger-Poisson data and which are needed in the following. We set

$$B_0^\pm := 2g^\pm(0) + \frac{1}{2\pi}\sqrt{|\Omega|\,\overline{m}^\pm}\int_0^\infty d\lambda\, \frac{g^\pm(\lambda)}{\sqrt{\lambda}} \tag{2.5}$$

and

$$B_1^\pm := \frac{1}{\pi}\, g(0)\sqrt{|\Omega|\,\overline{m}^\pm}. \tag{2.6}$$

We note that the quantities $B_0^\pm$ and $B_1^\pm$ depend only one the Schrödinger data and on the length $|\Omega|$ of the device.

The embedding operators from $W_0^{1,2}(\Omega)$ into $L^\infty(\Omega)$ and $L^1(\Omega)$ into $W_0^{-1,2}(\Omega)$ are denoted by E_∞ and E_1, respectively. We note that $E_1 = E_\infty^* \upharpoonright L^1(\Omega)$. Their norms are equal and are denoted by ε_1 in the sequel. A straightforward computation shows that $\varepsilon_1 \leq \sqrt{|\Omega|}$. Let $\widehat{\varphi}$ be the function

$$\Omega \ni x \longrightarrow \frac{1}{\int_a^b dt\, \frac{1}{\epsilon(t)}}\left\{\varphi_a \int_a^x dt\, \frac{1}{\epsilon(t)} + \varphi_b \int_x^b dt\, \frac{1}{\epsilon(t)}\right\}. \tag{2.7}$$

Clearly, $\widehat{\varphi} \in W^{1,2}(\Omega) \hookrightarrow L^\infty(\Omega)$. We set

$$\begin{aligned} D_0 := \varepsilon_1 \|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}\,\Bigg\{\|C\|_{W_0^{-1,2}} + \\ \varepsilon_1\left(B_0^+ + B_0^- + B_1^+\sqrt{\|V_0^+ + \widehat{\varphi}\|_{L^\infty}} + B_1^-\sqrt{\|V_0^- - \widehat{\varphi}\|_{L^\infty}}\right)\Bigg\} \end{aligned} \tag{2.8}$$

and

$$D_1 := \varepsilon_1^2 \|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}\left(B_1^+ + B_1^-\right). \tag{2.9}$$

Using D_0 and D_1 we introduce the radii

$$r_0 := \frac{1}{2}\left(D_1 + \sqrt{D_1^2 + 4D_0}\right) \tag{2.10}$$

and

$$r_1^\pm := \|V_0^\pm + \widehat{\varphi}\|_{L^\infty} + r_0 \tag{2.11}$$

If $h : [a,b] \longrightarrow \mathbb{R}$ is a function of finite total variation and $x, y \in [a,b]$, then the total variation of $h|_{[x,y]}$ is denoted by $\bigvee_x^y h$. If $\frac{1}{m^\pm}$ has a finite total variation, then we set

$$\mathfrak{M}^\pm := \sqrt{\overline{m}^\pm}\exp\left\{\frac{\overline{m}^\pm}{2}\bigvee_a^b \frac{1}{m^\pm}\right\}. \tag{2.12}$$

Next we introduce the functions

$$R_j^{\pm}(y) := \mathfrak{M}^{\pm}\left(1 + |\kappa_j^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right)\exp\left\{y\,|\Omega|\,(\mathfrak{M}^{\pm})^2\sqrt{\frac{2}{\underline{m}^{\pm}}}\right\} \tag{2.13}$$

for $y \geq 0$ and $j = a, b$. Further we set

$$L^{\pm}(y) := \sqrt{\frac{2}{\pi}}\left\{\frac{R_a^{\pm}[2y + 2 + \gamma_0^{\pm}]^2}{(\alpha_a^{\pm})^2} + \frac{R_b^{\pm}[2y + 2 + \gamma_0^{\pm}]^2}{(\alpha_b^{\pm})^2}\right\}^{1/2}. \tag{2.14}$$

for $y \geq 0$ where the representation

$$\kappa_a^{\pm} = q_a^{\pm} + i\frac{(\alpha_a^{\pm})^2}{2} \quad \text{and} \quad \kappa_b^{\pm} = q_b^{\pm} + i\frac{(\alpha_b^{\pm})^2}{2}. \tag{2.15}$$

is used. The constants $\gamma_0^{\pm}$ are given by

$$\gamma_0^{\pm} := 2\overline{m}^{\pm}(\mathfrak{q}^{\pm})^2\left\{\frac{1}{2} + \frac{1}{\mathfrak{q}^{\pm}|\Omega|\overline{m}^{\pm}} + \sqrt{\frac{1}{4} + \frac{1}{\mathfrak{q}^{\pm}|\Omega|\overline{m}^{\pm}}}\right\} \tag{2.16}$$

where

$$\mathfrak{q}^{\pm} := \max\{0, q_a^{\pm}, q_b^{\pm}\}. \tag{2.17}$$

We define

$$\mathfrak{G}^{\pm}(y) = \sqrt{B_0^{\pm} + B_1^{\pm}\sqrt{y}}, \quad y \geq 0. \tag{2.18}$$

and

$$\mathfrak{L}^{\pm}(x,y) := \mathfrak{c}^{\pm}(\mathfrak{G}^{\pm}(x) + \mathfrak{G}^{\pm}(y))^2 + 4\pi|\Omega|\,L^{\pm}(x)\,L^{\pm}(y)\,\mathfrak{G}^{\pm}(x)\,\mathfrak{G}^{\pm}(y), \tag{2.19}$$

for $x, y \geq 0$. Finally, we introduce the constant

$$\mathfrak{L} := \mathfrak{L}^{+}(r_1^{+}, r_1^{+}) + \mathfrak{L}^{-}(r_1^{-}, r_1^{-}). \tag{2.20}$$

and we set

$$\mathfrak{U} := \varepsilon_1^2\|1/\epsilon\|_{L^\infty}\sqrt{1 + |\Omega|}\;\mathfrak{L}. \tag{2.21}$$

We note again that the introduce constants (2.5)-(2.21) depend only on the Schrödinger-Poisson data which means that they are fixed for fixed Schrödinger-Poisson data.

3 Schrödinger-type operators

Since it is unimportant in this section whether we have to do with electrons or with holes we admit the superscript $\pm$ in this section. Further, throughout we assume that Schrödinger data $\mathfrak{Q} = \{m, \kappa_a, \kappa_b, V_0, \rho\}$ satisfy the Schrödinger assumptions mutatis mutandis.

3.1 Definitions

Following the suggestion of [16, 17] we consider the non-selfadjoint Schrödinger-type operator $H[V]$ on the Hilbert space $\mathfrak{H}$ defined by

$$\mathrm{dom}(H[\kappa_a,\kappa_b,V]) = \left\{ f \in W^{1,2} : \begin{array}{c} \frac{1}{m(x)} f'(x) \in W^{1,2}(\Omega), \\ \frac{1}{2m(a)} f'(a) = -\kappa_a f(a), \\ \frac{1}{2m(b)} f'(b) = \kappa_b f(b) \end{array} \right\}$$

and

$$(H[\kappa_a,\kappa_b,V]g)(x) = (l[V]g)(x), \quad g \in \mathrm{dom}(H[\kappa_a,\kappa_b,V]),$$

where

$$(l[V]g)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}g(x) + V(x)g(x),$$

cf. [18, 19], where $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \overline{\mathbb{C}_+} := \{z \in \mathbb{C} : \Im\mathrm{m}(z) \geq 0\}$, are called the boundary coefficients. The operator $H[\kappa_a,\kappa_b,V]$ is maximal dissipative if either $\kappa_a \in \mathbb{C}_+$ or $\kappa_b \in \mathbb{C}_+$. In both cases the operator is completely non-selfadjoint, see [18]. In the following we consider the case $\kappa_a, \kappa_b \in \mathbb{C}_+$. In this case we usually write $H[V]$ instead of $H[\kappa_a,\kappa_b,V]$. The spectrum of $H[V]$ consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity, i.e $\mathrm{spec}(H[V]) \subseteq \overline{\mathbb{C}_-} := \{z \in \mathbb{C} : \Im\mathrm{m}(z) \leq 0\}$. Since the operator $H[V]$ is completely non-selfadjoint, its eigenvalues are non-real.

Besides the operator $H[V]$ we consider the operator $H_{\Re}[V] := H[q_a,q_b,V]$, $V \in L^\infty_{\mathbb{R}}(\Omega)$, $q_a, q_b \in \mathbb{R}$. The operator $H_{\Re}[V]$ is self-adjoint and semi-bounded from below. In some sense the operator $H_{\Re}[V]$ can be regarded as the real part of the maximal dissipative $H[V]$. By $\gamma[V]$ we denote the bottom of the spectrum of $H_{\Re}[V]$, i.e. $\gamma[V] := \inf \mathrm{spec}(H_{\Re}[V])$.

Lemma 3.1 *Let the Schrödinger assumptions Q_1 be satisfied. If $q_a, q_b \in \mathbb{R}$, then*

$$\gamma[V] \geq -\gamma_0 - \|V_-\|_{L^\infty} \tag{3.1}$$

where $V_-(x) := \frac{1}{2}\{|V(x)| - V(x)\}$, $x \in \Omega$, and γ_0 is given by (2.16).

Proof. We consider the quadratic form $\mathfrak{h}[q_a,q_b](\cdot,\cdot)$,

$$\mathfrak{h}[q_a,q_b](f,f) := -q_a|f(a)|^2 - q_b|f(b)|^2 + \int_a^b \frac{1}{2m(x)}|f'(x)|^2\,dx,$$

$f \in \mathrm{dom}(\mathfrak{h}[q_a,q_b,V]) = W^{1,2}(\Omega)$, which is associated with the self-adjoint operator $H[q_a,q_b,0]$. The quadratic form $\mathfrak{h}[q_a,q_b](\cdot,\cdot)$ admits the estimate

$$\mathfrak{h}[q_a,q_b](f,f) \geq \widehat{\mathfrak{h}}(f,f) := -\mathfrak{q}\{|f(a)|^2 + |f(b)|^2\} + \frac{1}{2\overline{m}}\int_a^b |f'(x)|^2\,dx$$

where $\mathfrak{q} := \max\{0,q_a,q_b\}$, cf. (2.17). The quadratic form $\widehat{\mathfrak{h}}$ corresponds to the self-adjoint operator $\widehat{H}$,

$$(\widehat{H}f)(x) = -\frac{1}{2\overline{m}}\frac{d^2}{dx^2}f(x), \quad f \in \mathrm{dom}(\widehat{H}),$$

$$\operatorname{dom}(\widehat{H}) = \left\{ f \in W^{2,2}(\Omega) : \frac{1}{2\overline{m}} f'(a) = -\mathfrak{q} f(a), \quad \frac{1}{2\overline{m}} f'(b) = \mathfrak{q} f(b) \right\}.$$

A straightforward computation shows that $\lambda = -\mu^2$, $\mu \geq \mathfrak{q}\sqrt{2\overline{m}}$, is an eigenvalue of $\widehat{H}$ if and only if μ satisfies the equation

$$\mu|\Omega|\sqrt{2\overline{m}} = \ln\left(\frac{\mu + \mathfrak{q}\sqrt{2\overline{m}}}{\mu - \mathfrak{q}\sqrt{2\overline{m}}}\right).$$

Hence, if $\lambda = -\mu^2$ is an eigenvalue, then the estimate

$$\mu|\Omega|\sqrt{2\overline{m}} \leq \frac{2\mathfrak{q}\sqrt{2\overline{m}}}{\mu - \mathfrak{q}\sqrt{2\overline{m}}}$$

holds. This yields

$$\lambda = -\mu^2 \geq -2\overline{m}\mathfrak{q}^2 \left\{ \frac{1}{2} + \frac{1}{\mathfrak{q}|\Omega|\overline{m}} + \sqrt{\frac{1}{4} + \frac{1}{\mathfrak{q}|\Omega|\overline{m}}} \right\}.$$

Using this estimate we immediately verify (3.1). □

3.2 Elementary solutions and estimates

An important tool to investigate the dissipative operator $H[V]$ are the so-called elementary solutions defined by

$$l[V](v_a(x,z)) = zv_a(x,z), \quad v_a(a,z) = 1, \quad \frac{1}{2m(a)} v_a'(a,z) = -\kappa_a \tag{3.2}$$

$$l[V](v_b(x,z)) = zv_b(x,z), \quad v_b(b,z) = 1, \quad \frac{1}{2m(b)} v_b'(b,z) = \kappa_b. \tag{3.3}$$

The existence of these solutions for each $z \in \mathbb{C}$ can be proved by writing (3.2) and (3.3) in integral form

$$v_a(x,z) = 1 - 2\kappa_a M_a(x) + 2\int_a^x dt\,(M_a(x) - M_a(t))(V(t) - z)v_a(t,z) \tag{3.4}$$

and

$$v_b(x,z) = 1 - 2\kappa_b M_b(x) + 2\int_x^b dt\,(M_b(x) - M_b(t))(V(t) - z)v_b(t,z) \tag{3.5}$$

where

$$M_a(x) := \int_a^x dt\; m(t) \quad \text{and} \quad M_b(x) := \int_x^b dt\; m(t)$$

Since (3.4) and (3.5) are Volterra-type equations they have always solutions for any $z \in \mathbb{C}$, in particular, for $z = \lambda \in \mathbb{R}$. Moreover, one gets that v_a and v_b as well as $\frac{1}{m}v_a'$ and $\frac{1}{m}v_b'$ are absolutely continuous.

In the following the estimates are based on Gronwall's lemma which we need in a slightly generalized form.

Lemma 3.2 (Gronwall's lemma) *Let μ be a finite Borel measure on $[a,b]$. If the non-negative continuous function $g(\cdot) : [a,b] \longrightarrow \mathbb{R}$ obeys*

$$0 \le g(x) \le C + \int_{[a,x]} g(t)\, d\mu(t), \quad x \in [a,b], \quad C > 0, \tag{3.6}$$

then the estimate

$$g(x) \le C \exp\left\{ \int_{[a,x]} d\mu(t) \right\}, \quad x \in [a,b], \tag{3.7}$$

holds.

The proof follows immediately from Lemma 5 of [15]. Using Gronwall's lemma we are going to establish bounds for the elementary solutions if $\lambda > 0$. At first we prove this for the special case $V = 0$ and later on we extend the result to $V \neq 0$.

Let $V = 0$. We consider the the boundary value problem

$$l[0]w(x,\lambda) = \lambda w(x,\lambda), \quad w(a,\lambda) = p, \quad \frac{1}{2m(a)} w'(a,\lambda) = q,$$

where $p, q \in \mathbb{C}$.

Lemma 3.3 *Let the Schrödinger assumption Q_1 be satisfied. If m has a finite total variation, then*

$$|w(x,\lambda)| \le \sqrt{|p|^2 + \frac{2}{\lambda m(a)} |q|^2}\ \mathfrak{M}, \tag{3.8}$$

for $x \in [a,b]$ and $\lambda > 0$, where $\mathfrak{M}$ is defined by (2.12).

Proof. We note that

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} w(x,\lambda) = \lambda w(x,\lambda)$$

is satisfied for a.e. $x \in [a,b]$ with respect of the Lebesgue measure. Multiplying by $\overline{\frac{1}{m(x)} w'(x,\lambda)}$ we get

$$-\frac{1}{2}\overline{\frac{1}{m(x)} w'(x,\lambda)}\frac{d}{dx}\frac{1}{m(x)} w'(x,\lambda) = \lambda w(x,\lambda)\overline{\frac{1}{m(x)} w'(x,\lambda)}$$

which yields

$$\frac{1}{2}\frac{d}{dx}\left|\frac{1}{m(x)} w'(x,\lambda)\right|^2 = -\frac{\lambda}{m(x)}\frac{d}{dx}\left|w(x,\lambda)\right|^2$$

for a.e. $x \in [a,b]$. Since $\frac{1}{m(x)} w'(x,\lambda)$ is absolutely continuous we obtain

$$\frac{1}{2}\left|\frac{1}{m(x)} w'(x,\lambda)\right|^2 = \frac{1}{2}\left|\frac{1}{m(a)} w'(a,\lambda)\right|^2 - \lambda \int_a^x \frac{1}{m(t)}\frac{d}{dt}\left|w(t,\lambda)\right|^2 dt$$

for $x \in [a,b]$. Since m has a finite total variation, the limits $m(x-0) := \lim_{y \uparrow x} m(y)$ for $x \in (a,b]$ and $m(x+0) := \lim_{y \downarrow x} m(y)$ for $x \in [a,b)$ exist. Further, we set $m(a-0) := m(a)$

and $m(b+0) := m(b)$. Notice that $m(x)$ and $m(x-0)$ are different only on a countable set. Hence we can replace $\frac{1}{m(t)}$ by $\frac{1}{m(t-0)}$ above. Using the boundary conditions we get

$$\left|\frac{1}{m(x)}w'(x,\lambda)\right|^2 = 4\left|q\right|^2 - 2\lambda\int_{[a,x]}\frac{1}{m(t-0)}\,d\left|w(t,\lambda)\right|^2$$

for all $x \in [a,b]$ where the integral on the right-hand side is regarded as a Lebesgue-Stieltjes integral. If m has a finite total variation, then by assumption Q_1 the function $\frac{1}{m}$ has a finite total variation, too. By Theorem 21.67 and Remark 21.68 of [13] we get

$$\left|\frac{1}{m(x)}\frac{d}{dx}w(x,\lambda)\right|^2 + \frac{2\lambda}{m(x+0)}\left|w(x,\lambda)\right|^2 = \tag{3.9}$$
$$4\left|q\right|^2 + \frac{2\lambda}{m(a)}\left|w(a,\lambda)\right|^2 + 2\lambda\int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu(t)$$

where μ is the signed measure associated with $\frac{1}{m}$. Since $\frac{1}{m}$ is of bounded variation, the functions $\varpi(x) := \bigvee_a^x \frac{1}{m}$ and $\nu(x) := \varpi(x) - \frac{1}{m(x)}$, $x \in [a,b]$, are non-decreasing. Notice that $\frac{1}{m(x)} = \varpi(x) - \nu(x)$. Thus we find

$$\int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu(t) = \int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\varpi(t) - \int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\nu(t),$$

where μ_ϖ and μ_ν the measures associated with ϖ and ν, respectively. Hence

$$\int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu(t) \le \int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\varpi(t), \quad x \in [a,b].$$

Inserting this estimate into (3.9) and using the boundary condition $w(a,\lambda) = p$ we get

$$\frac{1}{m(x+0)}\left|w(x,\lambda)\right|^2 \le \frac{2}{\lambda}\left|q\right|^2 + \frac{1}{m(a)}|p|^2 + \int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\varpi(t), \quad x \in [a,b],$$

which yields

$$\left|w(x,\lambda)\right|^2 \le m(x+0)\left(\frac{2}{\lambda}\left|q\right|^2 + \frac{1}{m(a)}|p|^2\right) + m(x+0)\int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\varpi(t)$$

for $x \in [a,b]$. Since $m(x) \le \overline{m}$, $x \in [a,b]$, we obtain

$$\left|w(x,\lambda)\right|^2 \le \overline{m}\left(\frac{2}{\lambda}\left|q\right|^2 + \frac{1}{m(a)}|p|^2\right) + \overline{m}\int_{[a,x]}\left|w(t,\lambda)\right|^2\,d\mu_\varpi(t)$$

Applying Lemma 3.2, we immediately get

$$\left|w(x,\lambda)\right|^2 \le \left(\frac{2}{\lambda}\left|q\right|^2 + \frac{1}{m(a)}|p|^2\right)\exp\left\{\overline{m}\int_{[a,x]}\,d\mu_\varpi(t)\right\}$$

for $x \in [a,b]$. Hence

$$\left|w(x,\lambda)\right| \le \sqrt{|p|^2 + \frac{2}{\lambda m(a)}|q|^2}\,\sqrt{\overline{m}}\,\exp\left\{\frac{\overline{m}}{2}\int_{[a,x]}\,d\mu_\varpi(t)\right\}$$

for $x \in [a,b]$. Finally, taking into account

$$\int_{[a,x]} d\mu_\varpi(t) \le \int_{[a,b]} d\mu_\varpi(t) \le \bigvee_a^b \frac{1}{m}$$

we prove (3.8). □

We note that a similar lemma holds if the end point a is replaced by b.

In the following we consider the solutions $w_0(x,\lambda)$ and $w_1(x,\lambda)$ of the boundary value problems

$$\begin{aligned} (l[0]w_1)(x) &= \lambda w_1(x,\lambda), \quad w_1(a,\lambda)=1, \quad \frac{1}{2m(a)}w_1'(a,\lambda)=0,\\ (l[0]w_0)(x) &= \lambda w_0(x,\lambda), \quad w_0(a,\lambda)=0, \quad \frac{1}{2m(a)}w_0'(a,\lambda)=1. \end{aligned}$$

By Lemma 3.3 we have the estimates

$$|w_1(x,\lambda)| \le \mathfrak{M} \quad \text{and} \quad |w_0(x,\lambda)| \le \sqrt{\frac{2}{\lambda m(a)}}\ \mathfrak{M}, \quad x \in [a,b], \quad \lambda > 0.$$

Lemma 3.4 *Let the Schrödinger assumption Q_1 be satisfied and let $V \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then*

$$|v_j(x,\lambda)| \le \begin{cases} R_j(\|V\|_{L^\infty}), & \lambda \ge 1, \\ R_j(\|V+1-\lambda\|_{L^\infty}), & \lambda < 1, \end{cases}, \quad j=a,b, \quad x \in \Omega, \tag{3.10}$$

where $R_j(\cdot)$ is defined by (2.13)

Proof. The solution $v_a(x,\lambda)$ satisfies the integral equation

$$\begin{aligned} v_a(x,\lambda) &= w_1(x,\lambda) - \kappa_a w_0(x,\lambda) + \\ &\int_a^x dt\ \{w_0(x,\lambda)w_1(t,\lambda) - w_0(t,\lambda)w_1(x,\lambda)\}V(t)v_a(t,\lambda), \end{aligned}$$

$x \in \Omega$ and $\lambda \in \mathbb{R}$. Therefore, we have the estimate

$$\begin{aligned} &|v_a(x,\lambda)| \le \\ &\mathfrak{M}\left(1 + |\kappa_a|\sqrt{\frac{2}{\lambda\, m(a)}}\right) + \mathfrak{M}^2\sqrt{\frac{2}{\lambda\, m(a)}}\int_a^x dt\ |V(t)|\ |v_a(t,\lambda)|, \end{aligned}$$

$x \in \Omega$ and $\lambda > 0$. Applying Gronwall's lemma we find

$$|v_a(x,\lambda)| \le \mathfrak{M}\left(1 + |\kappa_a|\sqrt{\frac{2}{\lambda\, m(a)}}\right)\exp\left\{\mathfrak{M}^2\sqrt{\frac{2}{\lambda\, m(a)}}\int_a^x dt\ |V(t)|\right\}$$

for $x \in \Omega$ and $\lambda > 0$. If $\lambda \ge 1$, then we immediately verify the first part of (3.10).

If $\lambda < 1$, then $v_j(x,\lambda)$ satisfies the equation $l[V+1-\lambda]v_a(x,\lambda) = v_a(x,\lambda)$. Taking into account the first estimate of (3.10) we prove the second estimate. The proof for $j=b$ is similar. □

3.3 Characteristic function

Let us introduce the operator-valued function $T(z) : \mathcal{H} \longrightarrow \mathbb{C}^2$,

$$T[V](z)f := \begin{pmatrix} \alpha_b((H[V]-z)^{-1}f)(b) \\ -\alpha_a((H[V]-z)^{-1})f(a) \end{pmatrix}, \quad \alpha_a, \alpha_b > 0,$$

for $z \in \mathrm{res}(H[V])$ and $f \in L^2(\Omega)$. Using Theorem 2.1 of [19], we find

$$T[V](z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\ v_a(y,z)f(y) \\ \alpha_a \int_a^b dy\ v_b(y,z)f(y) \end{pmatrix}$$

for $f \in L^2(\Omega)$ where $W(z)$ denotes the Wronskian of the solutions $v_a(x,z)$ and $v_b(x,z)$,

$$W(z) := v_a(x,z)\frac{1}{2m(x)}v_b'(x,z) - v_b(x,z)\frac{1}{2m(x)}v_a'(x,z),$$

which is independent from $x \in \Omega$. The adjoint operator is given by

$$\left(T[V](z)^*\xi\right)(x) = \frac{1}{\overline{W(z)}}\left(-\alpha_b\overline{v_a(x,z)}, \alpha_a\overline{v_b(x,z)}\right)\xi \tag{3.11}$$

$x \in \Omega$, where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{3.12}$$

and the right-hand side is regarded as a matrix multiplication. Similarly, we set

$$T_*[V](z)f := \begin{pmatrix} \alpha_b((H[V]^*-z)^{-1}f)(b) \\ -\alpha_a((H[V]^*-z)^{-1}f)(a) \end{pmatrix}$$

for $z \in \mathrm{res}(H^*)$ and $f \in L^2(\Omega)$. Using again Theorem 2.1 of [19]we find

$$T_*[V](z)f = \frac{1}{W_*(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\ v_{*a}(y,z)f(y) \\ \alpha_b \int_a^b dy\ v_{*b}(y,z)f(y) \end{pmatrix}.$$

where $W_*(z)$ is the Wronskian of the solutions $v_{*a}(x,z) := \overline{v_a(x,\overline{z})}$ and $v_{*b}(x,z) := \overline{v_b(x,\overline{z})}$,

$$W_*(z) := v_{*a}(x,z)\frac{1}{2m(x)}v_{*b}'(x,z) - v_{*b}(x,z)\frac{1}{2m(x)}v_{*a}'(x,z).$$

which also independent from $x \in \Omega$. The adjoint operator has the representation

$$\left(T_*[V](z)^*\xi\right)(x) = \frac{1}{\overline{W_*(z)}}\left(-\alpha_b\overline{v_{*a}(x,z)}, \alpha_a\overline{v_{*b}(x,z)}\right)\xi$$

$x \in \Omega$, $\xi \in \mathbb{C}^2$.

The operator $H[V]$ can be (up to unitary equivalence) characterized by its characteristic function $z \to \Theta[V](z)$, with $z \in \mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*)$, cf. [9]. The characteristic function $\Theta[V](\cdot)$ of the maximal dissipative operator $H[V]$ is a two-by-two matrix-valued function which satisfies the relation

$$\Theta[V](z)T[V](z)f = T_*[V](z)f, \quad z \in \mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*),$$

$f \in \mathfrak{H}$. In terms of the adjoint elementary solutions the characteristic function can be expressed as follows:

$$\Theta[V](z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)}\begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix},$$

which can be written as

$$\Theta[V](z) = I_{\mathbb{C}^2} - i\alpha T[V](\overline{z})^*,$$

$z \in \operatorname{res}(H[V]) \cap \operatorname{res}(H[V]^*)$, where the operator $\alpha : L^2(\Omega) \longrightarrow \mathbb{C}$, is defined by

$$\alpha f := \begin{pmatrix} \alpha_b f(b) \\ -\alpha_a f(a) \end{pmatrix}, \quad f \in \operatorname{dom}(\alpha) := C(\bar{\Omega}).$$

Notice that the operator α is not closed and not closable. The characteristic function $\Theta[V](\lambda)$ is a holomorphic on $\operatorname{res}(H[V]) \cap \operatorname{res}(H[V]^*)$ and contractive on $\mathbb{C}_- \cup \mathbb{R}$, i.e. it satisfies

$$\|\Theta[V](z)\| \le 1 \quad \text{for} \quad z \in \mathbb{C}_- \cup \mathbb{R}.$$

In particular, it is well-defined and continuous on $\mathbb{R}$, cf. [19]. We note that by Lemma 2.2 of [26] one has $\lim_{\lambda \to -\infty} \|\Theta[V](\lambda) - I_{\mathbb{C}^2}\|_{\mathcal{B}(\mathbb{C}^2)} = 0$.

3.4 Phase shift

The phase shift $\omega[V]$ is defined by

$$e^{2\pi i \omega[V](\lambda)} := \det(\Theta[V](\lambda)), \quad \lambda \in \mathbb{R},$$

where it is assumed that $\omega[V](\cdot) : \mathbb{R} \longrightarrow \mathbb{R}$ is continuous. Notice that the phase shift is determined modulo $\mathbb{Z}$. Since $\lim_{\lambda \to -\infty} \det(\Theta[V](\lambda)) = 1$ by Lemma 2.2 of [26] we fix the phase shift by the condition

$$\lim_{\lambda \to -\infty} \omega[V](\lambda) = 0.$$

Lemma 3.5 *[26, Lemma 4.1] Let the Schrödinger assumptions Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then the phase shift is holomorphic in a neighbourhood of $\mathbb{R}$ and satisfies*

$$\omega'[V](\lambda) := \frac{d}{d\lambda}\omega[V](\lambda) = -\frac{1}{2\pi}\operatorname{tr}(T[V](\lambda)T[V](\lambda)^*) \le 0 \tag{3.13}$$

for $\lambda \in \mathbb{R}$.

Lemma 3.5 shows that the phase shift is non-increasing. Moreover, since $\omega[V](-\infty) = 0$ the phase shift is always non-positive, i.e $\omega[V](\lambda) \le 0$ for $\lambda \in \mathbb{R}$. Let us introduce the counting function

$$\Phi[V](\lambda) := \operatorname{card}\{s \le \lambda : \det(\Theta[V](s)) = 1\}, \quad \lambda \in \mathbb{R}.$$

It turns out that the $\Phi[V](\cdot)$ is comparable with the counting function $N_D[V](\cdot)$,

$$N_D[V](\lambda) := \operatorname{card}\{s \le \lambda : s \in \operatorname{spec}(H_D[V])\}, \quad \lambda \in \mathbb{R}.$$

where $H_D[V]$ denotes the Schrödinger-type operator with Dirichlet boundary conditions.

Theorem 3.6 *[26, Theorem 4.7] Let the Schrödinger assumption Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$N_D[V](\lambda) \le \Phi[V](\lambda) \le N_D[V](\lambda) + 1, \quad \lambda \in \mathbb{R}.$$

Corollary 3.7 *Let the Schrödinger assumption Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$0 \le -\omega[V](\lambda) \le 2 + \frac{1}{\pi}\sqrt{2\overline{m}|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+} \tag{3.14}$$

for $\lambda \in \mathbb{R}$.

Proof. Since $-\omega[V](\lambda)$ is non-decreasing by Lemma 3.5 the estimate $-\omega[V](\lambda) \le 1 + \Phi[V](\lambda)$, $\lambda \in \mathbb{R}$, holds. By Remark 4.8 of [26] and Theorem 3.6 one gets

$$N_D[V](\lambda) \le \frac{1}{\pi}\sqrt{2\overline{m}|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+}, \quad \lambda \in \mathbb{R},$$

which yields (3.14). □

3.5 Lipschitz continuity of the phase shift

We are going to verify the Lipschitz continuity of the phase shift by giving bounds for the derivative of $\omega[V]$.

Proposition 3.8 *Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then*

$$|\omega[V](\lambda) - \omega[V](\lambda')| \le |\Omega|\ L(\ \|V\|_{L^\infty})^2\ |\lambda - \lambda'|, \tag{3.15}$$

$\lambda, \lambda' \in \mathbb{R}$ where $L(\cdot)$ is defined by (2.14).

Proof. Since the phase shift is continuously differentiable it is sufficient to show $-\omega'[V](\lambda) \le |\Omega|\ L(\ \|V\|_{L^\infty})^2$, $\lambda \in \mathbb{R}$. Taking into account Lemma 3.5 we get

$$\omega'[V](\lambda) = -\frac{1}{2\pi}\sum_{j=1}^{2}\|T[V](\lambda)^* e_j\|^2_{L^2}, \quad \lambda \in \mathbb{R}, \tag{3.16}$$

where

$$e_1 := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_2 := \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

By (3.11) we find

$$\|T[V](\lambda)^* e_1\|^2_{L^2} = \frac{\alpha_b^2}{|W(\lambda)|^2}\int_a^b dx\ |v_a(x,\lambda)|^2.$$

Let

$$E := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We note that $\|E\Theta[V](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \le 1$, $\lambda \in \mathbb{R}$, and

$$\mathrm{tr}(E\Theta[V](\lambda)) = -2i\frac{\alpha_a\alpha_b}{W(\lambda)}, \quad \lambda \in \mathbb{R},$$

which yields

$$\frac{\alpha_a\alpha_b}{|W(\lambda)|} \le 1, \quad \lambda \in \mathbb{R}.$$

Hence

$$\|T[V](\lambda)^*e_1\|^2_{L^2} \le \frac{1}{\alpha_a^2}\int_a^b dx\ |v_a(x,\lambda)|^2, \quad \lambda \in \mathbb{R}.$$

Applying Lemma 3.4 we get the estimate

$$\|T[V](\lambda)^*e_1\|^2_{L^2} \le |\Omega|\frac{R_a[\ \|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \quad \lambda \in [\lambda_0-1,\infty). \tag{3.17}$$

where $\lambda_0 := -\|V\|_{L^\infty} - \gamma_0$ and γ_0 is given by (2.16). By Lemma 3.1 one immediately gets that $(-\infty,\lambda_0) \subseteq \mathrm{res}(H[V])$. Using the resolvent formula

$$(H[V]-\lambda)^{-1} = (H[V]-\lambda_0)^{-1}\left\{I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\right\},$$

$\lambda \in (-\infty,\lambda_0)$, we find the representation

$$T[V](\lambda) = T[V](\lambda_0)\left\{I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\right\}, \tag{3.18}$$

$\lambda \in (-\infty,\lambda_0)$. By $\Gamma[V]$ we denote the numerical range of $H[V]$. One easily verifies that $\Gamma[V] \subseteq \{z \in \mathbb{C} : \Re\mathrm{e}(z) \ge \lambda_0\}$. Applying Theorem 3.1 of [18] we get the estimate

$$\|(H[V]-\lambda)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \le \frac{1}{\mathrm{dist}(\Gamma[V],\lambda)} \le \frac{1}{|\lambda-\lambda_0|} \le 1$$

for $\lambda \in (-\infty,\lambda_0-1)$. Hence we find the estimate

$$\|I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \le 1 + \frac{|\lambda-\lambda_0|}{|\lambda-\lambda_0|} = 2$$

for $\lambda \in (-\infty,\lambda_0-1)$. Further, from (3.18) we get

$$T[V](\lambda)^*e_1 = \{I + (\lambda-\lambda_0)(H[V]^*-\lambda)^{-1}\}T[V](\lambda_0)^*e_1$$

for $\lambda \in (-\infty,\lambda_0-1)$. Using (3.17)

$$\|T[V](\lambda)^*e_1\|^2_{L^2} \le 4\ \|T[V](\lambda_0)^*e_1\|^2_{L^2} \le 4\ |\Omega|\ \frac{R_a[\ \|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \tag{3.19}$$

$\lambda \in (-\infty,\lambda_0-1)$. Taking into account (3.17) and (3.19) we finally get

$$\|T[V](\lambda)^*e_1\|^2_{L^2} \le 4\ |\Omega|\ \frac{R_a[\ \|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \quad \lambda \in \mathbb{R}. \tag{3.20}$$

Similarly, we prove

$$\|T[V](\lambda)^*e_2\|^2_{L^2} \le 4\ |\Omega|\ \frac{R_b[\ \|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_b^2}, \quad \lambda \in \mathbb{R}. \tag{3.21}$$

From (3.16), (3.20) and (3.21) we obtain

$$-\omega'[V](\lambda) \leq \frac{2}{\pi}\,|\Omega|\,\left\{\frac{R_a[\,\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2} + \frac{R_b[\,\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_b^2}\right\}$$

for $\lambda \in \mathbb{R}$. Inserting $\lambda_0 = -\|V\|_{L^\infty} - \gamma_0$ into this formula and using the definition (2.14) we obtain (3.15). □

3.6 Dilations

Since $H[V]$ is a maximal dissipative operator there is a larger Hilbert space $\mathfrak{K} \supseteq \mathfrak{H}$ and a self-adjoint operator $K[V]$ on $\mathfrak{K}$ such that

$$P_{\mathfrak{H}}^{\mathfrak{K}}(K[V]-z)^{-1}\restriction\mathfrak{H} = (H[V]-z)^{-1}, \quad \Im\mathrm{m}(z) > 0, \tag{3.22}$$

see [9]. The operator $K[V]$ is called a self-adjoint dilation of the maximal dissipative operator $H[V]$. Obviously, from the condition (3.22) one gets

$$P_{\mathfrak{H}}^{\mathfrak{K}}(K[V]-z)^{-1}\restriction\mathfrak{H} = (H[V]^*-z)^{-1}, \quad \Im\mathrm{m}(z) < 0.$$

If the condition

$$\mathrm{clospan}\{z \in \mathbb{C}\setminus\mathbb{R} : (K[V]-z)^{-1}\mathfrak{H}\} = \mathfrak{K}$$

is satisfied, then $K[V]$ is called a minimal self-adjoint dilation of $H[V]$. Minimal self-adjoint dilations of maximal dissipative operators are determined up to an isomorphism, in particular, all minimal self-adjoint dilations are unitarily equivalent. The self-adjoint operator $K[V]$ is absolutely continuous and its spectrum coincides with the real axis, i.e. $\mathrm{spec}(K) = \mathbb{R}$. The multiplicity of its spectrum is two. For more details the reader is referred to [19].

Definition 3.9 (c.f. [22]) Let K be a selfadjoint, absolutely continuous operator on a Hilbert space $\mathcal{H}$ and A be a bounded operator on $\mathcal{H}$. Then A is called K-smooth if there is a constant $C_A > 0$ such that

$$\int_{-\infty}^{+\infty} dt\,\|Ae^{-itK}\vec{f}\|_{\mathcal{H}}^2 \leq 2\pi\, C_A^2\|\vec{f}\|_{\mathcal{H}}^2 \tag{3.23}$$

for all $\vec{f} \in \mathcal{H}$. The smallest constant C_A is denoted by $\|A\|_K$.

Let us verify that the projection $P_{\mathfrak{H}}^{\mathfrak{K}}$ is $K[V]$-smooth. To this end we need the following lemma which was proved in [26].

Lemma 3.10 *[26, Lemma 5.3] Let the Schrödinger assumptions Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$\frac{d}{d\lambda}(E_{K[V]}(\lambda)P_{\mathfrak{H}}^{\mathfrak{K}}\vec{f}, P_{\mathfrak{H}}^{\mathfrak{K}}\vec{g})_{\mathfrak{K}} = (T[V](\lambda)P_{\mathfrak{H}}^{\mathfrak{K}}\vec{f}, T[V](\lambda)P_{\mathfrak{H}}^{\mathfrak{K}}\vec{g})_{\mathbb{C}^2}$$

for a.e $\lambda \in \mathbb{R}$ and $\vec{f}, \vec{g} \in \mathfrak{K}$ where $E_{K[V]}(\cdot)$ denotes the spectral measure of the the self-adjoint dilation $K[V]$.

Proposition 3.8 and Lemma 3.10 imply the smoothness of $P^{\mathfrak{K}}_{\mathfrak{H}}$:

Theorem 3.11 *Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then the projection $P^{\mathfrak{K}}_{\mathfrak{H}}$ is $K[V]$-smooth and the estimate*

$$\|P^{\mathfrak{K}}_{\mathfrak{H}}\|_{K[V]} \le \sqrt{|\Omega|}\; L(\,\|V\|_{L^\infty}) \tag{3.24}$$

holds where $L(\cdot)$ is defined by (2.14).

Proof. In accordance with [22] we set

$$a_2 := \sup_{\Delta\subseteq\mathbb{R},\vec{f}\in\mathfrak{K},\vec{f}\neq 0} \frac{\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2}{|\Delta|\;\|\vec{f}\|^2}$$

where $\Delta = (\lambda_1,\lambda_2) \subseteq \mathbb{R}$ are bounded intervals of $\mathbb{R}$ and $|\Delta| := \lambda_2 - \lambda_1$ denotes their length. Then Theorem 5.1 of [22] states $\|P^{\mathfrak{K}}_{\mathfrak{H}}\|_{K[V])} = \sqrt{a_2}$. Thus, the $K[V]$-smoothness of the projection $P^{\mathfrak{K}}_{\mathfrak{H}}$ including the estimate (3.24) is shown if we verify

$$a_2 \le |\Omega|\; L(\|V\|_{L^\infty})^2.$$

Using Lemma 3.10 we get that

$$\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2_{\mathfrak{K}} = \frac{1}{2\pi}\int_\Delta d\lambda\; \|T[V](\lambda)f\|^2_{\mathfrak{H}}.$$

We note that

$$\|T[V](\lambda)f\|^2_{\mathfrak{H}} \le \|f\|^2_{\mathfrak{H}}\mathrm{tr}(T[V](\lambda)^*T[V](\lambda)) = \|f\|^2_{\mathfrak{H}}\;\mathrm{tr}(T[V](\lambda)T[V](\lambda)^*),$$

$\lambda \in \mathbb{R}$. Hence

$$\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2_{\mathfrak{K}} \le \|\vec{f}\|^2_{\mathfrak{K}}\;\frac{1}{2\pi}\int_\Delta d\lambda\;\mathrm{tr}(T[V](\lambda)T[V](\lambda)^*).$$

Taking into account Lemma 3.5 we obtain the estimate

$$\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2_{\mathfrak{K}} \le -\|\vec{f}\|^2_{\mathfrak{K}}\;\int_\Delta d\lambda\;\omega'[V](\lambda).$$

Hence we obtain

$$\frac{\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2_{\mathfrak{K}}}{\|\vec{f}\|^2_{\mathfrak{K}}} \le (\omega[V](\lambda_1) - \omega[V](\lambda_2))$$

Using (3.15) we find the estimate

$$\frac{\|E_{K[V]}(\Delta)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}\|^2_{\mathfrak{K}}}{|\Delta|\;\|f\|^2_{\mathfrak{K}}} \le |\Omega|\;L(\|V\|_{L^\infty})^2.$$

□

3.7 Lax-Phillips scattering theory

The dilation space $\mathfrak{K}$ admits the decomposition

$$\mathfrak{K} = \mathcal{D}_- \oplus \mathfrak{H} \oplus \mathcal{D}_+.$$

where $\mathcal{D}_\pm = L^2(\mathbb{R}_\pm, \mathbb{C}^2)$, see [19]. Since

$$e^{-itK[V]}\mathcal{D}_- \subseteq \mathcal{D}_-, \quad t \le 0,$$

$$e^{-itK[V]}\mathcal{D}_+ \subseteq \mathcal{D}_+, \quad t \ge 0$$

as well as

$$\bigcap_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_- = \bigcap_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_+ = \{0\},$$

$$\overline{\bigcup_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_-} = \overline{\bigcup_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_+} = \mathfrak{K} \tag{3.25}$$

the subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces with respect to $e^{-itK[V]}$, cf. [1, Ch. XII] or [24]. Further, introducing the Hilbert space $\mathfrak{K}_0$,

$$\mathfrak{K}_0 = L^2(\mathbb{R}, \mathbb{C}^2) = \mathcal{D}_- \oplus \mathcal{D}_+ \subseteq \mathfrak{K} = \mathcal{D}_- \oplus \mathfrak{H} \oplus \mathcal{D}_+,$$

and the self-adjoint differentiation operator K_0,

$$(K_0 f)(x) = -i\frac{d}{dx}f(x), \quad f \in \mathrm{dom}(K_0) = W^{1,2}(\mathbb{R}, \mathbb{C}^2),$$

one easily verifies that $\mathcal{D}_-$ and $\mathcal{D}_+$ are incoming and outgoing subspaces with respect to e^{-itK_0}. The Lax-Phillips wave operators are defined by

$$W_\pm(K[V], K_0; J_\pm) := s - \lim_{t\to\pm\infty} e^{itK[V]} J_\pm e^{-itK_0}$$

where the identification operators $J_\pm : \mathfrak{K}_0 \longrightarrow \mathfrak{K}$ are given by

$$\vec{f} = J_- f := P^{\mathfrak{K}_0}_{\mathcal{D}_-} f \oplus 0 \oplus 0, \quad f \in \mathfrak{K}_0,$$

$$\vec{f} = J_+ f := 0 \oplus 0 \oplus P^{\mathfrak{K}_0}_{\mathcal{D}_+} f, \quad f \in \mathfrak{K}_0.$$

Since

$$e^{-itK[V]}|\mathcal{D}_- = e^{-itK_0}|\mathcal{D}_-, \quad t \le 0,$$

$$e^{-itK[V]}|\mathcal{D}_+ = e^{-itK_0}|\mathcal{D}_+, \quad t \ge 0,$$

the wave operators $W_\pm(K[V], K_0; J_\pm)$ exist. Using (3.25) one proves the completeness of the wave operators, i.e. $\mathrm{ran}(W_\pm(K[V], K_0; J_\pm)) = \mathfrak{K}$. For for details see [1, Ch. XII] or [24]. Defining the Fourier transform $F : \mathfrak{K}_0 \longrightarrow \widehat{\mathfrak{K}}_0 = L^2(\mathbb{R}, \mathbb{C}^2)$ by

$$(Ff)(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx\; e^{-ix\lambda} f(x), \quad f \in \mathfrak{K}_0, \quad \lambda \in \mathbb{R}.$$

one defines the generalized Fourier transform $\Phi[V] : \mathfrak{K} \longrightarrow \widehat{\mathfrak{K}}_0$ by

$$\Phi[V] := FW_-(K[V], K_0; J_-)^*, \tag{3.26}$$

cf. Remark 5.2 of [20], which is an isometry. Moreover, if M is the multiplication operator defined by

$$(M\widehat{f}) = \lambda \widehat{f}(\lambda), \quad \widehat{f} \in \mathrm{dom}(M) = \{\widehat{f} \in \widehat{\mathfrak{K}}_0 : \lambda \widehat{f}(\lambda) \in \widehat{\mathfrak{K}}_0\}.$$

on the Hilbert space $\mathfrak{K}_0$, then $M = \Phi[V]K[V]\Phi[V]^{-1}$.

Lemma 3.12 *Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V, W \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then the estimate*

$$\|(W_-(K[W], K[V]) - I_{\mathfrak{K}})\|_{\mathcal{B}(\mathfrak{K})} \le 2\pi\ |\Omega|\ L(\|V\|_{L^\infty})\ L(\|W\|_{L^\infty})\ \|V - W\|_{L^\infty} \tag{3.27}$$

holds where $L(\cdot)$ is given by (2.14).

Proof. Similar to formula (X.3.24) of [22] one has

$$\Big((W_-(K[W], K[V]) - I_{\mathfrak{K}})\vec{f}, \vec{g}\Big)_{\mathfrak{K}} = \\ -i\int_{-\infty}^{0} dt\ \Big([W - V]P^{\mathfrak{K}}_{\mathfrak{H}} e^{-itK[V]}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}} e^{-itK[W]}\vec{g}\Big),$$

for $\vec{f}, \vec{g} \in \mathrm{dom}(K[V]) = \mathrm{dom}(K[W])$. Hence, we obtain the estimate

$$\left|\Big((W_-(K[W], K[V]) - I_{\mathfrak{K}})\vec{f}, \vec{g}\Big)_{\mathfrak{K}}\right| \le \\ \|V - W\|_{L^\infty} \left(\int_{\mathbb{R}} dt\ \|P^{\mathfrak{K}}_{\mathfrak{H}} e^{-itK[V]}\vec{f}\|^2\right)^{1/2} \left(\int_{\mathbb{R}} dt\ \|P^{\mathfrak{K}}_{\mathfrak{H}} e^{-itK[W]}\vec{g}\|^2\right)^{1/2},$$

$\vec{f}, \vec{g} \in \mathfrak{K}$. Applying (3.23) and (3.24) we obtain

$$\left|\Big((W_-(K[W], K[V]) - I_{\mathfrak{K}})\vec{f}, \vec{g}\Big)_{\mathfrak{K}}\right| \le \\ 2\pi|\Omega|\ L(\|V\|_{L^\infty})\ L(\|W\|_{L^\infty})\ \|V - W\|_{L^\infty}\ \|\vec{f}\|\|\vec{g}\|$$

for $\vec{f}, \vec{g} \in \mathfrak{K}$ which proves (3.27). □

4 Carrier density operator and continuity

4.1 Carrier density operator

In the following an operator $\varrho : \mathfrak{K} \longrightarrow \mathfrak{K}$ is called a density operator if ϱ is a bounded, non-negative, self-adjoint operator. The operator ϱ is called a steady state, if ϱ commutes with $K[V]$, see [20]. Thus any steady state ϱ is unitarily equivalent to a multiplication operator $\widehat{\rho}$ on the Hilbert space $L^2(\mathbb{R}, \mathbb{C}^2)$ induced by a density matrix $\rho(\cdot) \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$. In the following we assume that the function $\rho(\cdot)$ is fixed. This leads to a steady state of the form

$$\varrho[V] = \Phi[V]^{-1}\widehat{\rho}\ \Phi[V], \tag{4.1}$$

which depends on V. The reduced density operator $\varrho_{\mathfrak{H}}[V] \in \mathcal{B}(\mathfrak{H})$ is defined

$$\varrho_{\mathfrak{H}}[V] := P^{\mathfrak{K}}_{\mathfrak{H}} \varrho[V] \upharpoonright \mathfrak{H}.$$

Similarly, we define the reduced density operator $g_{\mathfrak{H}}(K[V]) \in \mathcal{B}(\mathfrak{H})$ by

$$g_{\mathfrak{H}}(K[V]) := P^{\mathfrak{K}}_{\mathfrak{H}} g(K[V]) \upharpoonright \mathfrak{H}.$$

Notice that by the Schrödinger assumption (2.1) one has

$$0 \le \varrho_{\mathfrak{H}}[V] \le g_{\mathfrak{H}}(K[V]). \tag{4.2}$$

Lemma 4.1 *Let the Schrödinger assumptions Q_1, Q_2 and Q_4 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then $g_{\mathfrak{H}}(K[V])$ is a trace class operator such that*

$$0 \le \mathrm{tr}(g_{\mathfrak{H}}(K[V])) \le \mathfrak{G}(\|V_-\|_{L^\infty})^2 \tag{4.3}$$

where $\mathfrak{G}(\cdot)$ is defined by (2.18).

Proof. Let $\{\psi_k\}_{k=1}^\infty$ be an orthonormal basis in $\mathfrak{H}$. By the spectral theorem

$$\sum_{k=1}^n (g_{\mathfrak{H}}(K[V])\psi_k, \psi_k) = \sum_{k=1}^n (g(K[V])\psi_k, \psi_k) = \int_{\mathbb{R}} d\lambda\, g(\lambda) \sum_{k=1}^n \frac{d}{d\lambda}(E_{K[V]}(\lambda)\psi_k, \psi_k)$$

where we have used that the spectral measure $E_{K[V]}(\cdot)$ of $K[V]$ is absolutely continuous with respect to the Lebesgue measure. Applying Lemma 3.10 we find

$$\int_{\mathbb{R}} d\lambda\, g(\lambda) \frac{d}{d\lambda}(E_{K[V]}(\lambda)\psi_k, \psi_k) = \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)(T[V](\lambda)\psi_k, T[V](\lambda)\psi_k), \quad k \in \mathbb{N},$$

which yields

$$\sum_{k=1}^n (g(K[V])\psi_k, \psi_k) = \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda) \sum_{k=1}^n (T[V](\lambda)\psi_k, T[V](\lambda)\psi_k).$$

Hence we obtain

$$\sum_{k=1}^n (g(K[V])\psi_k, \psi_k) \le \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}(T[V](\lambda)^* T[V](\lambda))$$

or

$$\sum_{k=1}^n (g(K[V])\psi_k, \psi_k) \le \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda) T[V](\lambda)^*) \tag{4.4}$$

By (3.13) we get

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda) T[V](\lambda)^*) = -\int d\lambda\, g(\lambda)\omega'[V](\lambda), \quad \lambda \in \mathbb{R},$$

which yields

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda) T[V](\lambda)^*) = -g(\lambda)\omega[V](\lambda)\big|_{\lambda=-\infty}^{\lambda=+\infty} + \int_{\mathbb{R}} d\lambda\, g'(\lambda)\omega[V](\lambda).$$

By Corollary 3.7 we have

$$-\omega[V](\lambda) \le 2 + \frac{1}{\pi}\sqrt{m|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+}$$

for $\lambda \in \mathbb{R}$. We note that the conditions (2.2) and (2.3) imply

$$\lim_{\lambda\to\infty} \sqrt{\lambda}\, g(\lambda) = 0.$$

Taking into account this property we obtain

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}\left(T[V](\lambda)T[V](\lambda)^*\right) = \int_{\mathbb{R}} d\lambda\, g'(\lambda)\omega[V](\lambda).$$

Since $g'(\lambda) \ge 0$ for $\lambda \le 0$ and $g'(\lambda) \le 0$ for $\lambda \ge 0$ as well as $\omega[V](\lambda) \le 0$, $\lambda \in \mathbb{R}$, we get

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}\left(T[V](\lambda)T[V](\lambda)^*\right) \le$$
$$\int_0^{+\infty} d\lambda\, g'(\lambda)\omega[V](\lambda) \le -\int_0^\infty d\lambda\, g'(\lambda)\left(2 + \frac{1}{\pi}\sqrt{m|\Omega|}\sqrt{\lambda + \|V_-\|_{L^\infty}}\right).$$

Integrating by parts we find

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}\left(T[V](\lambda)T[V](\lambda)^*\right) \le$$
$$g(0)\left(2 + \frac{1}{\pi}\sqrt{m|\Omega|}\sqrt{\|V_-\|_{L^\infty}}\right) + \frac{1}{2\pi}\sqrt{m|\Omega|}\int_0^\infty d\lambda\, \frac{g(\lambda)}{\sqrt{\lambda + \|V_-\|_{L^\infty}}}$$

which yields the estimate

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\, \mathrm{tr}_{\mathbb{C}^2}\left(T[V](\lambda)T[V](\lambda)^*\right) \le$$
$$\left(2g(0) + \frac{1}{2\pi}\sqrt{m|\Omega|}\int_0^\infty d\lambda\, \frac{g(\lambda)}{\sqrt{\lambda}}\right) + \frac{1}{\pi}\, g(0)\sqrt{m|\Omega|}\sqrt{\|V_-\|_{L^\infty}}.$$

From (4.4) we get the estimate

$$\sum_{k=1}^n (g(K[V])\psi_k, \psi_k) \le \left(2g(0) + \frac{1}{2\pi}\sqrt{m|\Omega|}\int_0^\infty d\lambda\, \frac{g(\lambda)}{\sqrt{\lambda}}\right) + \frac{1}{\pi}\, g(0)\sqrt{m|\Omega|}\sqrt{\|V_-\|_{L^\infty}}.$$

for $n \in \mathbb{N}$ which shows that $\sum_{k=1}^\infty (g(K[V])\psi_k, \psi_k)$ is finite for any orthonormal basis of $\mathfrak{H}$. Hence, the restriction $g_{\mathfrak{H}}(K[V])$ is a trace class operator. Using the notation (2.5), (2.6) and (2.18) we obtain (4.3). □

In the Hilbert space $\mathfrak{H}$ let us introduce the multiplication operator

$$(M(h)f)(x) := h(x)f(x), \quad f \in \mathrm{dom}(M(h)) = \mathfrak{H},$$

for functions $h \in L^\infty(\Omega)$. Since $\varrho_{\mathfrak{H}}[V]$ is a trace class operator the functional Ξ_ρ given by $h \longrightarrow \mathrm{tr}(\varrho_{\mathfrak{H}}[V]M(h))$ is well-defined on $L^\infty(\Omega)$. Moreover, setting $\nu_\rho(\Delta) := \Xi(\chi_\Delta)$ for

Borel subsets Δ of Ω one defines a Borel measure on Ω which is absolutely continuous with respect to the Lebesgue measure, cf. [20]. Its Radon-Nikodym derivative $u_\rho[V] \in L^1(\Omega)$ obeys the relation

$$\operatorname{tr}(\varrho[V]M(h)) = \int_a^b dx\; u_\rho[V](x)h(x), \quad h \in L^\infty(\Omega). \tag{4.5}$$

The function $u_\rho[V](\cdot)$ is not negative and is called the carrier density for a given potential $V \in L^\infty$. The operator $\mathcal{N}_\rho(V) : L^\infty_{\mathbb{R}}(\Omega) \longrightarrow L^1_{\mathbb{R}}(\Omega)$ defined by

$$\mathcal{N}_\rho(V) := u_\rho[V], \quad V \in \operatorname{dom}(\mathcal{N}_\rho) := L^\infty_{\mathbb{R}}(\Omega),$$

is called the carrier density operator.

Proposition 4.2 *Let the Schrödinger assumptions Q_1, Q_2 and Q_4 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$\|\mathcal{N}_\rho(V)\|_{L^1} \le \mathfrak{G}(\|V_-\|_{L^\infty})^2 \tag{4.6}$$

where $\mathfrak{G}(\cdot)$ is defined by (2.18).

Proof. From (4.5) one gets the estimate

$$\|u_\rho[V]\|_{L^1} \le \|\varrho_{\mathfrak{H}}[V]\|_{\mathcal{B}_1(\mathfrak{H})} = \operatorname{tr}(\varrho_{\mathfrak{H}}[V]).$$

Using (4.2) we obtain the estimate

$$\|u_\rho[V]\|_{L^1} \le \operatorname{tr}(g_{\mathfrak{H}}(K[V])).$$

Finally, taking into account Lemma 4.1 we verify (4.6). □

4.2 Lipschitz continuity

Further, it was shown that the carrier density operator is continuous, i.e., if $V_n \xrightarrow{L^\infty} V$, then $\mathcal{N}_\rho(V_n) \xrightarrow{L^1} \mathcal{N}_\rho(V)$. We are going to show that the continuity of the carrier density operator can be improved to bounded Lipschitz continuity, cf. Definition III.1.2 of [12].

At first let us prove the following lemma.

Lemma 4.3 *Let $g(\cdot)$ be non-negative, continuously differentiable even functions obeying* (2.2)*. The condition* (2.4) *is satisfied if and only if*

$$|g(\lambda) - g(\mu)| \le \mathfrak{c}\; \max\{g(\lambda), g(\mu)\}|\lambda - \mu| \tag{4.7}$$

holds for $\lambda, \mu \in \mathbb{R}$.

Proof. We assume $\lambda \le \mu$. Obviously, we have

$$g(\mu) - g(\lambda) = \int_\lambda^\mu g'(t)\; dt, \quad \lambda, \mu \in \mathbb{R},$$

which yields

$$|g(\mu) - g(\lambda)| \le \mathfrak{c} \int_\lambda^\mu g(t)\, dt$$

where we have used (2.4). Let $\lambda \in \mathbb{R}_+$. Since $g(\lambda)$, $\lambda \in \mathbb{R}_+$, is decreasing by (2.2) we find

$$|g(\mu) - g(\lambda)| \le \mathfrak{c} g(\lambda)(\mu - \lambda), \quad 0 \le \lambda \le \mu,$$

which yields (4.7). If $\lambda \le 0 \le \mu$, then

$$|g(\mu) - g(\lambda)| = |g(\mu) - g(-\lambda)| \le \mathfrak{c} \max\{g(\mu), g(-\lambda)\}|\mu + \lambda| \le \mathfrak{c} \max\{g(\mu), g(\lambda)\}|\mu - \lambda|$$

which also yields (4.7). The case $\lambda \le \mu \le 0$ follows from the case $0 \le \lambda \le \mu$.

Conversely, if (4.7) is satisfied, then tending μ to λ we obtain

$$|g'(\lambda)| \le \mathfrak{c} \max\{g(\lambda), g(\lambda)\} = \mathfrak{c}\, g(\lambda), \quad \lambda \in \mathbb{R},$$

which proves (2.4). □

Next we consider the operator $G[V] := \sqrt{g(K[V])} \restriction \mathfrak{H}$ acting from $\mathfrak{H}$ into $\mathfrak{K}$.

Lemma 4.4 *Let the Schrödinger assumptions Q_1, Q_2 and Q_4 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then $G[V] \in \mathcal{B}_2(\mathfrak{H}, \mathfrak{K})$ and*

$$\|G[V]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} \le \mathfrak{G}(\|V_-\|_{L^\infty}) \tag{4.8}$$

where $\mathfrak{G}(\cdot)$ is defined by (2.18). If $V, W \in L^\infty_{\mathbb{R}}(\Omega)$, then

$$\|G[V] - G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} \le \mathfrak{c}\, (\mathfrak{G}(\|V_-\|_{L^\infty}) + \mathfrak{G}(\|W_-\|_{L^\infty}))\, \|V - W\|_{L^\infty}. \tag{4.9}$$

Proof. By

$$\|G[V]\|^2_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} = \mathrm{tr}(G[V]^* G[V]) = \mathrm{tr}(g_{\mathfrak{H}}(K[V]))$$

and Lemma 4.1 one gets (4.8). Further, from (2.4) and Lemma 4.3 we obtain that

$$|g(\lambda) - g(\mu)| \le \mathfrak{c} \max\{g(\lambda), g(\mu)\}|\lambda - \mu| \le \mathfrak{c}\, (g(\lambda) + g(\mu))\, |\lambda - \mu|, \quad \lambda, \mu \in \mathbb{R},$$

which yields

$$\left|\sqrt{g(\lambda)} - \sqrt{g(\mu)}\right| \left(\sqrt{g(\lambda)} + \sqrt{g(\mu)}\right) \le \mathfrak{c} \left(\sqrt{g(\lambda)} + \sqrt{g(\mu)}\right)^2 |\lambda - \mu|. \quad \lambda, \mu \in \mathbb{R},$$

Therefore we get

$$\left|\sqrt{g(\lambda)} - \sqrt{g(\mu)}\right| \le \mathfrak{c} \left(\sqrt{g(\lambda)} + \sqrt{g(\mu)}\right) |\lambda - \mu|, \quad \lambda, \mu \in \mathbb{R}.$$

Hence, if we put

$$h(\lambda, \mu) := \frac{\sqrt{g(\lambda)} - \sqrt{g(\mu)}}{(\lambda - \mu)\left(\sqrt{g(\lambda)} + \sqrt{g(\mu)}\right)}, \quad \lambda, \mu \in \mathbb{R},$$

then $|h(\lambda, \mu)| \le \mathfrak{c}$, $\lambda, \mu \in \mathbb{R}$. Since the operators V and W act only on the subspace $\mathfrak{H}$ we get $\sqrt{G[V]}(V - W) + (V - W)\sqrt{G[W]} \in \mathcal{B}_2(\mathfrak{K})$. Applying the technique of double operator spectral integrals [5, 6, 7] we find the representation

$$\sqrt{g(K[V])} - \sqrt{g(K[W])} = \int_{\mathbb{R}} \int_{\mathbb{R}} h(\lambda, \mu)\, dE_{K[V]}(\lambda)\, \{G[V](V - W) + (V - W)G[W]^*\}\, dE_{K[W]}(\mu).$$

which yields $\sqrt{g(K[V])} - \sqrt{g(K[W])} \in \mathcal{B}_2(\mathfrak{K})$. Moreover, we find the estimate

$$\left\| \sqrt{g(K[V])} - \sqrt{g(K[W])} \right\|_{\mathcal{B}_2(\mathfrak{K})} \leq \mathfrak{c} \left\{ \|G[V]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} + \|G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} \right\} \|V - W\|_{\mathcal{B}(\mathfrak{H})}.$$

Since $G[V] := \sqrt{g(K[V])} \restriction \mathfrak{H}$ and $G[W] := \sqrt{g(K[W])} \restriction \mathfrak{H}$ we obtain

$$\|G[V] - G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} \leq \mathfrak{c} \left\{ \|G[V]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} + \|G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})} \right\} \|V - W\|_{\mathcal{B}(\mathfrak{H})}.$$

Using (4.8) we finally get (4.9). □

Proposition 4.5 *Let the Schrödinger assumptions Q_1, Q_2 and Q_4 be satisfied. If m has a finite total variation and $V, W \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$\|\mathcal{N}_\rho(V) - \mathcal{N}_\rho(W)\|_{L^1} \leq \mathfrak{L}(\|V\|_{L^\infty}, \|W\|_{L^\infty}) \, \|V - W\|_{L^\infty} \tag{4.10}$$

where $\mathfrak{L}(\cdot, \cdot)$ is given by (2.19).

Proof. By (4.5) we get

$$\int_a^b dx \, (u_\rho[V](x) - u_\rho[W](x))h(x) = \operatorname{tr}((\varrho_{\mathfrak{H}}[V] - \varrho_{\mathfrak{H}}[W])M(h))$$

for any $h \in L^\infty(\Omega)$ where $\varrho[V]$ and $\varrho[W]$ are defined in accordance with (4.1). By (3.26) we have

$$\varrho[V] = W_-(K[V], K_0) \, F^* \, \widehat{\rho} \, F \, W_-(K[V], K_0)^*$$

and

$$\varrho[W] = W_-(K[W], K_0) \, F^* \, \widehat{\rho} \, F \, W_-(K[W], K_0)^*$$

The wave operators $W_-(K[V], K_0)$ and $W_-(K[W], K_0)$ exist and are complete; consequently, the wave operator $W_-(K[W], K[V])$ exists and is complete. Moreover, the representation

$$W_-(K[W], K_0) = W_-(K[W], K[V])W_-(K[V], K_0)$$

holds. For brevity we set $W_-[W, V] := W_-(K[W], K[V])$ as well as $W_-[W] := W_-(K[W], K_0)$ and $W_-[V] := W_-(K[V], K_0)$. Let us introduce the matrix valued function

$$\rho_0(\lambda) := g(\lambda)^{-1}\rho(\lambda), \quad \lambda \in \mathbb{R}.$$

By assumption Q_4 one has

$$0 \leq \rho_0(\lambda) \leq I_{\mathbb{C}^2}, \quad \lambda \in \mathbb{R}.$$

Using this notation we find the representation

$$\begin{aligned}\varrho_{\mathfrak{H}}[V] - \varrho_{\mathfrak{H}}[W] &= G[V]^*\varrho_0[V]G[V] - G[W]^*\varrho_0[W]G[W] = \\ &(G[V]^* - G[W]^*) \, \varrho_0[V]G[V] + G[W]^*\varrho_0[V] \, (G[V] - G[W]) + \\ &G[W] \, (\varrho_0[V] - \varrho_0[W]) \, G[W].\end{aligned}$$

Hence, we get the estimate

$$\begin{aligned}&\|\varrho_{\mathfrak{H}}[V]-\varrho_{\mathfrak{H}}[W]\|_{\mathcal{B}_1(\mathfrak{H},\mathfrak{K})}\le\\ &\quad\left\{\|G[V]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})}+\|G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})}\right\}\|G[V]-G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})}+\\ &\quad\|G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})}\;\|G[W]\|_{\mathcal{B}_2(\mathfrak{H},\mathfrak{K})}\;\|\varrho_0[V]-\varrho_0[W]\|_{\mathcal{B}(\mathfrak{H})}.\end{aligned}$$

By the representation

$$\begin{aligned}&\varrho_0[V]-\varrho_0[W]=\varrho_0[V]-W_-[W,V]\varrho_0[V]W_-[W,V]^*=\\ &\quad(I_{\mathfrak{K}}-W_-[W,V])\varrho_0[V]W_-[W,V]^*+\varrho_0[V](I_{\mathfrak{K}}-W_-[W,V]^*)\end{aligned}$$

and Lemma 3.12 we obtain the estimate

$$\|\varrho_0[V]-\varrho_0[W]\|_{\mathcal{B}(\mathfrak{K})}\le 4\pi\;|\Omega|\;L[V]\,L[W]\;\|V-W\|_{L^\infty}.$$

By Lemma 4.4 we get

$$\begin{aligned}&\|\varrho_{\mathfrak{H}}[V]-\varrho_{\mathfrak{H}}[W]\|_{\mathcal{B}_1(\mathfrak{H},\mathfrak{K})}\le\Big(\mathfrak{c}\;\left(\mathfrak{G}(\|V\|_{L^\infty})+\mathfrak{G}(\|W\|_{L^\infty})\right)^2+\\ &\quad 4\pi\;|\Omega|\;L(\|V\|_{L^\infty})\;L(\|W\|_{L^\infty})\;\mathfrak{G}(\|V\|_{L^\infty})\;\mathfrak{G}(\|W\|_{L^\infty})\Big)\|V-W\|_{L^\infty}\end{aligned}$$

which proves (4.10). Taking into account the definition (2.19) we verify(4.10). □

5 Dissipative Schrödinger-Poisson system

5.1 Rigorous definition

By $W^{1,2}_0(\Omega)$ we denote the subspace of $W^{1,2}(\Omega)$ given by $W^{1,2}_0(\Omega):=\{f\in W^{1,2}(\Omega): f(a)=f(b)=0\}$. Its dual space with respect to the scalar product $<\cdot,\cdot>$ of $L^2(\Omega)$ is denoted by $W^{-1,2}_0(\Omega)$.

At first we will give a rigorous definition of Poisson's equation and afterwards define what we will call a solution of the dissipative Schrödinger Poisson system. We define the Poisson operator $\mathcal{P}: W^{1,2}_{\mathbb{R}}(\Omega)\longrightarrow W^{-1,2}_{0,\mathbb{R}}(\Omega)$ as usual by

$$<\mathcal{P}\upsilon,\varsigma>=\int_a^b dx\;\epsilon\;\frac{d\upsilon}{dx}\frac{d\varsigma}{dx},\qquad \upsilon\in W^{1,2}_{\mathbb{R}}(\Omega),\;\varsigma\in W^{1,2}_{0,\mathbb{R}}(\Omega).$$

Further, we set $\mathcal{P}_0:=\mathcal{P}\restriction W^{1,2}_{0,\mathbb{R}}(\Omega)$. The operators $\mathcal{P}$ and $\mathcal{P}_0$ are linear and bounded. We have

$$|<\mathcal{P}\upsilon,\varsigma>|\le\|\epsilon\|_{L^\infty}\|\upsilon\|_{W^{1,2}}\|\varsigma\|_{W^{1,2}_0}.$$

Hence $\mathcal{P}$ is continuous. Furthermore, one has the estimate

$$\|\varphi\|_{W^{1,2}_0}\le\sqrt{1+|\Omega|}\;\|\varphi'\|_{L^2},\quad \varphi\in W^{1,2}_0(\Omega).$$

Thus, we get by (5.1)

$$\|\varphi\|^2_{W^{1,2}_0}\le\|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}<\mathcal{P}_0\varphi,\varphi>,\quad \varphi\in W^{1,2}_0(\Omega).$$

By the Lax-Milgram lemma the inverse operator $\mathcal{P}_0^{-1}$ exists and its norm does not exceed $\|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}$, i.e.

$$\|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2},W_0^{1,2})} \le \|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}\,. \tag{5.1}$$

Definition 5.1 Let $u^\pm \in L^1$. We say that $\varphi \in W^{1,2}_{\mathbb{R}}$ satisfies Poisson's equation with boundary conditions $\varphi(a) = \varphi_a$ and $\varphi(b) = \varphi_b$ if $\zeta := \varphi - \widehat{\varphi} \in W_0^{1,2}(\Omega)$ and the equation

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

is fulfilled, where $\widehat{\varphi}$ is defined by (2.7).

Definition 5.2 We say that $\varphi \in W^{1,2}_{\mathbb{R}}(\Omega)$ is a solution of the dissipative Schrödinger-Poisson system if

1. the carrier densities $u^\pm \in L^1(\Omega)$ are given by $u^\pm = \mathcal{N}^\pm_{\rho^\pm}(V_0^\pm \pm \widehat{\varphi} \pm E_\infty\zeta)$, $\zeta := \varphi - \widehat{\varphi}$, and

2. φ satisfies the Poisson equation.

5.2 Existence of solutions and estimates

Let us introduce the non-linear mappings $\mathcal{Q} : L^\infty_{\mathbb{R}}(\Omega) \longrightarrow W^{1,2}_{0,\mathbb{R}}(\Omega)$,

$$\mathcal{Q}(\psi) := \mathcal{P}_0^{-1}\Big(C + E_1\mathcal{N}^+_{\rho^+}(V_0^+ + \widehat{\varphi} + \psi) - E_1\mathcal{N}^-_{\rho^-}(V_0^- - \widehat{\varphi} - \psi)\Big)\,, \tag{5.2}$$

$\psi \in \mathrm{dom}(\mathcal{Q}) = L^\infty_{\mathbb{R}}(\Omega)$, and $\mathcal{Q}_\infty : L^\infty_{\mathbb{R}}(\Omega) \longrightarrow L^\infty_{\mathbb{R}}(\Omega)$,

$$\mathcal{Q}_\infty(\psi) = E_\infty \mathcal{Q}(\psi),$$

$\psi \in \mathrm{dom}(\mathcal{Q}_\infty) = L^\infty_{\mathbb{R}}(\Omega)$. It was shown in [2] that the dissipative Schrödinger-Poisson system admits a solution if and only if $\mathcal{Q}_\infty$ admits a fixed point. Moreover, if $\zeta_\infty \in L^\infty_{\mathbb{R}}(\Omega)$ is a fixed point, i.e., $\mathcal{Q}_\infty(\zeta_\infty) = \zeta_\infty$, then $\varphi := \widehat{\varphi} + \mathcal{Q}(\zeta_\infty)$ is a solution of the dissipative Schrödinger-Poisson system. If $\zeta_\infty \in L^\infty_{\mathbb{R}}(\Omega)$ is a fixed point, i.e. $\zeta_\infty = \mathcal{Q}_\infty(\zeta_\infty)$, then one has the estimate

$$\|\zeta_\infty\|_{L^\infty} = \|\mathcal{Q}_\infty(\zeta_\infty)\|_{L^\infty(\Omega)} \le \varepsilon_1\|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2},W_0^{1,2})} \times \Big(\|C\|_{W_0^{-1,2}} + \varepsilon_1\|\mathcal{N}^+_{\rho^+}(V_0^+ + \widehat{\varphi} + \zeta_\infty)\|_{L^1} + \varepsilon_1\|\mathcal{N}^-_{\rho^-}(V_0^- - \widehat{\varphi} - \zeta_\infty)\|_{L^1}\Big)\,.$$

Taking into account (5.1) we obtain

$$\|\zeta_\infty\|_{L^\infty} = \|\mathcal{Q}_\infty(\zeta_\infty)\|_{L^\infty(\Omega)} \le \varepsilon_1\|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|} \times \Big(\|C\|_{W_0^{-1,2}} + \varepsilon_1\|\mathcal{N}^+_{\rho^+}(V_0^+ + \widehat{\varphi} + \zeta_\infty)\|_{L^1} + \varepsilon_1\|\mathcal{N}^-_{\rho^-}(V_0^- - \widehat{\varphi} - \zeta_\infty)\|_{L^1}\Big)\,. \tag{5.3}$$

Applying Proposition 4.2 we find

$$\|\mathcal{N}^+_{\rho^+}(V_0^+ + \widehat{\varphi} + \zeta_\infty)\|_{L^1} \le B_0^+ + B_1^+\sqrt{\|(V_0^+ + \widehat{\varphi} + \zeta_\infty)_-\|_{L^\infty}}$$

which yields

$$\|\mathcal{N}^+_{\rho^+}(V_0^+ + \widehat{\varphi} + \zeta_\infty)\|_{L^1} \le B_0^+ + B_1^+\sqrt{\|V_0^+ + \widehat{\varphi}\|_{L^\infty}} + B_1^+\sqrt{\|\zeta_\infty\|_{L^\infty}}.$$

Similarly, we obtain

$$\|\mathcal{N}^-_{\rho^-}(V_0^- - \widehat{\varphi} - \zeta_\infty)\|_{L^1} \le B_0^- + B_1^-\sqrt{\|V_0^- - \widehat{\varphi}\|_{L^\infty}} + B_1^-\sqrt{\|\zeta_\infty\|_{L^\infty}}.$$

Inserting these estimates into (5.3) we find

$$\|\zeta_\infty\|_{L^\infty} \le D_0 + D_1\sqrt{\|\zeta_\infty\|_{L^\infty}} \tag{5.4}$$

where D_0 and D_1 are given by (2.8) and (2.9). From (5.4) we obtain the estimate

$$\|\zeta_\infty\|_{L^\infty} \le r_0 \tag{5.5}$$

for any fixed point of the map $\mathcal{Q}_\infty$ where r_0 is defined by (2.10). So the following theorem is proven:

Theorem 5.3 *[3, Theorem 4.8] If the Schrödinger and Poisson assumptions are satisfied, then the dissipative Schrödinger-Poisson system always admits a solution. Moreover, for any solution $\varphi \in W^{1,2}_{\mathbb{R}}(\Omega)$ the estimate $\|\varphi_\infty - \widehat{\varphi}\|_{L^\infty} \le r_0$ holds.*

We note that the radius r_0 depends only on the Schrödinger and Poisson data. Therefore, if the Schrödinger and Poisson data are fixed, then the radius r_0 is fixed.

However, Theorem (5.3) does not answer the question whether this solution is unique.

5.3 Uniqueness

Now we are going to give conditions under which the solution of the dissipative Schrödinger-Poisson system is unique.

Theorem 5.4 *Let the Schrödinger and Poisson assumptions be satisfied. If $m^\pm$ have finite total variations and the condition $\mathfrak{U} < 1$ is valid, where $\mathfrak{U}$ is given by (2.21), then the dissipative Schrödinger-Poisson system admits only one solution.*

Proof. Let ζ_∞ and ζ'_∞ two fixed points of $\mathcal{Q}_\infty$. From (5.2) we get the representation

$$\zeta_\infty - \zeta'_\infty = E_\infty \mathcal{P}_0^{-1} E_1 \left\{ \left(\mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+)\right) - \left(\mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-)\right)\right\}$$

where

$$V^+ := V_0^+ + \widehat{\varphi} + \zeta_\infty \quad \text{and} \quad W^+ := V_0^+ + \widehat{\varphi} + \zeta'_\infty$$

and

$$V^- := V_0^- + \widehat{\varphi} + \zeta_\infty \quad \text{and} \quad W^- := V_0^- + \widehat{\varphi} + \zeta'_\infty.$$

Hence we find

$$\begin{aligned} \|\zeta_\infty - \zeta'_\infty\|_{L^\infty} &\le \varepsilon_1^2 \|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2}, W_0^{1,2})} \times \\ &\times \left\{ \left\|\mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+)\right\|_{L^1} + \left\|\mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-)\right\|_{L^1} \right\} \end{aligned}$$

Using (5.1) we obtain

$$\begin{aligned}\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} &\le \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1+|\Omega|} \times \\ &\times \left\{ \left\| \mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+) \right\|_{L^1} + \left\| \mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-) \right\|_{L^1} \right\}\end{aligned}$$

Applying Proposition 4.5 we get

$$\begin{aligned}\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} &\le \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1+|\Omega|} \times \\ &\times \left\{ \mathfrak{L}^+(\|V^+\|_{L^\infty}, \|W^+\|_{L^\infty}) + \mathfrak{L}^-(\|V^-\|_{L^\infty}, \|W^-\|_{L^\infty}) \right\} \ \|\zeta_\infty - \zeta'_\infty\|_{L^\infty}\end{aligned}$$

We have

$$\|V^+\|_{L^\infty} \le \|V_0^+ + \widehat{\varphi}\|_{L^\infty} + \|\zeta_\infty\|_{L^\infty} \le r_1^+$$

where we have used the estimate (5.5) and r_1^+ is defined by (2.11). Similarly we prove that

$$\|W^+\|_{L^\infty} \le r_1^+$$

and

$$\|V^-\|_{L^\infty} \le r_1^- \quad \text{and} \quad \|W^-\|_{L^\infty} \le r_1^-$$

where we have used the definitions (2.11). Since

$$\mathfrak{L}^\pm(\|V^\pm\|_{L^\infty}, \|W^\pm\|_{L^\infty}) \le \mathfrak{L}^\pm(r_1^\pm, r_1^\pm)$$

we obtain

$$\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} \le \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1+|\Omega|}\ \mathfrak{L}\ \|\zeta_\infty - \zeta'_\infty\|_{L^\infty}$$

where $\mathfrak{L}$ is given by (2.20). Hence, if condition (2.21) is satisfied, then $\|\zeta_\infty - \zeta'_\infty\|_{L^\infty}$ has to be zero which proves the uniqueness. □

5.4 Uniqueness and shrinking

Our next aim is to show that a dissipative Schrödinger-Poisson system admits always a solution if $|\Omega|$ is small. To this end we introduce the following

Definition 5.5 Let $\Omega' \subseteq \Omega$ and let $\mathfrak{D} = \mathfrak{Q} \cap \mathfrak{P}$ be Schrödinger-Poisson data of the device Ω. We say $\mathfrak{D}' := \mathfrak{Q}' \cap \mathfrak{P}'$ are shrunken Schrödinger-Poisson data of $\mathfrak{D}$ if

$$\mathfrak{Q}' := \{m^\pm \restriction \Omega', \kappa_a^\pm, \kappa_b^\pm, V_0^\pm \restriction \Omega', \rho^\pm\} \quad \text{and} \quad \mathfrak{P}' := \{C \restriction \Omega', \epsilon \restriction \Omega', \varphi_a, \varphi_b\}.$$

The corresponding dissipative Schrödinger-Poisson system is called a shrunken dissipative Schrödinger-Poisson system.

Definition 5.5 means that we leave unchanged the boundary coefficients $\kappa_a^\pm, \kappa_b^\pm$ of the dissipative Schrödinger operators and the density matrices as well as the boundary values of the inhomogeneous Poisson equation but we restrict the effective masses $m^\pm$, the external potentials $V_0^\pm$, the doping profile C and dielectric permittivity ϵ to the subinterval Ω'.

We note that the quantities (2.5)-(2.21) except (2.15) in fact depend on the interval Ω. We express this fact by adding in notation the term $[\Omega]$, for instance, $B_0^\pm[\Omega]$, $B_1^\pm[\Omega]$, $\widehat{\varphi}[\Omega](x), \ldots, \mathfrak{U}[\Omega]$.

Theorem 5.6 *Let the Schrödinger and Poisson assumptions be satisfied and let $m^\pm$ have finite total variations. A shrunken dissipative Schrödinger-Poisson system admits a unique solution if $|\Omega'|$, $\Omega' \subseteq \Omega$, is sufficiently small.*

Proof. By Theorem 5.4 it is sufficiently to show that $\limsup_{|\Omega'|\to 0} \mathfrak{U}[\Omega'] = 0$. Since

$$\underline{m}^\pm \le m^\pm(x) \le \overline{m}^\pm, \quad x \in \Omega',$$

we obtain from (2.5) and (2.6) that

$$\lim_{|\Omega'|\to 0} B_0^\pm[\Omega'] = 2g^\pm(0) \quad \text{and} \quad \lim_{|\Omega'|\to 0} B_1^\pm[\Omega'] = 0.$$

Since

$$\|\widehat{\varphi}[\Omega']\|_{L^\infty(\Omega')} \le \max\{|\varphi_a|, |\varphi_b|\}$$

we find

$$\|V_0^\pm \restriction \Omega' + \widehat{\varphi}[\Omega']\|_{L^\infty(\Omega')} \le \|V_0^\pm\|_{L^\infty(\Omega)} + \max\{|\varphi_a|, |\varphi_b|\}.$$

Taking into account this estimate and using $\|C \restriction \Omega'\|_{W^{-1,2}} \le \|C\|_{W^{-1,2}}$, $\varepsilon_1[\Omega'] \le \sqrt{|\Omega'|}$ we obtain

$$\lim_{|\Omega'|\to 0} D_0^\pm[\Omega'] = 0 \quad \text{and} \quad \lim_{|\Omega'|\to 0} D_1^\pm[\Omega'] = 0$$

which yields

$$\lim_{|\Omega'|\to 0} r_0^\pm[\Omega'] = 0$$

and

$$\limsup_{|\Omega'|\to 0} r_1^\pm[\Omega'] \le \|V_0^\pm\|_{L^\infty(\Omega)} + \max\{|\varphi_a|, |\varphi_b|\}. \tag{5.6}$$

Since $\bigvee_{a'}^{b'} \left(\frac{1}{m^\pm} \restriction \Omega'\right) \le \bigvee_a^b \frac{1}{m^\pm}$, $\Omega' = (a', b')$, we get

$$\limsup_{|\Omega'|\to 0} \mathfrak{M}^\pm[\Omega'] \le \mathfrak{M}^\pm[\Omega].$$

Further, we have

$$\limsup_{|\Omega'|\to 0} R_j^\pm(r_1^\pm[\Omega']) \le \mathfrak{M}^\pm[\Omega] \left(1 + |\kappa_j^\pm| \sqrt{\frac{2}{\underline{m}^\pm}}\right), \quad j = a, b.$$

using Lemma 3.1, (2.16) and (5.6) one gets

$$\lim_{|\Omega'|\to 0} \{2r_1^\pm[\Omega'] + 2\gamma_0[\Omega']\}|\Omega| = 4\mathfrak{q}^\pm \overline{m}^\pm$$

which yields

$$\limsup_{|\Omega'|\to 0} R_j^\pm(2r_1^\pm[\Omega'] + 2\gamma_0[\Omega']) \le$$
$$\mathfrak{M}^\pm[\Omega] \left(1 + |\kappa_j^\pm| \sqrt{\frac{2}{\underline{m}^\pm}}\right) \exp\left\{4\mathfrak{q}^\pm \overline{m}^\pm (\mathfrak{M}^\pm[\Omega])^2 \sqrt{\frac{2}{\underline{m}^\pm}}\right\}, \quad j = a, b.$$

Using that we obtain

$$\limsup_{|\Omega'|\to 0} L^{\pm}(r^{\pm}[\Omega']) \le \mathfrak{M}^{\pm}[\Omega] \exp\left\{4\mathfrak{q}^{\pm}\overline{m}^{\pm}(\mathfrak{M}^{\pm}[\Omega])^2\sqrt{\frac{2}{\underline{m}^{\pm}}}\right\} \times$$
$$\times \left\{\frac{1}{(\alpha_a^{\pm})^2}\left(1+|\kappa_a^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right) + \frac{1}{(\alpha_b^{\pm})^2}\left(1+|\kappa_b^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right)\right\}.$$

By

$$\lim_{|\Omega'|\to 0} \mathfrak{G}^{\pm}(r_1^{\pm}[\Omega']) = \sqrt{2g^{\pm}(0)}.$$

we have

$$\lim_{|\Omega'|\to 0} \mathfrak{L}^{\pm}(r^{\pm}[\Omega'], r^{\pm}[\Omega']) = 8\mathfrak{c}^{\pm}g^{\pm}(0).$$

Therefore, we finally obtain

$$\lim_{|\Omega'|\to 0} \mathfrak{L}[\Omega'] = 8(\mathfrak{c}^{+}g^{+}(0) + \mathfrak{c}^{-}g^{-}(0))$$

where

$$\mathfrak{L}[\Omega'] := \mathfrak{L}^{+}(r_1^{+}[\Omega'], r_1^{+}[\Omega']) + \mathfrak{L}^{-}(r_1^{-}[\Omega'], r_1^{-}[\Omega']).$$

Since $\lim_{|\Omega'|\to 0} \varepsilon_1[\Omega'] = 0$ we find $\lim_{|\Omega'|\to 0} \mathfrak{U}[\Omega'] = 0$ where

$$\mathfrak{U}[\Omega'] := \varepsilon_1^2[\Omega']\sqrt{1+|\Omega'|}\mathfrak{L}[\Omega'].$$

Applying Theorem 5.4 we see that for sufficiently small domains $\Omega' \subseteq \Omega$ the solution of the dissipative Schrödinger-Poisson system is unique. □

6 Remarks

Let us comment the results.

1. Comparing the existence Theorem 5.3 with Theorem 4.8 of [2] one observes that Theorem 5.3 proves the existence under weaker assumptions. In particular, the Schrödinger assumption Q_4 is weaker than Assumption 4.2 $A_4^{\pm}$ of [2]. The assumption Q_4 is close to a necessary condition. However, both proofs use the Schauder fixed point theorem.

2. In contrast to [2] the proof of the crucial estimate (4.6) of Proposition 4.2, cf. Theorem 3.1 of [2], is now based on the phase shift and its asymptotic behaviour at $-\infty$ and $+\infty$.

3. The asymptotic properties of the phase shift are established by a detailed investigation in [26].

4. The uniqueness proof is essentially based on the Lipschitz continuity of the carrier density operator, cf. Proposition 4.5 which heavily rests on the Lipschitz continuity of the Lax-Phillips wave operators, cf. Section 3.7. This continuity relies on Kato's theory of smooth operators, cf. [22, 23].

5. The results of the paper, in particular the results of Section 5.4, suggest the possibility that the solution of the dissipative hybrid model, cf. [4], is also unique provided the quantum zone is sufficiently small.

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