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A quantum transmitting Schrödinger-Poisson system

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Abstract

We consider a stationary Schrödinger-Poisson system on a bounded interval of the real axis. The Schrödinger operator is defined on the bounded domain with transparent boundary conditions. This allows to model a non-zero current flow trough the boundary of the interval. We prove that the system always admits a solution and give explicit a priori estimates for the solutions.

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1 Introduction

The nonlinear interactions between an electric field and charged carriers, electrons and holes within a semiconductor device, are commonly modeled by a nonlinear Poisson equation, see [G] and references cited there. In the 1D case, which we consider here, the Poisson equation reads

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}\varphi(x) = q\left(C(x) + \mathcal{N}_+(\varphi)(x) - \mathcal{N}_-(\varphi)(x)\right), \quad x \in (a,b), \tag{1.1}$$

where $(a,b) \subset \mathbb{R}$ is the bounded spatial domain occupied by the semiconductor device, q denotes the magnitude of the elementary charge, C is the density of ionized dopants in the semiconductor device, $\epsilon > 0$ denotes the dielectric permittivity function and φ the electrostatic potential. $\mathcal{N}_\pm(\varphi)$ are the (in general nonlinear) operators which associate a density of positive and negative charge (holes and electrons) to an electrostatic potential. Therefore $\mathcal{N}_\pm(\varphi)$ are called the carrier density operators. The boundary conditions for (1.1) are usually of mixed type, see [G], allowing for Ohmic (metal) contacts on some parts of the boundary while other parts of the boundary of the device are insulated.

Depending on the underlying physical model, the operators $\mathcal{N}_\pm(\varphi)$ are set up in different ways. In this article we are interested in the case, where the carrier density operators are determined by Schrödinger-type operators of the form

$$H^\pm(v) = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m_\pm}\frac{d}{dx} + v, \tag{1.2}$$

on the interval (a,b); $\hbar$ is the reduced Planck constant, and $m_\pm > 0$ are the position dependent effective masses of electron and holes, respectively. The operators $H^\pm(v)$ are usually regarded with homogeneous, selfadjoint boundary conditions, including mixed ones, on the boundary of the device domain. Let us denote the operator $H^\pm(v)$ with some selfadjoint boundary conditions by $H^\pm_{sa}(v)$. If $f_\pm$ are equilibrium distribution functions such that the operators

$$\varrho_\pm(v) := f_\pm(H^\pm_{sa}(v)),$$

are selfadjoint, non-negative, and of trace class, i.e. density matrices, for all admissible potentials v, then the densities $\mathcal{N}^{sa}_\pm(\varphi)$ are given by the Radon-Nikodym derivative of the absolutely continuous measures (with respect to the Lebesgue measure)

$$\int_\omega dx\,\mathcal{N}^{sa}_\pm(\varphi)(x) = \mathbb{E}_{\varrho_\pm(v)}(\omega) := \operatorname{tr}\left(\varrho_\pm(v_\pm)M(\chi_\omega)\right),$$

where $M(\chi_\omega)$ denotes the multiplication operator by the indicator function χ_ω of a set $\omega \subset (a,b)$, and $v_\pm$ are given by

$$v_\pm = w_\pm \pm q\varphi,$$

with prescribed potentials $w_\pm$. Schrödinger-Poisson systems on bounded spatial domains in which the carrier density operators are described in the above form, have been intensively studied, see [CZF, N2, KR].

The selfadjointness of the operators $H^\pm_{sa}(v)$ reflects that the corresponding quantum systems of positively and negatively charged carriers are closed. Hence, there is no flow of carriers through the boundary of the device. However, the operation of semiconductor devices is characterized by the flow of electrons and holes. Therefore one passes to open quantum systems. One way to do so is to regard the Schrödinger operator with certain non-selfadjoint boundary conditions thus, allowing a flow through the boundary, see [F2, KL, BDM, KR, KNR3]. Since the current is constituted by scattering states, on has to find boundary conditions for the operators $H^\pm(v)$ which allow a particle to scatter through the device domain. Such boundary conditions are called transparent boundary conditions, see [F2, KL, BDM]. They make the operators $H^\pm(v)$ essentially non-selfadjoint. Thus, it is not clear how to determine the carrier and current densities, which are well defined only for closed quantum systems, see [LL].

In [KNR1] the following dissipative boundary conditions have been suggested

$$\frac{\hbar}{2m(a)}f'(a) = -i\alpha_a^2 f(a) \qquad \text{and} \qquad \frac{\hbar}{2m(b)}f'(b) = i\alpha_b^2 f(b),$$

where $\alpha_a, \alpha_b \in \mathbb{R}$, $\alpha_a, \alpha_b > 0$. Let us denote the operator with these boundary conditions by $H^\pm_{dis}(v)$. The operators $H^\pm_{dis}(v)$ with the above boundary conditions are essentially non-selfadjoint. But these operators are maximal dissipative, which allows an embedding of the open quantum system described by the non-selfadjoint operators $H^\pm_{dis}(v)$ into a larger closed quantum system described by the selfadjoint dilation operator, denoted by $K^\pm_{dis}(v)$, which exists for every maximal dissipative operator [FN]. Using the selfadjoint dilations $K^\pm_{dis}(v)$ the carrier density operators can be defined in a similar way as described above for $H^\pm_{sa}(v)$ (see [KNR1, KNR2, BN] for details), which leads to the so-called dissipative Schrödinger-Poisson system. This system has been investigated in [BKNR].

Another ansatz to introduce carrier and current densities for an open quantum system on an interval was made by Ben Abdallah, Degond, and Markowich, see [BDM]. Their approach is to extend the effective masses $m^\pm$ and the potential $v_\pm$ to the whole real line by setting them constant outside the interval (a, b). This leads to selfadjoint operators $K^\pm_{v_\pm}$ on $\mathcal{K} := \mathsf{L}^2(\mathbb{R})$ called Buslaev-Fomin operators. The boundary conditions for the non-selfadjoint Schrödinger operator on the bounded spatial domain (a, b) are obtained by a projection onto (a, b), see also [F2, F1, KL]. The carrier and current densities for the open system are defined in terms of the generalized eigenfunctions corresponding to the Buslaev-Fomin operators $K^\pm_{v_\pm}$, see [BDM] for details. The existence of a solution for a very special case of this model, more precisely $\mathcal{N}^- \equiv 0$, $C \equiv 0$, $\epsilon \equiv 1$ and $m_\pm \equiv 1$, was proved in [BDM]. But the mathematical techniques used there to prove the existence do not apply in the general case which we consider here. In this paper we will show that the model used by Ben Abdallah, Degond and Markowich in [BDM] also allows an interpretation in terms of a family of dissipative operators the so-called *quantum transmitting boundary operator* *family*, or QTB family, which leads to the quantum transmitting Schrödinger-Poisson system. We will show that this Schrödinger-Poisson system always admits a solution and give some a priori estimates for this solution. The quantum transmitting Schrödinger-Poisson system is closely related to the dissipative Schrödinger-Poisson system considered in [BKNR]. We will point out the relation between the two systems throughout this paper. In particular we show that the dissipative Schrödinger-Poisson system and the quantum transmitting Schrödinger-Poisson system coincide, modulo a unitary transformation, for fixed energy.

The paper is organized as follows: In Section 2 we define the Buslaev-Fomin operator, derive the QTB family and show the relation between the QTB family and the Buslaev-Fomin operator. In Section 3 we calculate the generalized eigenfunctions of the Buslaev-Fomin operator, define the corresponding Fourier transform and show that the eigenfunctions can be expressed in terms of the QTB family. Section 4 is devoted to the scattering matrix of the Buslaev-Fomin operator. In Section 5 we define the carrier and current density for the open quantum system related to the QTB family and show that these densities are completely characterized by the QTB family. Section 6 is devoted to the carrier density operator of the QTB family and its properties. In Section 7 we investigate the Schrödinger-Poisson system with the carrier density operator of the QTB family.

2 Buslaev-Fomin operator and QTB family

Let us first introduce some notation which will be used throughout this paper: $\mathbb{N}$, $\mathbb{R}$ and $\mathbb{C}$ denote the natural, the real and the complex numbers, respectively; $\mathbb{C}_+ := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) > 0\}$, $\mathbb{C}_- := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) < 0\}$; if $z \in \mathbb{C}$, then $\overline{z}$ denotes the complex conjugate number. $\mathsf{L}^p(\Omega, X, \nu)$, $1 \le p < \infty$ is the space of ν-measurable, p-integrable functions with values in the Banach space X; $\mathsf{L}^\infty(\Omega, X, \nu)$ is the corresponding space of essentially bounded functions. If $\Omega \subseteq \mathbb{R}$ is a domain, ν the Lebesgue measure, and $X = \mathbb{C}$, then we write short $\mathsf{L}^p(\Omega)$, $1 \le p \le \infty$. Furthermore we denote by $\mathsf{W}^{1,2}(\Omega)$ the usual Sobolev space of complex-valued functions on Ω, by $\mathsf{C}(\Omega)$ the space of continuous complex-valued functions on Ω and by $\mathsf{C}^{\mathsf{b}}(\Omega)$ the space of continuous bounded complex-valued functions on Ω equipped with the supremum norm. If $\Omega = (a, b)$ we will abbreviate L^p, $\mathsf{W}^{1,2}$, ... for $\mathsf{L}^p(\Omega)$, $\mathsf{W}^{1,2}(\Omega)$, ...; moreover, we introduce $\mathcal{K} := \mathsf{L}^2(\mathbb{R})$ and $\mathcal{H} := \mathsf{L}^2 = \mathsf{L}^2(a, b)$. The real part of a function space will be indexed by $\mathbb{R}$, i.e. the real part of L^p, $\mathsf{W}^{1,2}$, ... will be denoted by $\mathsf{L}^p_{\mathbb{R}}$, $\mathsf{W}^{1,2}_{\mathbb{R}}$, ... For Banach spaces X and Y, we denote by $\mathfrak{B}(X, Y)$ the space of all linear, continuous operators from X into Y; if $X = Y$ we write $\mathfrak{B}(X)$ and $\mathbb{I}_X \in \mathfrak{B}(X)$ for the identity operator. If X, Y are Hilbert spaces, then $\mathfrak{B}_1(X, Y)$ denotes the space of trace class operators and $\mathfrak{B}_2(X, Y)$ denotes the space of Hilbert Schmidt operators; if $X = Y$ we abbreviate $\mathfrak{B}_1(X) := \mathfrak{B}_1(X, X)$ and $\mathfrak{B}_2(X) := \mathfrak{B}_2(X, X)$. For a densely defined linear operator $A : X \to Y$ we denote by A^* the adjoint operator and by $|A|$ the absolute value, if A is closed. If A is a selfadjoint operator in a Hilbert space we denote by $\sigma(A)$, $\sigma_p(A)$, $\sigma_{ac}(A)$ the spectrum of A, its point spectrum, and its absolutely continuous spectrum, respectively.

Let and v_a, $v_b \in \mathbb{R}$, $v_a > v_b$, be given. We define the operator $E : \mathsf{L}^\infty_\mathbb{R} \longrightarrow \mathsf{L}^\infty_\mathbb{R}(\mathbb{R})$ by

$$(Ev)(x) := \begin{cases} v_a, & -\infty < x \le a, \\ v(x), & x \in (a,b), \\ v_b, & b \le x < \infty, \end{cases} \qquad v \in \mathsf{D}(E) := \mathsf{L}^\infty_\mathbb{R} = \mathsf{L}^\infty_\mathbb{R}(a,b). \tag{2.1}$$

Moreover, we assume that $m \in \mathsf{L}^\infty_\mathbb{R}$ and $m_a, m_b \in \mathbb{R}$ are given, with $m_a, m_b > 0$, $m > 0$ and $1/m \in \mathsf{L}^\infty$. We set

$$\widehat{m}(x) := \begin{cases} m_a, & -\infty < x \le a, \\ m(x), & x \in (a,b), \\ m_b, & b \le x < \infty, \end{cases} \tag{2.2}$$

and define the operator K_v by

$$K_v f := l_v(f), \qquad f \in \mathsf{D}(K_v) := \left\{ f \in \mathsf{W}^{1,2}(\mathbb{R}) \mid \frac{1}{\widehat{m}} f' \in \mathsf{W}^{1,2}(\mathbb{R}) \right\}, \tag{2.3}$$

where

$$l_v(f)(x) := -\frac{\hbar^2}{2} \frac{d}{dx} \frac{1}{\widehat{m}(x)} \frac{d}{dx} f(x) + (Ev)(x) f(x).$$

K_v is selfadjoint on $\mathcal{K} = \mathsf{L}^2(\mathbb{R})$. We call K_v the Buslaev-Fomin operator (see [BF] or [W, chapter 17]). We set

$$q_a(z) := \sqrt{\frac{z - v_a}{2m_a}} \quad \text{and} \quad q_b(z) := \sqrt{\frac{z - v_b}{2m_b}}, \quad z \in \mathbb{C}, \tag{2.4}$$

where the cut of the square root is taken along $[0, \infty)$. We note that in this case we have $\mathrm{Im}(\sqrt{z}) > 0$ for $z \in \mathbb{C} \setminus [0, \infty)$ and $\sqrt{z} > 0$ for $z \in (0, \infty)$. To construct the resolvent of K_v we proceed as in [W, chapter17] and introduce the functions

$$g_1(x,z) = \exp\left(i \tfrac{2m_b}{\hbar} q_b(z) x\right), \qquad x \in (b, \infty),$$
$$h_1(x,z) = \exp\left(-i \tfrac{2m_a}{\hbar} q_a(z) x\right), \quad x \in (-\infty, a),$$

for $z \in \mathbb{C}$. Furthermore let $g_2(v)(x,z)$ be the solution of the integral equation

$$g_2(v)(x,z) = c_1(z) - \frac{2}{\hbar} c_2(z) \int_x^b dt\, \widehat{m}(t) + \frac{2}{\hbar^2} \int_x^b dt\, \widehat{m}(t) \int_t^b ds\, ((Ev)(s) - z) g_2(v)(s,z),$$

$x \in (-\infty, b)$, $z \in \mathbb{C}$, where

$$c_1(z) := \exp\left(i \frac{2m_b}{\hbar} q_b(z) b\right), \qquad c_2(z) := i q_b(z) \exp\left(i \frac{2m_b}{\hbar} q_b(z) b\right).$$

Similarly we introduce $h_2(v)(x,z)$ as the solution of

$$h_2(v)(x,z) = d_1(z) + \frac{2}{\hbar} d_2(z) \int_a^x dt\, \widehat{m}(t) + \frac{2}{\hbar^2} \int_a^x dt\, \widehat{m}(t) \int_a^t ds\, ((Ev)(s) - z) h_2(v)(s,z),$$

$x \in (a,\infty)$, $z \in \mathbb{C}$, with

$$d_1(z) := \exp\left(-i\frac{2m_a}{\hbar}q_a(z)a\right), \qquad d_2(z) := -iq_a(z)\exp\left(-i\frac{2m_a}{\hbar}q_a(z)a\right).$$

Then we define

$$f_+(v)(x,z) := \begin{cases} g_2(v)(x,z), & -\infty < x < b, \\ g_1(x,z), & b \le x < \infty, \end{cases}, \qquad z \in \mathbb{C}, \tag{2.5}$$

and

$$f_-(v)(x,z) := \begin{cases} h_1(x,z), & -\infty < x \le a, \\ h_2(v)(x,z), & a < x < \infty, \end{cases}, \qquad z \in \mathbb{C}. \tag{2.6}$$

The $f_\pm(v)$ obey the equations

$$l_v(f_+(v)(x,z)) = zf_+(v)(x,z), \qquad l_v(f_-(v)(x,z)) = zf_-(v)(x,z), \qquad z \in \mathbb{C},$$

for almost every $x \in \mathbb{R}$. We note that $f_\pm(v)(x,\cdot)$ are holomorphic on $\mathbb{C} \setminus [0,\infty)$ and continuous on $\mathbb{C}$.

If $\psi_1, \psi_2 \in \mathsf{W}^{1,2}_{loc}(\mathbb{R})$, then we define the Wronskian by

$$W(\psi_1(x),\psi_2(x)) := \psi_1(x)\frac{\hbar}{2\widehat{m}(x)}\psi_2'(x) - \psi_2(x)\frac{\hbar}{2\widehat{m}(x)}\psi_1'(x). \tag{2.7}$$

We define the restrictions of $f_\pm(v)$ to the cut complex plane:

$$k_1(v)(x,z) := f_+(v)(x,z), \quad z \in \mathbb{C} \setminus (v_b,\infty),$$

and

$$k_2(v)(x,z) := f_-(v)(x,z), \quad z \in \mathbb{C} \setminus (v_b,\infty),$$

$x \in \mathbb{R}$. In the sequel the Wronskian $W(k_1(v)(x,z),k_2(v)(x,z))$ for $z \in \mathbb{C} \setminus (v_b,\infty)$ is of interest to us, for short we write $W_v(z)$. Indeed, this Wronskian does not depend on x.

Lemma 2.1. *The resolvent $(K_v - z)^{-1}$ of the Buslaev-Fomin operator (2.3) admits the representation*

$$((K_v - z)^{-1}f)(x) = \frac{k_1(v)(x,z)}{\hbar W_v(z)}\int_{-\infty}^{x} dy\, k_2(v)(y,z)f(y) + \frac{k_2(v)(x,z)}{\hbar W_v(z)}\int_{x}^{\infty} dy\, k_1(v)(y,z)f(y), \tag{2.8}$$

for all $f \in \mathcal{K}$ and all z from the resolvent set of K_v.

Proof. For convenience we will not indicate the dependence on v throughout the proof. Setting

$$g(x) := \frac{1}{\hbar W(z)}\left(k_1(x,z)\int_{-\infty}^{x} dy\, k_2(y,z)f(y) + k_2(x,z)\int_{x}^{\infty} dy\, k_1(y,z)f(y)\right),$$

for $f \in \mathcal{K}$, we get

$$\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{\widehat{m}(x)}\frac{d}{dx}g(x) = \frac{1}{\hbar W(z)}\Big(((Ev)(x) - z)\, k_1(x,z) \int_{-\infty}^{x} dy\, k_2(y,z) f(y) + ((Ev)(x) - z)\, k_2(x,z) \int_{x}^{\infty} dy\, k_1(y,z) f(y) - \hbar W(z) f(x)\Big).$$

Hence,

$$l(g(x)) - zg(x) = f(x),$$

i.e. $g \in \mathsf{D}(K)$ and $(K - z)g = f$. □

The spectrum of K_v is given by $\sigma(K_v) = \sigma_{ac}(K_v) \cup \sigma_p(K_v)$, where the absolutely continuous part is $\sigma_{ac}(K_v) = [v_b, \infty)$ and the point spectrum $\sigma_p(K_v)$ consists of finitely many simple eigenvalues $\lambda_j(v)$, $j = 1, \cdots, N(v)$, with $\lambda_j(v) < v_b$. $\sigma_{ac}(K_v)$ is simple on $[v_b, v_a)$ and has multiplicity two on $[v_a, \infty)$, see [BF] or [W, Theorem 17.C.1].

With respect to (2.4) we define

$$\kappa_a(z) := iq_a(z), \qquad \kappa_b(z) := iq_b(z), \qquad z \in \mathbb{C}_+. \tag{2.9}$$

Definition 2.2. (see [KL]) The quantum transmitting boundary operator family, short QTB family, $\{H_v(z)\}_{z\in\mathbb{C}_+}$ is the family of maximal dissipative operators on $\mathcal{H} = \mathsf{L}^2$ given by

$$\mathsf{D}(H_v(z)) := \left\{ f \in \mathsf{W}^{1,2} \;\middle|\; \begin{array}{l} \frac{1}{m} f' \in \mathsf{W}^{1,2}, \\ \frac{\hbar}{2m(a)} f'(a) = -\kappa_a(z) f(a), \\ \frac{\hbar}{2m(b)} f'(b) = \kappa_b(z) f(b) \end{array} \right\},$$

and

$$H_v(z) f := -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx} f + vf, \qquad f \in \mathsf{D}(H_v(z)),$$

for all $z \in \mathbb{C}_+$.

Since $\mathrm{Re}(q_j(z)) > 0$ for $z \in \mathbb{C}_+$, we have $\mathrm{Im}(\kappa_j(z)) > 0$, $j = a, b$. Thus the operator $H_v(z)$ is dissipative for each fixed z, i.e. $\mathrm{Im}(H_v(z)f, f) \le 0$ for all $f \in \mathsf{D}(H_v(z))$. Furthermore, for each $z \in \mathbb{C}+$ the spectrum of $H_v(z)$ is contained in the lower half plain $\mathbb{C}_-$ and $H_v(z)$ is maximal dissipative and completely non-selfadjoint, see [KNR1, Theorems 4.6 and 5.2].

Proposition 2.3. *Let $P_{\mathcal{H}}^{\mathcal{K}}$ denote the projection operator from $\mathcal{K}$ onto $\mathcal{H}$. Then*

$$P_{\mathcal{H}}^{\mathcal{K}}(K_v - z)^{-1}\Big|_{\mathcal{H}} = (H_v(z) - z)^{-1} \qquad \textit{for all } z \in \mathbb{C}_+, \tag{2.10}$$

$$P_{\mathcal{H}}^{\mathcal{K}}(K_v - z)^{-1}\Big|_{\mathcal{H}} = (H_v(\overline{z})^* - z)^{-1} \qquad \textit{for all } z \in \mathbb{C}_-. \tag{2.11}$$

Proof. We will again omit the subscript v within the proof. It suffices to show that $g := P^{\mathcal{K}}_{\mathcal{H}}(K-z)^{-1}f$ satisfies the boundary condition for every $f \in \mathcal{H}$ and $z \in \mathbb{C}_+$. We will only prove that the boundary condition at b is satisfied; the corresponding statement at a is proven similarly. By equation (2.5) we get $k_1(x,z) = \exp(i2m_b q_b(z)x)$, for $x \geq b$. Thus,

$$k_1(b,z) = \exp\left(i\frac{2m_b}{\hbar}q_b(z)b\right) \quad \text{and} \quad \frac{\hbar}{2m(b)}k_1'(b,z) = iq_b(z)k_1(b,z).$$

Using the expression (2.8) for the resolvent of K we get

$$\begin{aligned} g(b) &= \frac{1}{\hbar W(z)}\left(k_1(b,z)\int_{-\infty}^{b} dy\, k_2(y,z)f(y) + k_2(b,z)\int_b^{\infty} dy\, k_1(y,z)f(y)\right)\\ &= \frac{k_1(b,z)}{\hbar W(z)}\int_a^b dy\, k_2(y,z)f(y), \end{aligned}$$

since $f(y) = 0$ for $y \in (b,\infty)$. Similarly we obtain

$$\begin{aligned} &\frac{\hbar}{2m(b)}g'(b)\\ &\quad= \frac{1}{\hbar W(z)}\left(iq_b(z)\, k_1(b,z)\int_{-\infty}^{b} dy\, k_2(y,z)f(y) + \frac{\hbar}{2m(b)}k_2'(b,z)\int_b^{\infty} dy\, k_1(y,z)f(y)\right)\\ &\quad= iq_b(z)\frac{k_1(b,z)}{\hbar W(z)}\int_a^b dy\, k_2(y,z)f(y) = \kappa_b(z)g(b). \end{aligned}$$

Now (2.11) follows from (2.10) by passing to the adjoints. □

Remark 2.4. The QTB family $\{H_v(z)\}_{z\in\mathbb{C}_+}$ describes an open quantum system on $\mathcal{H}$. The expression (2.10) is interpreted as the embedding of this open system into the larger quantum system described by the Buslaev-Fomin operator K_v.

Remark 2.5. The relation (2.10) looks similar to a relation between maximal dissipative operators and their dilations, see [FN]. More precisely: Let $v \in \mathsf{L}^\infty_{\mathbb{R}}$ and $\lambda_0 \in \mathbb{R}$ with $\lambda_0 > v_b$ be given. We set $H_{dis}(v) := H_v(\lambda_0)$. $H_{dis}(v)$ is maximal dissipative and completely non-selfadjoint. By the dilation theory we get the existence of a larger Hilbert space $\mathcal{K}_{dis}$ with $\mathcal{H} \subseteq \mathcal{K}_{dis}$ and the existence of a selfadjoint operator $K_{dis}(v)$ on $\mathcal{K}_{dis}$, such that

$$P^{\mathcal{K}_{dis}}_{\mathcal{H}}(K_{dis}(v)-z)^{-1}\Big|_{\mathcal{H}} = (H_{dis}(v)-z)^{-1} \qquad \text{for all} \qquad z \in \mathbb{C}_+, \tag{2.12}$$

where $P^{\mathcal{K}_{dis}}_{\mathcal{H}}$ denotes the projection from $\mathcal{K}_{dis}$ onto $\mathcal{H}$, see [FN]. The operator $K_{dis}(v)$ is called the dilation corresponding to $H_{dis}(v)$. Note that the equation (2.12) differs from the expression (2.10), since $H_{dis}(v)$ is independent of $z \in \mathbb{C}_+$. The Hilbert space $\mathcal{K}_{dis}$ and the operator K_{dis} have been explicitly calculated in [KNR2]. We remark that the Hilbert space $\mathcal{K}_{dis}$ differs from the space $\mathcal{K}$. Furthermore, the operator $K_{dis}(v)$ is not bounded from below and its spectrum is completely absolutely continuous, i.e. $\sigma(K_{dis}(v)) = \sigma_{ac}(K_{dis}(v)) = \mathbb{R}$ (see [KNR2] for details).

Proposition 2.6. *If* $v \in \mathsf{L}^\infty_\mathbb{R}$ *and* K_v *is the operator* (2.3), *then* $(K_v - i)^{-1}P^\mathcal{K}_\mathcal{H}$ *is trace class and its trace norm can be estimated by*

$$\|(K_v - i)^{-1}P^\mathcal{K}_\mathcal{H}\|_{\mathfrak{B}_1(\mathcal{K})} \le 3 + \left(8 + 4\sqrt{\|m\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar}\right)\sqrt{1 + \|v\|_{\mathsf{L}^\infty}}.$$

For the proof we need the subsequent lemma. We set

$$r_a := \mathrm{Re}(\kappa_a(i)), \quad r_b := \mathrm{Re}(\kappa_b(i)), \quad \alpha_a := \mathrm{Im}(\kappa_a(i)), \quad \alpha_b := \mathrm{Im}(\kappa_b(i)).$$

We note that $r_a, r_b \le 0$ and $\alpha_a, \alpha_b \ge 0$. Furthermore we abbreviate $H_v := H_v(i)$. Following [KNR2] we introduce the (unclosed) operator $\alpha : \mathcal{H} \longrightarrow \mathbb{C}^2$ by

$$\alpha f = \begin{pmatrix} \sqrt{\alpha_b} f(b) \\ -\sqrt{\alpha_a} f(a) \end{pmatrix}, \qquad \mathsf{D}(\alpha) = \mathsf{W}^{1,2}, \tag{2.13}$$

and the operator $U_v(z) : \mathcal{H} \longrightarrow \mathbb{C}^2$ given by

$$U_v(z) = \alpha(H_v - z)^{-1}, \quad \mathsf{D}(U_v(z)) = \mathcal{H}$$

for z from the resolvent set of the operator H_v.

Lemma 2.7. *For every* $v \in \mathsf{L}^\infty_\mathbb{R}$ *we have the estimates*

$$\|(H_v - i)^{-1}\|_{\mathfrak{B}_1(\mathcal{H})} \le 3 + 4\sqrt{\|m\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar}\sqrt{1 + \|v\|_{\mathsf{L}^\infty}}, \tag{2.14}$$

and

$$\|U_v(i)\|_{\mathfrak{B}_1(\mathcal{H},\mathbb{C}^2)} \le 8\sqrt{1 + \|v\|_{\mathsf{L}^\infty}}. \tag{2.15}$$

Proof. We define the selfadjoint operator H_0 by

$$\mathsf{D}(H_0) := \left\{ f \in \mathsf{W}^{1,2} \mid \frac{1}{m}f' \in \mathsf{W}^{1,2}, \quad \frac{\hbar}{2m(b)}f'(b) = \frac{\hbar}{2m(a)}f'(a) = 0 \right\},$$

$$H_0 f = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}f + f, \quad f \in \mathsf{D}(H_0).$$

Note that $H_0 \ge I$. Similar to the operator α we define the operator $r : \mathcal{H} \longrightarrow \mathbb{C}^2$ by

$$rf = \begin{pmatrix} \sqrt{-r_b} f(b) \\ -\sqrt{-r_a} f(a) \end{pmatrix}, \quad \mathsf{D}(r) = \mathsf{W}^{1,2}.$$

The operators $V_\alpha(\mu), V_r(\mu) : \mathcal{H} \longrightarrow \mathbb{C}^2$ are given by

$$V_\alpha(\mu) = \alpha(H_0 + \mu)^{-1/2}, \qquad V_r(\mu) = r(H_0 + \mu)^{-1/2}, \qquad \mu \ge 0.$$

Furthermore we introduce the operator $B_v(\mu) : \mathcal{H} \longrightarrow \mathcal{H}$ by

$$B_v(\mu) := (H_0 + \mu)^{-1/2}(v - 1)(H_0 + \mu)^{-1/2} + V_r(\mu)^* V_r(\mu) - iV_\alpha(\mu)^* V_\alpha(\mu),$$

for $\mu \geq 0$, see [BKNR]. There is

$$\|(H_0+\mu)^{-1/2}(v-1)(H_0+\mu)^{-1/2}\|_{\mathfrak{B}(\mathcal{H})} \leq \frac{1+\|v\|_{\mathsf{L}^\infty}}{1+\mu}.$$

Hence,

$$\|(H_0+\mu)^{-1/2}(v-1)(H_0+\mu)^{-1/2}\| \leq \frac{1}{2}, \quad \text{for } \mu \geq 1+2\|v\|_{\mathsf{L}^\infty}.$$

We set

$$R_v(\mu) := (H_0+\mu)^{-1/2}(v-1)(H_0+\mu)^{-1/2} + V_r(\mu)^* V_r(\mu),$$

for $\mu \geq 1+2\|v\|_{\mathsf{L}^\infty}$. $R_v(\mu)$ is selfadjoint and there is $1+R_v(\mu) \geq \frac{1}{2}$. Hence, $(1+R_v(\mu))^{-1/2}$ exists and its norm does not exceed $\sqrt{2}$. Now a straightforward calculation shows that

$$\begin{aligned}(1+B_v(\mu))^{-1} &= (1+R_v(\mu))^{-1/2}\times \\ &\times \left(1 - i(1+R_v(\mu))^{-1/2}V_\alpha(\mu)^* V_\alpha(\mu)(1+R_v(\mu))^{-1/2}\right)^{-1}(1+R_v(\mu))^{-1/2}.\end{aligned}$$

Hence,

$$\|(1+B_v(\mu))^{-1}\|_{\mathfrak{B}(\mathcal{H})} \leq 2, \quad \text{for } \mu \geq 1+2\|v\|_{\mathsf{L}^\infty}. \tag{2.16}$$

By Lemma 2.3 from [BKNR] we have the representation

$$(H_v+\mu)^{-1} = (H_0+\mu)^{-1/2}(1+B_v(\mu))^{-1}(H_0+\mu)^{-1/2}, \tag{2.17}$$

for large, positive μ. Because both sides depend on μ analytically, this operator equality extends to all real μ for which $(1+B_v(\mu))^{-1} \in \mathfrak{B}(\mathcal{H})$. This is true for any $\mu \geq 1+2\|v\|_{\mathsf{L}^\infty}$; hence, (2.17) extends to all these μ. Using the first resolvent equation we obtain

$$(H_v-i)^{-1} = (H_v+\mu)^{-1}\left(1+(\mu+i)(H_v-i)^{-1}\right),$$

and we get by (2.17) that

$$\|(H_v-i)^{-1}\|_{\mathfrak{B}_1(\mathcal{H})} \leq (2+\mu)\|(H_v+\mu)^{-1}\|_{\mathfrak{B}_1(\mathcal{H})} \leq 2(2+\mu)\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{B}_2(\mathcal{H})}. \tag{2.18}$$

According to the proof of Proposition 2.4 in [BKNR] we have

$$\|(H_0+\mu)^{-1/2}\|^2_{\mathfrak{B}_2(\mathcal{H})} \leq \frac{1}{1+\mu} + \sqrt{\|m\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar\sqrt{2}}\frac{1}{\sqrt{1+\mu}}.$$

Thus, from (2.18) we obtain for $\mu = 1+2\|v\|_{\mathsf{L}^\infty}$:

$$\|(H_v-i)^{-1}\|_{\mathfrak{B}_1(\mathcal{H})} \leq 3 + 4\sqrt{\|m\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar}\sqrt{1+\|v\|_{\mathsf{L}^\infty}},$$

i.e. the first assertion (2.14) of the lemma. To prove the second assertion we estimate for $\mu \geq 1+2\|v\|_{\mathsf{L}^\infty}$

$$\|U_v(i)\|_{\mathfrak{B}_1(\mathcal{H},\mathbb{C}^2)} \leq 2\|U_v(i)\|_{\mathfrak{B}(\mathcal{H},\mathbb{C}^2)} \leq 2(2+\mu)\|U_v(\mu)\|_{\mathfrak{B}(\mathcal{H},\mathbb{C}^2)}. \tag{2.19}$$

Using the definition of $U_v(\mu)$ and the representation (2.17) for the resolvent of H_v we get

$$U_v(\mu) = V_\alpha(\mu)(1 + B_v(\mu))^{-1}(H_0 + \mu)^{-1/2} = V_\alpha(\mu)(1 + R_v(\mu))^{-1/2} \times \\ \times \left(1 - i(1 + R_v(\mu))^{-1/2} V_\alpha(\mu)^* V_\alpha(\mu)(1 + R_v(\mu))^{-1/2}\right)^{-1} \times \\ \times (1 + R_v(\mu))^{-1/2}(H_0 + \mu)^{-1/2}.$$

Because the operator norm of

$$V_\alpha(\mu)(1 + R_v(\mu))^{-1/2} \left(1 - i(1 + R_v(\mu))^{-1/2} V_\alpha(\mu)^* V_\alpha(\mu)(1 + R_v(\mu))^{-1/2}\right)^{-1}$$

is not bigger than one, we get

$$\|U_v(\mu)\|_{\mathfrak{B}(\mathcal{H},\mathbb{C}^2)} \le \sqrt{2}\|(H_0 + \mu)^{-1/2}\|_{\mathfrak{B}(\mathcal{H})} \le \sqrt{\frac{2}{1+\mu}}$$

and with (2.19):

$$\|U_v(i)\|_{\mathfrak{B}_1(\mathcal{H},\mathbb{C}^2)} \le 2\sqrt{2}\frac{2+\mu}{\sqrt{1+\mu}} \le 4\sqrt{2}\sqrt{1+\mu}.$$

Setting $\mu = 1 + 2\|v\|_{\mathsf{L}^\infty}$ we finally obtain the inequality (2.15). □

Proof of Proposition 2.6. Using Proposition 2.3 we get

$$\begin{aligned} \left|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\right|^2 &= P^{\mathcal{K}}_{\mathcal{H}}(K_v + i)^{-1}(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}} \\ &= \frac{1}{2i}P^{\mathcal{K}}_{\mathcal{H}}\left((K_v + i)^{-1} - (K_v - i)^{-1}\right)P^{\mathcal{K}}_{\mathcal{H}} \\ &= \frac{1}{2i}\left((H_v^* + i)^{-1} - (H_v - i)^{-1}\right). \end{aligned}$$

By Lemma 3.2 from [KNR2] we get

$$\left|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\right|^2 = U_v(i)^*U_v(i) + (H_v^* + i)^{-1}(H_v - i)^{-1}.$$

Therefore we find

$$\|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\|_{\mathfrak{B}_1(\mathcal{K})} = \|\,|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}|\,\|_{\mathfrak{B}_1(\mathcal{K})} \\ \le \|U_v(i)\|_{\mathfrak{B}_1(\mathcal{H},\mathbb{C}^2)} + \|(H_v - i)^{-1}\|_{\mathfrak{B}_1(\mathcal{H})}.$$

Now using Lemma 2.7 the proof is finished. □

Proposition 2.8. *Assume that $v \in \mathsf{L}^\infty_{\mathbb{R}}$ and let K_v be given by (2.3). The number of eigenvalues $N(v)$ of K_v is estimated by*

$$N(v) \le 1 + \frac{\sqrt{2\|m\|_{\mathsf{L}^\infty}}(b-a)}{\pi\hbar}\sqrt{\|v\|_{\mathsf{L}^\infty} + |v_b|}.$$

Proof. We define the operator K_1 by

$$K_1 := -\frac{d^2}{dx^2} - \frac{2\|m\|_{\mathsf{L}^\infty}(\|v\|_{\mathsf{L}^\infty} + |v_b|)}{\hbar^2}\chi_{(a,b)}, \qquad \mathsf{D}(K_1) = \mathsf{W}^{2,2}(\mathbb{R}),$$

where $\chi_{(a,b)} \in \mathsf{L}^\infty_{\mathbb{R}}(\mathbb{R})$ is the indicator function of the set (a,b). The number of eigenvalues of K_1, which we will denote by $N(K_1)$, can be estimated, see [W, p. 274]:

$$N(K_1) \le 1 + \frac{\sqrt{2\|m\|_{\mathsf{L}^\infty}}(b-a)}{\pi\hbar}\sqrt{\|v\|_{\mathsf{L}^\infty} + |v_b|}.$$

Therefore it suffices to show that $N(v) \le N(K_1)$. A straightforward calculation shows that $\frac{\hbar^2}{2\|m\|_{\mathsf{L}^\infty}}K_1 \le K_v$. By the min-max principle, see e.g. [RS2, Theorem XIII.2], this implies $N(v) \le N(K_1)$. □

3 Eigenfunction expansion

In this section we investigate the generalized eigenfunctions of the Buslaev-Fomin operator K_v, see (2.3). These eigenfunctions will be important for the definition of the carrier and current densities, which we will introduce in Section 5. Furthermore we will introduce the Fourier transform corresponding to K_v and show that the eigenfunctions of the Buslaev-Fomin operator can be expressed in terms of the QTB family. The first part of this section slightly generalizes results of Buslaev and Fomin [BF], see also [W, chapter 17].

We define

$$f_1(v)(x,\lambda) := f_+(v)(x,\lambda), \qquad \text{for} \qquad \lambda \in (v_b, \infty), \quad x \in \mathbb{R},$$

and

$$f_2(v)(x,\lambda) := f_-(v)(x,\lambda), \qquad \text{for} \qquad \lambda \in (v_b, \infty), \quad x \in \mathbb{R}.$$

In the following investigations Wronskians—as defined in (2.7)—will repeatedly appear. First, a straightforward calculation shows that

$$W(\overline{f_1(v)(x,\lambda)}, f_1(v)(x,\lambda)) = 2iq_b(\lambda), \qquad \lambda \in (v_b,\infty), \tag{3.1}$$

$$W(\overline{f_2(v)(x,\lambda)}, f_2(v)(x,\lambda)) = -2iq_a(\lambda), \qquad \lambda \in (v_a,\infty). \tag{3.2}$$

Furthermore we define the coefficients

$$C_{11}(v)(\lambda) := \frac{1}{2iq_b(\lambda)}W(\overline{f_1(v)(x,\lambda)}, f_2(v)(x,\lambda)), \quad \lambda \in (v_b,\infty),$$

$$C_{12}(v)(\lambda) := \frac{1}{2iq_b(\lambda)}W(f_2(v)(x,\lambda), f_1(v)(x,\lambda)), \quad \lambda \in (v_b,\infty),$$

$$C_{21}(v)(\lambda) := \frac{1}{2iq_a(\lambda)}W(f_2(v)(x,\lambda), f_1(v)(x,\lambda)), \quad \lambda \in (v_a,\infty),$$

$$C_{22}(v)(\lambda) := \frac{1}{2iq_a(\lambda)}W(f_1(v)(x,\lambda), \overline{f_2(v)(x,\lambda)}), \quad \lambda \in (v_a,\infty).$$

Thus,

$$f_1(v)(x,\lambda) = C_{22}(v)(\lambda)f_2(v)(x,\lambda) + C_{21}(v)(\lambda)\overline{f_2(v)(x,\lambda)}, \qquad \lambda \in (v_a,\infty), \tag{3.3}$$

$$f_2(v)(x,\lambda) = C_{11}(v)(\lambda)f_1(v)(x,\lambda) + C_{12}(v)(\lambda)\overline{f_1(v)(x,\lambda)}, \qquad \lambda \in (v_b,\infty). \tag{3.4}$$

There are the following equations:

$$\begin{aligned} q_b(\lambda)C_{12}(v)(\lambda) &= q_a(\lambda)C_{21}(v)(\lambda), \\ q_b(\lambda)C_{11}(v)(\lambda) &= -q_a(\lambda)\overline{C_{22}(v)(\lambda)}, \end{aligned} \qquad \lambda \in (v_a,\infty), \tag{3.5}$$

and

$$\frac{q_b(\lambda)}{q_a(\lambda)}|C_{12}(v)(\lambda)|^2 = 1 + \frac{q_b(\lambda)}{q_a(\lambda)}|C_{11}(v)(\lambda)|^2 = 1 + \frac{q_a(\lambda)}{q_b(\lambda)}|C_{22}(v)(\lambda)|^2 \tag{3.6}$$

for $\lambda \in (v_a,\infty)$. Moreover, we have

$$C_{11}(v)(\lambda) = \overline{C_{12}(v)(\lambda)}, \qquad \lambda \in (v_b, v_a). \tag{3.7}$$

The scattering coefficients $S_{ij}(v)(\lambda)$ are given by

$$S_{ba}(v)(\lambda) := \frac{1}{C_{21}(v)(\lambda)}, \qquad S_{aa}(v)(\lambda) := \frac{C_{22}(v)(\lambda)}{C_{21}(v)(\lambda)}, \qquad \lambda \in (v_a,\infty), \tag{3.8}$$

$$S_{bb}(v)(\lambda) := \frac{C_{11}(v)(\lambda)}{C_{12}(v)(\lambda)}, \qquad S_{ab}(v)(\lambda) := \frac{1}{C_{12}(v)(\lambda)}, \qquad \lambda \in (v_b,\infty). \tag{3.9}$$

Using (3.5) and (3.6) we obtain the following relations for $\lambda \in (v_a,\infty)$:

$$\begin{aligned} q_a(\lambda)S_{ab}(v)(\lambda) &= q_b(\lambda)S_{ba}(v)(\lambda), \\ q_b(\lambda)S_{ba}(v)(\lambda)\overline{S_{bb}(v)(\lambda)} &= -q_a(\lambda)S_{aa}(v)(\lambda)\overline{S_{ab}(v)(\lambda)} \end{aligned} \tag{3.10}$$

and

$$\frac{q_b(\lambda)}{q_a(\lambda)}|S_{ba}(v)(\lambda)|^2 + |S_{aa}(v)(\lambda)|^2 = \frac{q_a(\lambda)}{q_b(\lambda)}|S_{ab}(v)(\lambda)|^2 + |S_{bb}(v)(\lambda)|^2 = 1. \tag{3.11}$$

Equation (3.10) implies

$$|S_{aa}(v)(\lambda)| \le 1, \qquad \text{and} \qquad |S_{bb}(v)(\lambda)| \le 1, \qquad \text{for } \lambda \in (v_a,\infty). \tag{3.12}$$

Furthermore, we get from (3.7)

$$|S_{bb}(v)(\lambda)| = 1, \qquad \text{for } \lambda \in (v_b, v_a). \tag{3.13}$$

The boundary values of $S_{ij}(\lambda)$, $i,j = a,b$, are given by

$$\lim_{\lambda\to v_a} S_{ab}(v)(\lambda) = \lim_{\lambda\to v_b} S_{ba}(v)(\lambda) = 0, \quad \lim_{\lambda\to v_a} S_{aa}(v)(\lambda) = \lim_{\lambda\to v_b} S_{bb}(v)(\lambda) = -1.$$

Now we define

$$\begin{aligned}\psi_a(v)(x,\lambda) &:= S_{ba}(v)(\lambda)f_1(v)(x,\lambda), \quad \lambda \in (v_a,\infty),\\ \psi_b(v)(x,\lambda) &:= S_{ab}(v)(\lambda)f_2(v)(x,\lambda), \quad \lambda \in (v_b,\infty).\end{aligned} \tag{3.14}$$

By (3.3) and (3.4) we get

$$\begin{aligned}\psi_a(v)(x,\lambda) &= \overline{f_2(v)(x,\lambda)} + S_{aa}(v)(\lambda)f_2(v)(x,\lambda) \qquad \text{for } \lambda \in (v_a,\infty),\\ \psi_b(v)(x,\lambda) &= \overline{f_1(v)(x,\lambda)} + S_{bb}(v)(\lambda)f_1(v)(x,\lambda) \qquad \text{for } \lambda \in (v_b,\infty).\end{aligned}$$

Thus, outside the interval (a,b) the functions $\psi_a(v)$ and $\psi_b(v)$ are given by

$$\psi_a(v)(x,\lambda) = \begin{cases}\exp\left(i\frac{2m_a}{\hbar}q_a(\lambda)x\right) + S_{aa}(v)(\lambda)\exp\left(-i\frac{2m_a}{\hbar}q_a(\lambda)x\right), & x \in (-\infty,a),\\ S_{ba}(v)(\lambda)\exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)x\right), & x \in (b,\infty)\end{cases} \tag{3.15}$$

for $\lambda \in (v_a,\infty)$ and

$$\psi_b(v)(x,\lambda) = \begin{cases}S_{ab}(v)(\lambda)\exp\left(-i\frac{2m_a}{\hbar}q_a(\lambda)x\right), & x \in (-\infty,a),\\ \exp\left(-i\frac{2m_b}{\hbar}q_b(\lambda)x\right) + S_{bb}(v)(\lambda)\exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)x\right), & x \in (b,\infty)\end{cases} \tag{3.16}$$

for $\lambda \in (v_b,\infty)$, respectively.

Remark 3.1. Formulae (3.15) and (3.16) have the following physical interpretation: The wave $\exp(i\frac{2m_a}{\hbar}q_a(\lambda)x)$ coming from $-\infty$ is scattered at the potential v. During the scattering the wave is partially reflected and partially transmitted by v. The reflection and the transmission part is given by

$$S_{aa}(v)(\lambda)\exp(-i\frac{2m_a}{\hbar}q_a(\lambda)x) \qquad \text{and} \qquad S_{ba}(v)(\lambda)\exp(i\frac{2m_b}{\hbar}q_b(\lambda)x),$$

respectively. Similarly, the wave $\exp(-i\frac{2m_b}{\hbar}q_b(\lambda)x)$ which comes from $+\infty$, splits up during the scattering into the reflection and transmission part

$$S_{bb}(v)(\lambda)\exp(i\frac{2m_b}{\hbar}q_b(\lambda)x) \qquad \text{and} \qquad S_{ab}(v)(\lambda)\exp(-i\frac{2m_a}{\hbar}q_a(\lambda)x),$$

respectively.

Lemma 3.2. *There are the following identities for the functions* (3.14)*:*

$$\int_{\mathbb{R}} dx\, \psi_a(v)(x,\lambda)\overline{\psi_a(v)(x,\mu)} = 4\pi\hbar q_a(\lambda)\delta(\lambda-\mu), \qquad \text{for } \lambda,\mu \in (v_a,\infty), \tag{3.17}$$

$$\int_{\mathbb{R}} dx\, \psi_b(v)(x,\lambda)\overline{\psi_b(v)(x,\mu)} = 4\pi\hbar q_b(\lambda)\delta(\lambda-\mu), \qquad \text{for } \lambda,\mu \in (v_b,\infty), \tag{3.18}$$

and

$$\int_{\mathbb{R}} dx\, \psi_a(v)(x,\lambda)\overline{\psi_b(v)(x,\mu)} = 0, \qquad \text{for } \lambda,\mu \in (v_a,\infty). \tag{3.19}$$

Proof. For the sake of simplicity we will omit the index v within the proof. Assume $\lambda, \mu \in (v_a, \infty)$. Then

$$\int_{-N}^{N} dx\, \psi_a(x,\lambda)\overline{\psi_a(x,\mu)} = \frac{\hbar}{\lambda-\mu}\Big(\int_{-N}^{N} dx\, \psi_a(x,\lambda)\overline{\frac{\partial}{\partial x}\frac{\hbar}{2m(x)}\frac{\partial}{\partial x}\psi_a(x,\mu)} - \int_{-N}^{N} dx\, \frac{\partial}{\partial x}\frac{\hbar}{2m(x)}\frac{\partial}{\partial x}\psi_a(x,\lambda)\overline{\psi_a(x,\mu)}\Big)$$
$$= \frac{\hbar}{\lambda-\mu}\left(W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)}) - W(\psi_a(-N,\lambda), \overline{\psi_a(-N,\mu)})\right).$$

For $N \geq b$ we get by (3.15)

$$W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)}) = -iS_{ba}(\lambda)\overline{S_{ba}(\mu)}(q_b(\lambda)+q_b(\mu))\exp\left(i\tfrac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))N\right). \tag{3.20}$$

Hence, we get by observing $\delta(\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))) = 2\hbar q_b(\lambda)\delta(\lambda-\mu)$, see [GS, chapter II §2 eq. II]:

$$\lim_{N\to\infty}\frac{\hbar}{\lambda-\mu}W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)}) = \pi|S_{ba}(\lambda)|^2\delta(\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu)))$$
$$= 2\pi\hbar|S_{ba}(\lambda)|^2 q_b(\lambda)\delta(\lambda-\mu),. \tag{3.21}$$

For $N \leq a$ one obtains, analogously to (3.20):

$$\frac{\hbar}{\lambda-\mu}W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)}) = -\, i\hbar\frac{\exp\left(-i\frac{2m_a}{\hbar}(q_a(\lambda)-q_a(\mu))N\right)}{2m_a(q_a(\lambda)-q_a(\mu))}$$
$$- i\hbar\overline{S_{aa}(\mu)}\frac{\exp\left(i\frac{2m_a}{\hbar}(q_a(\lambda)+q_a(\mu))N\right)}{2m_a(q_a(\lambda)+q_a(\mu))}$$
$$- i\hbar S_{aa}(\lambda)\frac{\exp\left(-i\frac{2m_a}{\hbar}(q_a(\lambda)+q_a(\mu))N\right)}{2m_a(q_a(\lambda)+q_a(\mu))}$$
$$+ i\hbar\overline{S_{aa}(\mu)}S_{aa}(\lambda)\frac{\exp\left(i\frac{2m_a}{\hbar}(q_a(\lambda)-q_a(\mu))N\right)}{2m_a(q_a(\lambda)-q_a(\mu))}.$$

Therefore

$$\lim_{N\to-\infty}\frac{1}{\lambda-\mu}W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)})$$
$$= -\pi q_a(\lambda)\left(1+\overline{S_{aa}(\mu)}S_{aa}(\lambda)\right)\delta(\frac{2m_a}{\hbar}(q_a(\lambda)-q_a(\mu)))$$
$$+ \pi\left(\overline{S_{aa}(\mu)} - S_{aa}(\lambda)\right)\delta(\frac{2m_a}{\hbar}(q_a(\lambda)+q_a(\mu))).$$

Since $q_a(\lambda') > 0$ for all $\lambda' \in (v_a, \infty)$ we get $\delta(\frac{2m_a}{\hbar}(q_a(\lambda)+q_a(\mu))) = 0$. Thus,

$$\lim_{N\to-\infty}\frac{\hbar}{\lambda-\mu}W(\psi_a(N,\lambda), \overline{\psi_a(N,\mu)}) = -2\pi\hbar q_a(\mu)\left(1+|S_{aa}(\mu)|^2\right)\delta(\lambda-\mu). \tag{3.22}$$

Putting (3.21) and (3.22) together yields

$$\int_{-\infty}^{\infty} \psi_a(x,\lambda)\overline{\psi_a(x,\mu)}\,dx = 2\pi\hbar\left(q_b(\lambda)|S_{ba}(\lambda)|^2 + q_a(\lambda) + q_a(\lambda)|S_{aa}(\lambda)|^2\right)\delta(\lambda-\mu).$$

By (3.11) we get

$$\int_{-\infty}^{\infty} \psi_a(x,\lambda)\overline{\psi_a(x,\mu)}\,dx = 4\pi\hbar q_a(\lambda)\delta(\lambda-\mu)$$

which proves (3.17). Analogously we obtain (3.18) and (3.19). □

The generalized eigenfunctions of the Buslaev-Fomin operator K_v, see (2.3), are given by

$$\begin{aligned}\phi_b(v)(x,\lambda) &:= \frac{1}{\sqrt{4\pi\hbar q_b(\lambda)}}\psi_b(v)(x,\lambda), \quad \lambda\in(v_b,\infty),\\ \phi_a(v)(x,\lambda) &:= \frac{1}{\sqrt{4\pi\hbar q_a(\lambda)}}\psi_a(v)(x,\lambda), \quad \lambda\in(v_a,\infty);\end{aligned} \tag{3.23}$$

the orthonormal eigenfunctions corresponding to the eigenvalues $\lambda_1(v), \ldots, \lambda_{N(v)}(v)$ are denoted by $\phi_p(v)(x,\lambda_j(v))$, $j=1,\ldots,N(v)$.

Corollary 3.3. *The functions*

$$\{\phi_a(v)(\cdot,\lambda)\}_{\lambda\in(v_a,\infty)} \cup \{\phi_b(v)(\cdot,\lambda)\}_{\lambda\in(v_b,\infty)} \cup \{\phi_p(v)(\cdot,\lambda)\}_{\lambda\in\sigma_p(K_v)}$$

constitute a complete system of orthonormal generalized eigenfunctions, i.e.

$$(\phi_\tau(v)(\cdot,\lambda), \phi_{\tau'}(v)(\cdot,\lambda'))_{\mathcal{K}} = \delta_{\tau,\tau'}\delta(\lambda-\lambda'), \quad \tau,\tau'\in\{a,b,p\},$$

where λ and λ' are from a part of $\sigma(K_v)$ which corresponds to τ and τ', respectively.

We now introduce the Hilbert space

$$\widehat{\mathcal{K}}_v := \mathsf{L}^2(\sigma(K_v), \mathfrak{h}(\lambda), \nu),$$

see [BW, chapter 4], where

$$\mathfrak{h}(\lambda) := \begin{cases} \mathbb{C}, & \lambda\in\sigma_p(K_v) = \cup_{j=1}^{N(v)}\{\lambda_j(v)\},\\ \mathbb{C}, & \lambda\in(v_b,v_a),\\ \mathbb{C}^2, & \lambda\in(v_a,\infty).\end{cases} \tag{3.24}$$

The measure $\nu(\cdot)$ decomposes

$$\nu(\cdot) = \nu_p(\cdot) + \nu_{ac}(\cdot) \tag{3.25}$$

into an atomic measure $\nu_p(\{\lambda_j(v)\}) = 1$, $j=1,\ldots,N(v)$, supported on $\sigma_p(K_v)$, and an absolutely continuous measure $d\nu_{ac}(\lambda) = \chi_{(v_b,\infty)}(\lambda)d\lambda$ supported on (v_b,∞). With respect to the decomposition (3.24) we define

$$\vec{\phi}_v(x,\lambda) := \begin{cases} \phi_p(v)(x,\lambda), & \lambda\in\sigma_p(K_v),\\ \phi_b(v)(x,\lambda), & \lambda\in(v_b,v_a),\\ \begin{pmatrix}\phi_b(v)(x,\lambda)\\ \phi_a(v)(x,\lambda)\end{pmatrix}, & \lambda\in(v_a,\infty).\end{cases} \tag{3.26}$$

By means of the functions $\vec{\phi}_v(x,\lambda)$ we now define the Fourier transform with respect to K_v as the unitary operator $\Phi_v : \mathcal{K} \longrightarrow \widehat{\mathcal{K}}_v$, see [W, Theorem 17.C.2]:

$$(\Phi_v f)(\lambda) = \int_{\mathbb{R}} dx\; f(x)\overline{\vec{\phi}_v(x,\lambda)}, \quad \lambda \in \sigma(K_v). \tag{3.27}$$

The inverse Fourier transform $\Phi_v^{-1} : \widehat{\mathcal{K}}_v \longrightarrow \mathcal{K}$ is given by

$$(\Phi_v^{-1}\hat{g})(x) = \int_{\sigma(K_v)} d\nu(\lambda)\; \left(\hat{g}(\lambda), \overline{\vec{\phi}_v(x,\lambda)}\right)_{\mathfrak{h}(\lambda)}, \quad x \in \mathbb{R}, \quad \hat{g} \in \widehat{\mathcal{K}}_v.$$

We note that

$$\Phi_v K_v \Phi_v^{-1} = M,$$

where M is the multiplication operator

$$(Mg)(\lambda) := \lambda g(\lambda) \quad \text{for } g \in \mathsf{D}(M) := \{g \in \widehat{\mathcal{K}}_v \mid \lambda g(\lambda) \in \widehat{\mathcal{K}}_v\}\ .$$

In the following we will give a description of the eigenfunctions of the Buslaev-Fomin operator K_v, see (2.3), on the interval (a,b) in terms of the QTB family. To that end we consider the QTB family $\{H_v(\lambda)\}_{\lambda\in\mathbb{R}}$ on the real axis. By the definition of $H_v(\lambda)$ we have to distinguish two cases:

$\lambda \in (-\infty, v_b)$: The coefficients $\kappa_a(\lambda)$ and $\kappa_b(\lambda)$ are real and negative. Therefore the operator family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ is a family of selfadjoint operators.

$\lambda \in (v_b, \infty)$: The imaginary part of $\kappa_b(\lambda)$ is strictly positive, $\mathrm{Im}(\kappa_b(\lambda)) > 0$. Hence, the operator family $\{H_v(\lambda)\}_{\lambda\in(v_b,\infty)}$ is a family of dissipative operators.

Let us first show that the generalized eigenfunctions of K_v are closely related to the family $\{H_v(\lambda)\}_{\lambda\in(v_b,\infty)}$. To that end we introduce the operators $\alpha(\lambda) : \mathcal{H} \longrightarrow \mathfrak{h}(\lambda)$, $\lambda \in (v_b,\infty)$, see also (2.13):

$$\alpha(\lambda)f := \begin{cases} \sqrt{2}\sqrt{q_b(\lambda)}f(b), & \lambda \in (v_b, v_a), \\ \sqrt{2}\begin{pmatrix} \sqrt{q_b(\lambda)}f(b) \\ -\sqrt{q_a(\lambda)}f(a) \end{pmatrix}, & \lambda \in (v_a,\infty), \end{cases} \qquad f \in \mathsf{D}(\alpha(\lambda)) = \mathsf{W}^{1,2} \tag{3.28}$$

Moreover, we define the vectors $e_b(\lambda)$, $e_a(\lambda) \in \mathfrak{h}(\lambda)$, $\lambda \in (v_b,\infty)$, by

$$e_b(\lambda) := \begin{cases} 1, & \lambda \in (v_b,v_a), \\ (1,0)^T, & \lambda \in (v_a,\infty), \end{cases} \qquad e_a(\lambda) := \begin{cases} 0, & \lambda \in (v_b,v_a), \\ (0,1)^T, & \lambda \in (v_a,\infty), \end{cases}$$

where T denotes the transposed of a vector. Furthermore we define the operators $T_v(\lambda) : \mathcal{H} \longrightarrow \mathfrak{h}(\lambda)$, $\lambda \in (v_b,\infty)$, by

$$T_v(\lambda)f := \alpha(\lambda)(H_v(\lambda)^* - \lambda)^{-1}f, \quad f \in \mathcal{H}. \tag{3.29}$$

Note that the definition makes sense, since the spectrum of $H_v(\lambda)$ does not intersect the real line, see [KNR1, Theorem 5.2].

Lemma 3.4. *For $x \in (a,b)$ there is the following representations of the eigenfunctions of the Buslaev-Fomin operator K_v:*

$$\phi_b(v)(x,\lambda) = -i\sqrt{\frac{\hbar}{2\pi}} \exp\left(-i\frac{2m_b}{\hbar}q_b(\lambda)b\right)(T_v(\lambda)^* e_b(\lambda))(x), \qquad \lambda \in (v_b,\infty), \tag{3.30}$$

$$\phi_a(v)(x,\lambda) = i\sqrt{\frac{\hbar}{2\pi}} \exp\left(i\frac{2m_a}{\hbar}q_a(\lambda)a\right)(T_v(\lambda)^* e_a(\lambda))(x), \qquad \lambda \in (v_a,\infty). \tag{3.31}$$

Proof. Using Lemma 2.1 and Proposition 2.3 we get for every $f \in \mathcal{H}$ and $x \in (a,b)$

$$((H_v(\lambda)^* - \lambda)^{-1} f)(x)$$
$$= \frac{\overline{f_1(v)(x,\lambda)}}{\hbar\overline{W_v(\lambda)}} \int_a^x dy\, \overline{f_2(v)(y,\lambda)} f(y) + \frac{\overline{f_2(v)(x,\lambda)}}{\hbar\overline{W_v(\lambda)}} \int_x^b dy\, \overline{f_1(v)(y,\lambda)} f(y).$$

Hence,

$$T_v(\lambda)f = \frac{\sqrt{2}}{\hbar\overline{W_v(\lambda)}} \begin{cases} \sqrt{q_b(\lambda)}\; \overline{f_1(v)(b,\lambda)} \int_a^b dy\, \overline{f_2(v)(y,\lambda)} f(y), & \lambda \in (v_b, v_a), \\ \begin{pmatrix} \sqrt{q_b(\lambda)}\; \overline{f_1(v)(b,\lambda)} \int_a^b dy\, \overline{f_2(v)(y,\lambda)} f(y) \\ -\sqrt{q_a(\lambda)}\; \overline{f_2(v)(a,\lambda)} \int_a^b dy\, \overline{f_1(v)(y,\lambda)} f(y) \end{pmatrix}, & \lambda \in (v_a,\infty). \end{cases}$$

Since

$$f_1(v)(b,\lambda) = \exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)b\right) \quad \text{and} \quad f_2(v)(a,\lambda) = \exp\left(-i\frac{2m_a}{\hbar}q_a(\lambda)a\right),$$

we obtain for all $x \in (a,b)$:

$$(T_v(\lambda)^* e_b(\lambda))(x) = \frac{\sqrt{2q_b(\lambda)} f_2(v)(x,\lambda)}{\hbar W_v(\lambda)} \exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)b\right), \qquad \lambda \in (v_b,\infty),$$

$$(T_v(\lambda)^* e_a(\lambda))(x) = -\frac{\sqrt{2q_a(\lambda)} f_1(v)(x,\lambda)}{\hbar W_v(\lambda)} \exp\left(-i\frac{2m_a}{\hbar}q_a(\lambda)a\right), \qquad \lambda \in (v_a,\infty).$$

By the definition (2.7) of the Wronskians $W_v(\lambda)$ we have

$$W_v(\lambda) = -2iq_a(\lambda)C_{21}(v)(\lambda) = -2iq_b(\lambda)C_{12}(v)(\lambda)$$

or in terms of the scattering coefficients (3.8) and (3.9)

$$\frac{1}{W_v(\lambda)} = \frac{i}{2q_a(\lambda)} S_{ba}(v)(\lambda) = \frac{i}{2q_b(\lambda)} S_{ab}(v)(\lambda).$$

Thus,

$$\frac{1}{\sqrt{2\pi}}(T_v(\lambda)^* e_b(\lambda))(x) = \frac{i\exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)b\right)}{\hbar\sqrt{4\pi q_b(\lambda)}} S_{ab}(v)(\lambda) f_2(v)(x,\lambda)$$
$$= \frac{i\exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)b\right)}{\hbar\sqrt{4\pi q_b(\lambda)}} \psi_b(v)(x,\lambda)$$
$$= \frac{i\exp\left(i\frac{2m_b}{\hbar}q_b(\lambda)b\right)}{\sqrt{\hbar}} \phi_b(x,\lambda),$$

which proves (3.31); similarly we get (3.30). ☐

By means of

$$\vec{\phi}_T(v)(x,\lambda) := \begin{cases} (T_v(\lambda)^* e_b(\lambda))(x), & \lambda \in (v_b, v_a), \\ \begin{pmatrix} (T_v(\lambda)^* e_b(\lambda))(x) \\ (T_v(\lambda)^* e_a(\lambda))(x) \end{pmatrix}, & \lambda \in (v_a, \infty), \end{cases}$$

and

$$Q(\lambda) := \begin{cases} -i \exp\left(-i \frac{2m_b}{\hbar} q_b(\lambda) b\right), & \lambda \in (v_b, v_a), \\ \begin{pmatrix} -i \exp\left(-i \frac{2m_b}{\hbar} q_b(\lambda) b\right) & 0 \\ 0 & i \exp\left(i \frac{2m_a}{\hbar} q_a(\lambda) a\right) \end{pmatrix}, & \lambda \in (v_a, \infty), \end{cases} \tag{3.32}$$

we can write the functions (3.26)

$$\vec{\phi}(v)(x,\lambda) = \sqrt{\frac{\hbar}{2\pi}} Q(\lambda) \vec{\phi}_T(v)(x,\lambda), \quad \lambda \in (v_b, \infty), \quad x \in (a,b).$$

Thus, we get the following

Corollary 3.5. *For $f \in \mathcal{H}$ we get*

$$(\Phi_v f)(\lambda) = \sqrt{\frac{\hbar}{2\pi}} Q(\lambda)^* T_v(\lambda) f, \qquad \lambda \in (v_b, \infty).$$

Remark 3.6. Let $v \in \mathsf{L}^\infty_{\mathbb{R}}$ and $\lambda_0 \in \mathbb{R}$, with $\lambda_0 > v_b$ be given. We set $H_{dis}(v) := H_v(\lambda_0)$ and denote by $K_{dis}(v)$ the selfadjoint dilation corresponding to $H_{dis}(v)$, see Remark 2.5. In [KNR2] it was shown, that the generalized eigenfunctions $\phi_{dis,b}(v), \phi_{dis,a}(v)$ of $K_{dis}(v)$ on the interval (a,b) are given by

$$\phi_{dis,b}(v)(x,\xi) = \frac{1}{\sqrt{2\pi}} (T_{dis}(v;\xi)^* e_b(\lambda_0))(x), \qquad \xi \in \mathbb{R}, \quad x \in (a,b)$$
$$\phi_{dis,a}(v)(x,\xi) = \frac{1}{\sqrt{2\pi}} (T_{dis}(v;\xi)^* e_a(\lambda_0))(x), \qquad \xi \in \mathbb{R}, \quad x \in (a,b),$$

where $T_{dis}(v;\xi) : \mathcal{H} \longrightarrow \mathbb{C}^2$ is defined by

$$T_{dis}(v;\xi) := \alpha(\lambda_0)(H_{dis}(v)^* - \xi)^{-1}, \qquad \xi \in \mathbb{C}_-,$$

see [KNR2, Theorem 5.1.]. Therefore we get by Lemma 3.4 ($\hbar$ scaled to 1)

$$\begin{pmatrix} \phi_b(v)(x,\lambda_0) \\ \phi_a(v)(x,\lambda_0) \end{pmatrix} = Q(\lambda_0) \begin{pmatrix} \phi_{dis,b}(v)(x,\lambda_0) \\ \phi_{dis,a}(v)(x,\lambda_0) \end{pmatrix}, \qquad x \in (a,b).$$

i.e. the generalized eigenfunctions of K_v and $K_{dis}(v)$ coincide, modulo a unitary transformation, for any *fixed* energy $\lambda_0 > v_b$.

We are now going to show that the eigenfunctions and eigenvalues of the operator family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ determine the eigenfunctions and eigenvalues of K_v in a unique way. Let us first define what we mean by the eigenvalues and eigenfunction of an operator family.

Definition 3.7. An element $f \in \mathcal{H}$ is called an eigenvector of the operator family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$, if $H_v(\mu(v))f = \mu(v)f$ for some $\mu(v) \in (-\infty, v_b)$; $\mu(v)$ is called the corresponding eigenvalue. The set of all these eigenvalues—the spectrum of $\{H_v(\lambda)\}$—is denoted by $\sigma(\{H_v(\lambda)\})$ and the normalized eigenfunctions of $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ corresponding to the eigenvalue $\mu(v)$ are denoted by $\eta(v)(\cdot, \mu(v))$.

For every $\mu(v) \in \sigma(\{H_v(\lambda)\})$ we set

$$\tilde{\phi}(v)(x,\mu(v)) = \begin{cases} \exp\left(-\kappa_a(\mu(v))\frac{2m_a}{\hbar}(x-a)\right)\eta(v)(a,\mu(v)), & x\in(-\infty,a],\\ \eta(v)(x,\mu(v)), & x\in(a,b),\\ \exp\left(\kappa_b(\mu(v))\frac{2m_b}{\hbar}(x-b)\right)\eta(v)(b,\mu(v)), & x\in[b,\infty).\end{cases}$$

Note that $\kappa_a(\lambda), \kappa_b(\lambda) < 0$ for all $\lambda \in (-\infty, v_b)$. Hence, $\tilde{\phi}(v)(\cdot,\mu(v)) \in \mathcal{K}$ for every $\mu(v) \in \sigma(\{H_v(\lambda)\})$. Since $\eta(v)(\cdot,\mu(v)) \in \mathsf{D}(H_v(\mu(v)))$, see Definition 2.2, it satisfies the quantum transmitting boundary condition and a straightforward calculation shows that

$$\left(\tilde{\phi}(v)(\cdot,\mu(v)), \tilde{\phi}(v)(\cdot,\xi(v))\right)_{\mathcal{K}} = 0, \quad \text{for } \mu(v),\xi(v)\in\sigma(\{H_v(\lambda)\}),\ \mu(v)\neq\xi(v). \tag{3.33}$$

The following Lemma states the relation between the eigenvalues and eigenfunctions of the family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ and the eigenvalues and eigenfunctions of the Buslaev-Fomin operator K_v.

Lemma 3.8. *Assume that $v \in \mathsf{L}^\infty_{\mathbb{R}}$.*

(i) If $\mu(v) \in \sigma(\{H_v(\lambda)\})$, then

$$\phi_p(v)(\cdot,\mu(v)) := \frac{\tilde{\phi}(v)(\cdot,\mu(v))}{\|\tilde{\phi}(v)(\cdot,\mu(v))\|_{\mathcal{K}}}, \tag{3.34}$$

is an eigenfunction of K_v corresponding to the eigenvalue $\mu(v)$. Furthermore, these eigenfunctions are mutually orthonormal for different eigenvalues $\mu(v)$.

(ii) If $\lambda_j(v) \in \sigma_p(K_v)$, then the function

$$\eta(v)(x,\lambda_j(v)) := \frac{\phi_p(v)(x,\lambda_j(v))}{\|\phi_p(v)(\cdot,\lambda_j(v))\chi_{(a,b)}\|_{\mathcal{K}}}, \qquad x\in(a,b),$$

is a normalized eigenfunction of the family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$.

(iii) The point spectrum of K_v and the spectrum of the operator family $\{H_v(\lambda)\}$ coincide, i.e.

$$\sigma_p(K_v) = \sigma(\{H_v(\lambda)\}).$$

Proof. Let us first prove (i). Assume that $\mu(v) \in \sigma(\{H_v(\lambda)\})$. Using the boundary conditions of $\eta(v)(\cdot, \mu(v))$ one verifies that $\tilde{\phi}(v)(\cdot, \mu(v)) \in \mathsf{D}(K_v)$. Since

$$H_v(\mu(v))\eta(v)(\cdot, \mu(v)) = \mu(v)\eta(v)(\cdot, \mu(v))$$

there is

$$K_v\tilde{\phi}(v)(\cdot, \mu(v)) = \mu(v)\tilde{\phi}(v)(\cdot, \mu(v)).$$

By means of (3.33) and (3.34) one now obtains that the $\phi_p(v)(\cdot, \mu(v))$ are indeed mutually orthogonal eigenfunctions of K_v for different eigenvalues of the family $\{H_v(\lambda)\}_{\lambda \in (-\infty, v_b)}$. Moreover, the $\phi_p(v)(\cdot, \mu(v))$ have norm one in $\mathcal{K}$.

Assume now $\lambda_j(v) \in \sigma_p(K_v)$. In order to prove (ii) it suffices to show that the functions $\phi_p(v)(\cdot, \lambda_j(v))$ satisfy the boundary condition at a and b imposed on functions from the domain of the QTB family $\{H_v(\lambda)\}_{\lambda \in (-\infty, v_b)}$, see Definition 2.2. We set

$$\tilde{\psi}(v)(x, \lambda_j(v)) := \begin{cases} \exp\left(-\kappa_a(\lambda_j(v))\frac{2m_a}{\hbar}(x-a)\right)\phi_p(v)(a, \lambda_j(v)), & x \in (-\infty, a], \\ \phi_p(v)(x, \lambda_j(v)), & x \in (a, b), \\ \exp\left(\kappa_b(\lambda_j(v))\frac{2m_b}{\hbar}(x-b)\right)\phi_p(v)(b, \lambda_j(v)), & x \in [b, \infty). \end{cases}$$

There is $\tilde{\psi}(v)(\cdot, \lambda_j(v)) \in \mathsf{D}(K_v)$ and $K_v\tilde{\psi}(v)(\cdot, \lambda_j(v)) = \lambda_j(v)\tilde{\psi}(v)(\cdot, \lambda_j(v))$. Since the eigenvalues of K_v are simple, there exists a constant $C(\lambda_j(v)) \in \mathbb{C}$ such that

$$\phi_p(v)(\cdot, \lambda_j(v)) = C(\lambda_j(v))\tilde{\psi}(v)(\cdot, \lambda_j(v)).$$

We have

$$\frac{\hbar}{2m(a)}\tilde{\psi}'(v)(a, \lambda_j(v)) = \frac{\hbar}{2m_a}\tilde{\psi}'(v)(a, \lambda_j(v)) = -\kappa_a(\lambda_j(v))\tilde{\psi}(v)(a, \lambda_j(v)),$$

i.e. $\tilde{\psi}(v)(\cdot, \lambda_j(v))$ satisfies the boundary condition at a. In the same way one gets that $\tilde{\psi}(v)(\cdot, \lambda_j(v))$ satisfies the boundary condition at b. Thus, (ii) has been proven. The statement (iii) follows directly from the statements (i) and (ii). □

4 Scattering matrix

In this section we investigate the scattering matrix corresponding to the Buslaev-Fomin operator (2.3). As we will see later, the scattering matrix plays an important role for the current. Furthermore, we will show that the scattering matrix can be completely expressed in terms of the QTB family. The scattering matrix $S_v(\lambda)$ is defined by

$$S_v(\lambda) := \begin{cases} S_{bb}(v)(\lambda), & \lambda \in (v_b, v_a), \\ \tilde{S}(v)(\lambda), & \lambda \in (v_a, \infty), \end{cases} \tag{4.1}$$

where

$$\tilde{S}(v)(\lambda) := \begin{pmatrix} S_{bb}(v)(\lambda) & \sqrt{\frac{q_b(\lambda)}{q_a(\lambda)}} S_{ba}(v)(\lambda) \\ \sqrt{\frac{q_a(\lambda)}{q_b(\lambda)}} S_{ab}(v)(\lambda) & S_{aa}(\lambda) \end{pmatrix}$$

and $S_{ij}(v)(\lambda)$, $i,j = a,b$ are the scattering coefficients (3.8), (3.9). By (3.10), (3.11) and (3.13) we get that $S_v(\lambda)S_v(\lambda)^* = S_v^*(\lambda)S_v(\lambda) = \mathbb{I}_{\mathfrak{h}(\lambda)}$, $\lambda \in (v_b, \infty)$, i.e. $S_v(\lambda)$ is unitary. We define $\widehat{\mathcal{K}}_{ac} := \mathsf{L}^2((v_b,\infty), \mathfrak{h}(\lambda), d\lambda)$. By $\widehat{S_v}$ we denote the—unitary—multiplication operator $\widehat{S_v} : \widehat{\mathcal{K}}_{ac} \longrightarrow \widehat{\mathcal{K}}_{ac}$ induced by $S_v(\lambda)$:

$$(\widehat{S_v} f)(\lambda) = S_v(\lambda) f(\lambda), \quad f \in \mathsf{D}(\widehat{S_v}) := \widehat{\mathcal{K}}_{ac}. \tag{4.2}$$

Since

$$(K_v - i)^{-1} - (K_w - i)^{-1} = (K_v - i)^{-1}(Ev - Ew)(K_w - i)^{-1} = (K_v - i)^{-1}(v - w)P_{\mathcal{H}}^{\mathcal{K}}(K_w - i)^{-1}$$

is trace class for all $v, w \in \mathsf{L}^\infty_{\mathbb{R}}$ the wave operators

$$W_\pm(K_v, K_w) := \operatorname*{s-lim}_{t\to\pm\infty} \exp(itK_v)\exp(-itK_w)P_{ac}(K_w),$$

exist and are asymptotically complete, where $P_{ac}(K_w)$ denotes the projection onto the absolutely continuous subspace of K_w, see [RS1, Theorem XI.9].

Lemma 4.1. *(For the case $v_a = v_b = 0$ and $\widehat{m} \equiv 1$ see also [W, 17.c].) For every v, $w \in \mathsf{L}^\infty_{\mathbb{R}}$ the wave operators obey*

$$\Phi_v W_+(K_v, K_w)\Phi_w^* = \widehat{S_v}^* \widehat{S_w}, \qquad \Phi_v W_-(K_v, K_w)\Phi_w^* = \mathbb{I}_{\widehat{\mathcal{K}}_{ac}},$$

where Φ_v is the Fourier transform with respect to K_v, see (3.27), and $\widehat{S_v}$ is the multiplication operator (4.2) induced by the scattering matrix.

Proof. We will only prove the first equation, the second one can be proven similarly. Let us define the projections $P_1(v) : \mathcal{K} \to \mathcal{K}$ and $P_2(v) : \mathcal{K} \to \mathcal{K}$ by

$$P_1(v) := \Phi_v^* \chi_{(v_b, v_a)} \Phi_v, \qquad P_2(v) := \Phi_v^* \chi_{(v_a, \infty)} \Phi_v, \qquad v \in \mathsf{L}^\infty_{\mathbb{R}}.$$

There is

$$W_+(K_v, K_w) = P_1(v) W_+(K_v, K_w) P_1(w) + P_2(v) W_+(K_v, K_w) P_2(w).$$

Hence, it suffices to show:

$$\left(\Phi_v W_+(K_v, K_w)\Phi_w^* \hat{f}\right)(\lambda) = \overline{S_{bb}(v)(\lambda)} S_{bb}(w) \hat{f}(\lambda), \qquad \hat{f} \in \mathsf{L}^2(v_b, v_a), \tag{4.3}$$

$$\left(\Phi_v W_+(K_v, K_w)\Phi_w^* \hat{f}\right)(\lambda) = \tilde{S}(v)(\lambda)^* \tilde{S}(w)(\lambda) \hat{f}(\lambda), \qquad \hat{f} \in \mathsf{L}^2((v_a, \infty), \mathbb{C}^2). \tag{4.4}$$

We will only prove (4.3); the proof of (4.4) is similar. Since $\chi_{(a,b)}(K_w+i)^{-1}$ is compact, in fact it is even trace class, we get by [BW, Proposition 6.70] that

$$\operatorname*{s-lim}_{t\to+\infty}\chi_{(a,b)}(K_w+i)^{-1}\exp(-itK_w)P_{ac}(K_w)=0.$$

Applying this to all vectors of the form $(K_w+i)f$ we obtain

$$\operatorname*{s-lim}_{t\to+\infty}\chi_{(a,b)}\exp(-itK_w)P_{ac}(K_w)=0. \tag{4.5}$$

Therefore

$$\Phi_v W_+(K_v,K_w)\Phi_w^*\hat{f}=\Phi_v W_a(K_v,K_w)\Phi_w^*\hat{f}+\Phi_v W_b(K_v,K_w)\Phi_w^*\hat{f} \tag{4.6}$$

for $\hat{f}\in \mathsf{L}^2(v_b,v_a)$, where

$$\begin{aligned} W_a(K_v,K_w) &:= \operatorname*{s-lim}_{t\to+\infty}\exp(itK_v)\chi_{(-\infty,a)}\exp(-itK_w)P_{ac}(K_w),\\ W_b(K_v,K_w) &:= \operatorname*{s-lim}_{t\to+\infty}\exp(itK_v)\chi_{(b,\infty)}\exp(-itK_w)P_{ac}(K_w). \end{aligned}$$

For every $\hat{g}\in \mathsf{L}^2(v_b,v_a)$ there is

$$(\chi_{(-\infty,a)}\Phi_w^*\hat{g})(x)=\chi_{(-\infty,a)}(x)\int_{v_b}^{v_a}d\lambda\,\phi_b(w)(x,\lambda)\hat{g}(\lambda).$$

Since $q_a(\lambda)$ is purely imaginary for $\lambda\in(v_b,v_a)$, we obtain by (3.16) that $\chi_{(-\infty,a)}\Phi_w^*$ is a compact operator from $\mathsf{L}^2(v_b,v_a)$ into $\mathcal{K}$. This yields

$$\lim_{t\to+\infty}\chi_{(-\infty,a)}\exp(-itK_w)\Phi_w^*\hat{f}=0 \qquad \text{for all } \hat{f}\in\mathsf{L}^2(v_b,v_a).$$

Therefore

$$\Phi_v W_a(K_v,K_w)\Phi_w^*\hat{f}=0 \qquad \text{for all } \hat{f}\in\mathsf{L}^2(v_b,v_a). \tag{4.7}$$

For every $\hat{f}\in \mathsf{C}_0^\infty(v_b,v_a)$ we have

$$\begin{aligned}&\Big(\Phi_v W_b(K_v,K_w)\Phi_w^* f\Big)(\lambda)\\ &\quad=\lim_{t\to+\infty}\lim_{N\to+\infty}\int_b^N dx\int_{v_b}^{v_a}d\mu\;\exp(it(\lambda-\mu))\overline{\phi_b(v)(x,\lambda)}\phi_b(w)(x,\mu)\hat{f}(\mu).\end{aligned} \tag{4.8}$$

Using (3.16) we find for $x\in(b,\infty)$

$$\begin{aligned}\overline{\phi_b(v)(x,\lambda)}\phi_b(v_0)(x,\mu)=\frac{1}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}\Big(&\exp\left(i\tfrac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)\\ &+\overline{S_{bb}(v)(\lambda)}\exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\\ &+S_{bb}(w)(\mu)\exp\left(i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\\ &+\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\mu)\exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)\Big).\end{aligned} \tag{4.9}$$

We have

$$\int_b^N dx \int_{v_b}^{v_a} d\mu \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(it(\lambda-\mu)\right)\hat{f}(\mu)$$

$$= \int_{v_b}^{v_a} d\mu \, \hat{f}(\mu)e^{it(\lambda-\mu)} \int_b^N dx \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\hbar\pi\sqrt{q_b(\lambda)q_b(\mu)}}.$$

There is in the sense of distributions

$$\frac{\hbar}{i\pi} \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))N\right)}{2m_b(q_b(\lambda)-q_b(\mu))} \longrightarrow \delta\left(\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))\right) \qquad \text{as } N\to\infty. \tag{4.10}$$

Hence,

$$\lim_{N\to+\infty}\int_b^N dx \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}$$

$$= \frac{\delta\left(\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))\right)}{4\hbar\sqrt{q_b(\lambda)q_b(\mu)}} - \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))b\right)}{4i\pi\sqrt{q_b(\lambda)q_b(\mu)}} \, \frac{(q_b(\lambda)+q_b(\mu))}{\lambda-\mu}$$

$$= \frac{1}{2}\delta(\lambda-\mu) - \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))b\right)}{4i\pi\sqrt{q_b(\lambda)q_b(\mu)}} \, \frac{(q_b(\lambda)+q_b(\mu))}{\lambda-\mu}.$$

Further we get

$$\lim_{N\to+\infty}\int_b^N dx \int_{v_b}^{v_a} d\mu \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}\hat{f}(\mu)$$

$$= \frac{1}{2}\hat{f}(\lambda) - \frac{1}{2}\int_{v_b}^{v_a} d\mu \, \hat{f}(\mu)\frac{\exp\left(it(\lambda-\mu)\right)}{2i\pi(\lambda-\mu)} \exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))b\right)\frac{(q_b(\lambda)+q_b(\mu))}{\sqrt{q_b(\lambda)q_b(\mu)}}.$$

Since in the sense of distributions

$$\frac{1}{i\pi}\frac{\exp\left(it(\lambda-\mu)\right)}{\lambda-\mu} \longrightarrow \delta(\lambda-\mu) \qquad \text{as } t\to\infty \tag{4.11}$$

we finally obtain

$$\lim_{t\to+\infty}\int_b^\infty dx \int_{v_b}^{v_a} d\mu \, \frac{\exp\left(i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(it(\lambda-\mu)\right)\hat{f}(\mu) = 0. \tag{4.12}$$

Furthermore we have

$$\lim_{N\to+\infty}\int_b^N dx \int_{v_b}^{v_a} d\mu\frac{\overline{S_{bb}(v)(\lambda)}}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\exp\left(it(\lambda-\mu)\right)\hat{f}(\mu)$$

$$= \overline{S_{bb}(v)(\lambda)}\int_{v_b}^{v_a} d\mu\hat{f}(\mu)\exp\left(it(\lambda-\mu)\right)\int_b^\infty dx \, \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}.$$

Since

$$\int_b^\infty dx \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} = \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))b\right)}{4\pi i\sqrt{q_b(\lambda)q_b(\mu)}}\,\frac{(q_b(\lambda)-q_b(\mu))}{\lambda-\mu}$$

one gets

$$\begin{aligned}\int_b^\infty dx \int_{v_b}^{v_a} d\mu \frac{\overline{S_{bb}(v)(\lambda)}}{4\pi\hbar\sqrt{q_b(\lambda)}\sqrt{q_b(\mu)}} \exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\exp\left(it(\lambda-\mu)\right)\hat{f}(\mu)\\ = \overline{S_{bb}(v)(\lambda)}\int_{v_b}^{v_a} d\mu \hat{f}(\mu)\frac{\exp\left(it(\lambda-\mu)\right)}{i\pi(\lambda-\mu)}\exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))b\right)\frac{(q_b(\lambda)-q_b(\mu))}{4\sqrt{q_b(\lambda)q_b(\mu)}}\end{aligned}$$

which yields

$$\lim_{t\to\infty}\int_b^\infty dx \int_{v_b}^{v_a} d\mu \frac{\overline{S_{bb}(v)(\lambda)}}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\exp\left(it(\lambda-\mu)\right)\hat{f}(\mu) = 0. \tag{4.13}$$

Similarly we prove

$$\lim_{t\to\infty}\int_b^\infty dx \int_{v_b}^{v_a} d\mu \frac{S_{bb}(w)(\mu)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(i\tfrac{2m_b}{\hbar}(q_b(\lambda)+q_b(\mu))x\right)\exp\left(it(\lambda-\mu)\right)\hat{f}(\mu) = 0. \tag{4.14}$$

We have

$$\begin{aligned}\lim_{N\to+\infty}\int_b^N dx \int_{v_b}^{v_a} d\mu \frac{\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\mu)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}} \exp\left(-i2m_b\left(q_b(\lambda)-q_b(\mu)\right)x\right)\times\\ \times\exp\left(it(\lambda-\mu)\right)\hat{f}(\mu)\\ = \int_{v_b}^{v_a} d\mu \hat{f}(\mu)\exp\left(it(\lambda-\mu)\right)\frac{\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\mu)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}\int_b^\infty dx\,\exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right).\end{aligned}$$

Since

$$\begin{aligned}\lim_{N\to+\infty}\int_b^N dx \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)}{4\pi\hbar\sqrt{q_b(\lambda)q_b(\mu)}}\\ = \frac{\delta\left(\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))\right)}{4\sqrt{q_b(\lambda)q_b(\mu)}} + \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))b\right)}{4i\pi\sqrt{q_b(\lambda)q_b(\mu)}}\,\frac{(q_b(\lambda)+q_b(\mu))}{\lambda-\mu}\\ = \frac{1}{2}\delta(\lambda-\mu) + \frac{\exp\left(-i\frac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))b\right)}{4i\pi\sqrt{q_b(\lambda)q_b(\mu)}}\,\frac{(q_b(\lambda)+q_b(\mu))}{\lambda-\mu}\end{aligned}$$

we obtain

$$\lim_{t\to+\infty}\int_b^\infty dx\int_{v_b}^{v_a} d\mu \frac{\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\mu)}{4\pi\sqrt{q_b(\lambda)q_b(\mu)}}\exp\left(-i\tfrac{2m_b}{\hbar}(q_b(\lambda)-q_b(\mu))x\right)\times$$
$$\times \exp\left(it(\lambda-\mu)\right)\hat{f}(\mu)$$
$$=\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\lambda)\hat{f}(\lambda). \quad (4.15)$$

Thus, we get by (4.8), (4.9), (4.12), (4.13), (4.14), and (4.15) that

$$\left(\Phi_v W_b(K_v,K_w)\Phi_w^*\hat{f}\right)(\lambda)=\overline{S_{bb}(v)(\lambda)}S_{bb}(w)(\lambda)\hat{f}(\lambda) \quad (4.16)$$

for $f\in \mathsf{C}_0^\infty(v_b,v_a)$ and $\lambda\in(v_b,v_a)$. Now (4.16), (4.7) and (4.6) imply the assertion (4.4). □

In the following we set $v_0\in \mathsf{L}^\infty_{\mathbb{R}}$, $v_0\equiv v_b$. Lemma 4.1 implies

Corollary 4.2. *If $v_0(x)=v_b$ for all $x\in\mathbb{R}$, then*

$$\Phi_v=\Phi_{v_0}W_-(K_v,K_{v_0})^*=\widehat{S_v}^*\widehat{S_{v_0}}\Phi_{v_0}W_+(K_v,K_{v_0})^*$$
$$\widehat{S_v}=\widehat{S_{v_0}}\Phi_{v_0}W_+(K_v,K_{v_0})^*W_-(K_v,K_{v_0})\Phi_{v_0}^*=\widehat{S_{v_0}}\Phi_{v_0}S(K_v,K_{v_0})\Phi_{v_0}^*$$

for all $v\in\mathsf{L}^\infty_{\mathbb{R}}$, where $S(K_v,K_{v_0})$ is the scattering operator

$$S(K_v,K_{v_0}):=W_+(K_v,K_{v_0})^*W_-(K_v,K_{v_0}).$$

The scattering matrix $S_v(\lambda)$ can be completely described by the QTB family:

Lemma 4.3. *Let $\alpha(\lambda)$, $T_v(\lambda)$, and $Q(\lambda)$ be given by (3.28), (3.29), and (3.32), respectively. The scattering matrix (4.1) obeys*

$$S_v(\lambda)=Q(\lambda)\left(\mathbb{I}_{\mathfrak{h}(\lambda)}+i\hbar\alpha(\lambda)T_v(\lambda)^*\right)Q(\lambda),\qquad \lambda\in(v_b,\infty). \quad (4.17)$$

Proof. Using the definitions of $\alpha(\lambda)$ and $T_v(\lambda)$ one gets

$$\alpha(\lambda)T_v(\lambda)^*=\sqrt{2}\begin{cases}\sqrt{q_b(\lambda)}(T_v(\lambda)^*e_b)(b), & \lambda\in(v_b,v_a),\\ \begin{pmatrix}\sqrt{q_b(\lambda)}(T_v(\lambda)^*e_b)(b) & \sqrt{q_b(\lambda)}(T_v(\lambda)^*e_a)(b)\\ -\sqrt{q_a(\lambda)}(T_v(\lambda)^*e_b)(a) & -\sqrt{qa(\lambda)}(T_v(\lambda)^*e_a)(a)\end{pmatrix}, & \lambda\in(v_a,\infty).\end{cases}$$

Taking into account (3.30) and (3.31) we obtain

$$\alpha(\lambda)T_v(\lambda)^*=i\sqrt{\frac{4\pi}{\hbar}}\begin{cases}p_b(\lambda)\sqrt{q_b(\lambda)}\phi_b(b,\lambda), & \lambda\in(v_b,v_a),\\ \begin{pmatrix}p_b(\lambda)\sqrt{q_b(\lambda)}\phi_b(b,\lambda) & -p_a(\lambda)\sqrt{q_b(\lambda)}\phi_a(b,\lambda)\\ -p_b(\lambda)\sqrt{q_a(\lambda)}\phi_b(a,\lambda) & p_a(\lambda)\sqrt{q_a(\lambda)}\phi_a(a,\lambda)\end{pmatrix}, & \lambda\in(v_a,\infty),\end{cases}$$

where

$$p_b(\lambda) := \exp\left(i\tfrac{2m_b}{\hbar}q_b(\lambda)b\right) \quad \text{and} \quad p_a(\lambda) := \exp\left(-i\tfrac{2m_a}{\hbar}q_a(\lambda)a\right).$$

By equations (3.15), (3.16), and (3.23) one has

$$\alpha(\lambda)T_v(\lambda)^* = \frac{i}{\hbar}\mathbb{I}_{\mathfrak{h}(\lambda)} + \frac{i}{\hbar}\begin{cases} S_{bb}(v)(\lambda)p_b(\lambda)^2, & \lambda \in (v_b, v_a), \\ \begin{pmatrix} S_{bb}(v)(\lambda)p_b(\lambda)^2 & -\sqrt{\frac{q_b(\lambda)}{q_a(\lambda)}}S_{ba}(v)(\lambda)p_b(\lambda)p_a(\lambda) \\ -\sqrt{\frac{q_a(\lambda)}{q_b(\lambda)}}S_{ab}(v)(\lambda)p_b(\lambda)p_a(\lambda) & S_{aa}(v)(\lambda)p_a(\lambda)^2 \end{pmatrix}, & \lambda \in (v_a, \infty) \end{cases}$$

which yields (4.17). □

Remark 4.4. Rewriting (4.17) formally as

$$S_v(\lambda) = Q(\lambda)\left(\mathbb{I}_{\mathfrak{h}(\lambda)} + i\hbar\alpha(\lambda)(H_v(\lambda) - \lambda)^{-1}\alpha(\lambda)^*\right)Q(\lambda)$$

one suspects, that the resonances of K_v are given by

$$\{z \in \mathbb{C}_- | z \text{ is eigenvalue of } H_v(z)\},$$

see also Definition 3.7.

Remark 4.5. Let $v \in \mathsf{L}^\infty_{\mathbb{R}}$ and $\lambda_0 \in \mathbb{R}$ with $\lambda_0 > v_b$ be given. As in Remarks 2.5 and 3.6 we set $H_{dis}(v) := H_v(\lambda_0)$. The adjoint of the so-called characteristic function $\Theta_{H_{dis}(v)}(z) : \mathbb{C}^2 \longrightarrow \mathbb{C}^2$, $z \in \overline{\mathbb{C}_+}$, corresponding to the dissipative operator $H_{dis}(v)$ (see [FN]) is given by

$$\Theta_{H_{dis}(v)}(z)^* = \mathbb{I}_{\mathbb{C}^2} + i\alpha(\lambda_0)T_{dis}(v;\overline{z})^*, \qquad z \in \overline{\mathbb{C}_+},$$

where $T_{dis}(v;z)$ is defined as in Remark 3.6, and $\hbar$ is scaled to 1, see [KNR2, Lemma 3.3]. Therefore we get by Lemma 4.3

$$S_v(\lambda_0) = Q(\lambda_0)\Theta_{H_{dis}(v)}(\lambda_0)^*Q(\lambda_0),$$

i.e. for any *fixed* energy λ_0 the characteristic function is equal to the scattering matrix $S_v(\lambda_0)$, modulo the transformation $Q(\lambda_0)$.

5 Carrier and current densities

In this section we introduce the carrier density and the current density corresponding to the QTB family $\{H_v(z)\}_{z\in\mathbb{C}_+}$ from Definition 2.2.

5.1 Carrier densities

We now assume that ρ is a function

$$\rho = \rho_p \oplus \rho_{ac} \quad \text{with} \quad \rho_p \in \mathsf{C}^{\mathsf{b}}_{\mathbb{R}}(-\infty, v_b), \quad \rho_{ac} \in \mathsf{L}^\infty((v_b,\infty), \mathfrak{B}(\mathfrak{h}(\lambda)), \nu_{ac}), \tag{5.1}$$

where ν_{ac} is given as in (3.25). Note that ν_{ac} does not depend on the potential v while ν_p in (3.25) does. We have $\rho(\cdot) \in \mathsf{L}^\infty(\sigma(K_v), \mathfrak{B}(\mathfrak{h}(\lambda)), \nu)$ for all $v \in \mathsf{L}^\infty_{\mathbb{R}}$. Furthermore we assume

$$\rho_{ac}(\lambda)^* = \rho_{ac}(\lambda), \quad \rho_{ac}(\lambda) \geq 0 \quad \text{for a.e. } \lambda \in (v_b, \infty), \quad \text{and} \quad \rho_p \geq 0. \tag{5.2}$$

By means of a function (5.1) we define the multiplication operator $\widehat{\rho}$ on $\widehat{\mathcal{K}}_v$ by

$$(\widehat{\rho} g)(\lambda) := \rho(\lambda) g(\lambda), \quad g \in \mathsf{D}(\widehat{\rho}) = \mathsf{L}^2(\sigma(K_v), \mathfrak{h}(\lambda), \nu) \tag{5.3}$$

and finally the steady state $\varrho(v) : \mathcal{K} \longrightarrow \mathcal{K}$ by

$$\varrho(v) = \Phi_v^* \widehat{\rho} \Phi_v. \tag{5.4}$$

Obviously $\varrho(v)$ is a bounded, non-negative, selfadjoint operator which commutes with K_v.

Remark 5.1. There is a one-to-one correspondence between bounded, non-negative, selfadjoint operators which commute with K_v and multiplication operators of the form (5.3), i.e. if $\varrho(v) : \mathcal{K} \longrightarrow \mathcal{K}$ is a bounded, non-negative, selfadjoint operator, which commutes with K_v, then there exists exactly one function $\rho \in \mathsf{L}^\infty(\sigma(K_v), \mathfrak{B}(\mathfrak{h}(\lambda)), \nu)$ such that $\varrho(v)$ has the representation given by (5.4), see [BW, Proposition 4.18].

Remark 5.2. Using Corollary 4.2 we can rewrite equation (5.4) in the form

$$\varrho(v) = \varrho_p(v) + \varrho_{ac}(v), \tag{5.5}$$

where

$$\varrho_{ac}(v) = W_-(K_v, K_{v_0}) \varrho(v_0) W_-(K_v, K_{v_0})^*, \qquad \varrho(v_0) = \Phi_{v_0}^* \widehat{\rho_{ac}} \Phi_{v_0}, \tag{5.6}$$

and K_{v_0} is the operator (2.3) and Φ_{v_0} the corresponding Fourier transform with respect to the constant potential $v_0 \equiv v_b$, see also Corollary 4.2. The operator $\varrho_p(v)$ admits the representation, see also [N1],

$$\varrho_p(v) = \sum_{j=1}^{N(v)} \rho_p(\lambda_j(v)) P(\lambda_j(v)), \tag{5.7}$$

where $P(\lambda_j(v))$ are the orthogonal projections of K_v onto the eigenspaces corresponding to the eigenvalues $\lambda_j(v)$, $j = 1, \ldots, N(v)$, i.e.

$$P(\lambda_j(v)) f = \left(f, \vec{\phi}_v(\cdot, \lambda_j(v))\right)_{\mathcal{K}} \vec{\phi}_v(\cdot, \lambda_j(v)), \qquad f \in \mathcal{K}.$$

In the following we assume

$$C_{ac} := \operatorname*{esssup}_{\lambda\in(v_b,\infty)} \|\rho_{ac}(\lambda)\|_{\mathfrak{B}(\mathfrak{h}(\lambda))}\sqrt{\lambda^2+1} < \infty \tag{5.8}$$

and we define

$$C_p := \sup_{\lambda\in(-\infty,v_b)} \rho_p(\lambda). \tag{5.9}$$

(5.4) and (5.8) imply

$$\|\varrho_{ac}(v)(K_v - i)\|_{\mathfrak{B}(\mathcal{K})} = C_{ac} < \infty. \tag{5.10}$$

For every $h \in \mathsf{L}^\infty_{\mathbb{R}}$ we define the multiplication operator $M(h) : \mathcal{K} \longrightarrow \mathcal{K}$ by

$$(M(h)f)(x) = \begin{cases} h(x)f(x), & x \in (a,b), \\ 0, & x \in \mathbb{R}\setminus(a,b), \end{cases} \qquad f \in \mathsf{D}(M(h)) = \mathcal{K}; \tag{5.11}$$

note $\mathrm{ran}(M(h)) \subseteq \mathcal{H}$. For any Borel set $\omega \subseteq (a,b)$ we consider the observable $U(\omega) := M(\chi_\omega) : \mathcal{K} \longrightarrow \mathcal{K}$. Now we define the expectation value of $U(\omega)$ with respect to $\varrho(v)$ for any Borel set $\omega \subset (a,b)$ by

$$\mathbb{E}_{\varrho(v)}(\omega) := \mathrm{tr}(\varrho(v)U(\omega)).$$

The definition is justified since

$$|\mathrm{tr}(\varrho(v)U(\omega))| \le C_p N(v) + C_{ac}\|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\|_{\mathfrak{B}_1(\mathcal{K})} < \infty,$$

where (5.10) comes to bear. There is

$$\mathrm{tr}(\varrho(v)U(\omega)) = \mathrm{tr}(\widehat{\rho}\Phi_v U(\omega)\Phi_v^*) = \int_\omega dx \int_{\sigma(K_v)} d\nu(\lambda)\ \mathrm{tr}_{\mathfrak{h}(\lambda)}(\rho(\lambda)D(v)(x,\lambda)), \tag{5.12}$$

where

$$D(v)(x,\lambda) := \begin{cases} |\phi_p(v)(x,\lambda)|^2, & \lambda \in \sigma_p(K_v), \\ |\phi_b(v)(x,\lambda)|^2, & \lambda \in (v_b,v_a), \\ \begin{pmatrix} |\phi_b(v)(x,\lambda)|^2 & \phi_a(v)(x,\lambda)\overline{\phi_b(v)(x,\lambda)} \\ \phi_b(v)(x,\lambda)\overline{\phi_a(v)(x,\lambda)} & |\phi_a(v)(x,\lambda)|^2 \end{pmatrix}, & \lambda \in (v_a,\infty). \end{cases}$$

Hence, $\mathbb{E}_{\varrho(v)}(\cdot)$ defines a measure which is absolutely continuous with respect to the Lebesgue measure.

Definition 5.3. The Radon-Nikodym derivative of $\mathbb{E}_{\varrho(v)}(\cdot)$ is called the carrier density, with respect to $\varrho(v)$, of the open quantum system described by the QTB family $\{H_v(z)\}_{z\in\mathbb{C}_+}$ and will be denoted by $u_{\varrho(v)}$. Note the assumptions (5.1), (5.2), and (5.8).

(5.12) directly implies

$$u_{\varrho(v)}(x) = \int_{\sigma(K_v)} d\nu(\lambda)\ u_{\varrho(v)}(x,\lambda), \qquad x \in (a,b), \tag{5.13}$$

with

$$u_{\varrho(v)}(x,\lambda) := \left(\rho(\lambda)^T\vec{\phi}_v(x,\lambda),\vec{\phi}_v(x,\lambda)\right)_{\mathfrak{h}(\lambda)}, \qquad \lambda\in\sigma(K_v), \qquad x\in(a,b), \tag{5.14}$$

where $\rho(\lambda)^T$ denotes the transposed matrix. Since $\rho \geq 0$ the carrier density is positive, i.e. $u_{\varrho(v)}(x) \geq 0$ for a.e. $x \in (a,b)$. Note that in (5.14) enter only the values of the eigenfunctions for arguments $x \in (a,b)$. These can be expressed by the QTB family, see Lemma 3.4 and Lemma 3.8.

Remark 5.4. As in Remarks 2.5, 3.6, and 4.5 we fix a $\lambda_0 > v_b$ and define

$$\rho_{dis}(\lambda_0) := Q(\lambda_0)^*\rho(\lambda_0)Q(\lambda_0), \tag{5.15}$$

where $Q(\lambda_0)$ is given by (3.32). Remark 3.6 and the results from [KNR2, Section 3] imply

$$u_{dis,v}(x,\lambda_0) = u_{\varrho(v)}(x,\lambda),$$

where $u_{dis,v}(x,\xi)$, $\xi\in\mathbb{R}$, is defined as in [KNR2, Section 3] with the density matrix $\rho_{dis}(\lambda_0)$ given by (5.15). Thus, we get that the carrier density of the dissipative system and the carrier density of the QTB system coincide for fixed energy λ_0, if the density matrix for the dissipative system is transformed by (5.15).

Example 5.5. Let $f \in \mathrm{C}^{\mathrm{b}}_{\mathbb{R}}(\mathbb{R})$ be positive and

$$\operatorname*{ess\,sup}_{\lambda\in(v_b,\infty)} f(\lambda)\sqrt{\lambda^2+1} < \infty.$$

For $\varrho(v) = f(K_v)$ we obtain

$$u_{\varrho(v)}(x) = \int_{\sigma(K_v)} d\nu(\lambda)\; f(\lambda)\left\|\vec{\phi}_v(x,\lambda)\right\|^2_{\mathfrak{h}(\lambda)}, \qquad x\in(a,b).$$

Example 5.6. Assume that f is given as in the previous example. Furthermore, let $\epsilon_a,\epsilon_b,\epsilon_p\in\mathbb{R}$ be given constants. If

$$\rho(\lambda) := \begin{cases} f(\lambda-\epsilon_p), & \lambda\in(-\infty,v_b],\\ f(\lambda-\epsilon_b), & \lambda\in(v_b,v_a),\\ \begin{pmatrix} f(\lambda-\epsilon_b) & 0\\ 0 & f(\lambda-\epsilon_a)\end{pmatrix}, & \lambda\in[v_a,\infty),\end{cases}$$

then

$$\begin{aligned} u_{\varrho(v)}(x) &= \sum_{j=1}^{N(v)} f(\lambda_j(v)-\epsilon_p)|\phi_p(v)(x,\lambda_j(v))|^2 \\ &\quad + \int_{v_b}^{\infty} d\lambda\, f(\lambda-\epsilon_b)|\phi_b(v)(x,\lambda)|^2 + \int_{v_a}^{\infty} d\lambda\, f(\lambda-\epsilon_a)|\phi_a(v)(x,\lambda)|^2, \quad x\in(a,b). \end{aligned}$$

The function f can be interpreted as a distribution function and the constants ϵ_a, ϵ_b as the Fermi level of the reservoir at a, b, respectively, see [F1, MKS]; the constant ϵ_p is the Fermi level of the bounded states. If $\epsilon_a = \epsilon_b = \epsilon_p$, then one is in the situation of Example 5.5.

Lemma 5.7. *The carrier density $u_{\varrho(v)}$ from Definition 5.3 obeys*

$$\int_a^b dx\, u_{\varrho(v)}(x)h(x) = \mathrm{tr}(\varrho(v)M(h)), \quad \textit{for all } h \in \mathsf{L}^\infty_{\mathbb{R}}, \tag{5.16}$$

$M(h)$ being the multiplication operator (5.11). In particular there is

$$\|u_{\varrho(v)}\|_{\mathsf{L}^1} \le C_p N(v) + C_{ac}\|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\|_{\mathfrak{B}_1(\mathcal{K})}.$$

Proof. For any Borel set $\omega \subseteq (a,b)$ there is

$$\mathrm{tr}(\varrho(v)M(\chi_\omega)) = \mathbb{E}_\varrho(\omega) = \int_a^b dx\, u_{\varrho(v)}(x)\chi_\omega(x),$$

i.e. (5.16) for all $h = \chi_\omega$. By linearity (5.16) also holds for step functions on (a,b). Since $u_{\varrho(v)}$ is in $\mathsf{L}^1_{\mathbb{R}}$ and $\varrho M(\chi_{(a,b)})$ is a trace class operator (5.16) extends by density of the step functions in $\mathsf{L}^\infty_{\mathbb{R}}$ and continuity to all $h \in \mathsf{L}^\infty_{\mathbb{R}}$. Because $M(\chi_{(a,b)}) = P^{\mathcal{K}}_{\mathcal{H}}$ there is

$$\|u_{\varrho(v)}\|_{\mathsf{L}^1} = \mathrm{tr}(\varrho(v)P^{\mathcal{K}}_{\mathcal{H}}) \le C_p N(v) + C_{ac}\|(K_v - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\|_{\mathfrak{B}_1(\mathcal{K})}.$$

□

5.2 Current densities

For $x \in (a,b)$, $\lambda \in \sigma(K_v)$ the current density $j_{\varrho(v)}$ is defined by, see [LL],

$$\begin{aligned} j_{\varrho(v)}(x) &:= \int_{\sigma(K_v)} d\nu(\lambda)\, j_{\varrho(v)}(x,\lambda), \\ j_{\varrho(v)}(x,\lambda) &:= \mathrm{Im}\left(\left(\rho(\lambda)^T \frac{\hbar}{m(x)}\frac{\partial}{\partial x}\vec{\phi}_v(x,\lambda), \vec{\phi}_v(x,\lambda)\right)_{\mathfrak{h}(\lambda)}\right). \end{aligned} \tag{5.17}$$

Direct calculation shows that $\hbar\frac{\partial}{\partial x} j_{\varrho(v)}(x,\lambda) = 0$, i.e. $j_{\varrho(v)}$ is constant $j_{\varrho(v)}(x) \equiv j_{\varrho(v)}$.

Remark 5.8. The point spectrum and the simple spectrum do not contribute to the current:

$$j_{\varrho(v)}(\lambda) = 0, \qquad \lambda \in \sigma(K_v) \setminus (v_a, \infty).$$

Indeed, as $\mathrm{Im}(iq_a(\lambda)) = 0$ for $\lambda \in (v_b, v_a)$ we get by (3.16)

$$j_{\varrho(v)}(\lambda) = \mathrm{Im}\left(-i\frac{2m_a}{\hbar}q_a(\lambda)|S_{ab}(v)(\lambda)|^2 \exp\left(-i\frac{4m_a}{\hbar}q_a(\lambda)a\right)\right) = 0, \quad \lambda \in (v_b, v_a).$$

Now let us regard a $\mu \in \sigma_p(K_v)$. By Lemma 3.8 we have that $\mu \in \sigma(\{H_v(\lambda)\})$. Since $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ are selfadjoint operators, we get

$$\phi_p(v)(a,\mu) = \eta(v)(a,\mu) \quad \text{and} \quad \tfrac{\hbar}{2m(a)}\phi_p'(a,\mu) = -\kappa_a(\mu)\eta(v)(a,\mu),$$

where $\eta(v)(\cdot,\mu)$ is the eigenfunction of the family $\{H_v(\lambda)\}_{\lambda\in(-\infty,v_b)}$ corresponding to the eigenvalue μ. Therefore

$$j_{\varrho(v)}(\mu) = \operatorname{Im}\left(-\kappa_a(\mu)|\eta(v)(a,\mu)|^2\right) = 0, \quad \text{for all } \mu \in \sigma_p(K_v).$$

A straightforward calculation shows that

$$j_{\varrho(v)}(\lambda) = \operatorname{tr}_{\mathbb{C}^2}(\rho(\lambda)C(v)(\lambda)), \quad \lambda \in (v_a,\infty), \tag{5.18}$$

with

$$C(v)(\lambda) = \frac{1}{i}\begin{pmatrix} W(\overline{\phi_b(v)(x,\lambda)},\phi_b(x,\lambda)) & W(\overline{\phi_b(v)(x,\lambda)},\phi_a(x,\lambda)) \\ W(\overline{\phi_a(v)(x,\lambda)},\phi_b(x,\lambda)) & W(\overline{\phi_a(v)(x,\lambda)},\phi_a(x,\lambda)) \end{pmatrix}. \tag{5.19}$$

Lemma 5.9. *The operator $C(v)(\lambda)$ is selfadjoint and admits the representation*

$$C(v)(\lambda) = \frac{1}{2\pi\hbar}\begin{pmatrix} -\frac{q_b(\lambda)}{q_a(\lambda)}|S_{ba}(v)(\lambda)|^2 & \sqrt{\frac{q_a(\lambda)}{q_b(\lambda)}}S_{ab}(v)(\lambda)\overline{S_{bb}(v)(\lambda)} \\ -\sqrt{\frac{q_b(\lambda)}{q_a(\lambda)}}S_{ba}(v)(\lambda)\overline{S_{aa}(v)(\lambda)} & \frac{q_a(\lambda)}{q_b(\lambda)}|S_{ab}(v)(\lambda)|^2 \end{pmatrix}. \tag{5.20}$$

There is

$$C(v)(\lambda) = \frac{1}{2\pi\hbar}\left(P_aS_v(\lambda)^*P_b - P_bS_v(\lambda)^*P_a\right)S_v(\lambda) \qquad \text{for } \lambda\in(v_a,\infty), \tag{5.21}$$

where $P_a := (\cdot,e_a)_{\mathbb{C}^2}e_a$ and $P_b := (\cdot,e_b)_{\mathbb{C}^2}e_b$ with $e_b := (1,0)^T$, $e_a := (0,1)^T \in \mathbb{C}^2$.

Proof. By (3.23) and (3.16) for $x \le a$ we have

$$W(\overline{\phi_b(v)(x,\lambda)},\phi_b(x,\lambda)) = -\frac{1}{4\pi\hbar q_a(\lambda)}W(\overline{\psi_b(x,\lambda)},\psi_b(x,\lambda)) = -\frac{i}{2\pi\hbar}\frac{q_a(\lambda)}{q_b(\lambda)}|S_{ab}(v)(\lambda)|^2$$

Using (3.23) as well as (3.15) and (3.16) for $x \ge b$ we get

$$W(\overline{\phi_a(v)(x,\lambda)},\phi_b(x,\lambda)) = \frac{i}{2\pi\hbar}\sqrt{\frac{q_b(\lambda)}{q_a(\lambda)}}\overline{S_{ba}(v)(\lambda)}S_{bb}(v)(\lambda).$$

Similarly we obtain

$$W(\overline{\phi_b(v)(x,\lambda)},\phi_a(x,\lambda)) = -\frac{i}{2\pi\hbar}\sqrt{\frac{q_a(\lambda)}{q_b(\lambda)}}\overline{S_{ab}(v)(\lambda)}S_{aa}(v)(\lambda).$$

and

$$W(\overline{\phi_a(v)(x,\lambda)},\phi_a(x,\lambda)) = \frac{i}{2\pi\hbar}\frac{q_b(\lambda)}{q_a(\lambda)}|S_{ba}(v)(\lambda)|^2.$$

Using (5.19) and (3.10) we verify (5.20). The relation (5.21) immediately follows from (5.20). The selfadjointness of $C(v)(\lambda)$ follows from (3.10) and the identity (5.20). □

Note that the current depends only on the density matrix $\rho(\cdot)$ and the scattering matrix $S_v(\lambda)$. As has been shown in Lemma 4.3 the scattering matrix is completely described by the QTB family. Thus, the same is true for the current.

Remark 5.10. As in Remark 5.4 we assume that $\lambda_0 > v_b$ is fixed. Let $\rho_{dis}(\lambda_0)$ be given by (5.15) and let $j_{dis,v}$ denote the current density of the dissipative system corresponding to the density matrix ϱ_{dis} as defined in [KNR2, Section 4]. By Lemma 5.9 and [BN, Theorem 7.1.] we get $j_{dis,v}(\lambda_0) = j_{\varrho(v)}(\lambda_0)$, i.e. the current density of the dissipative system and of the QTB system coincide for fixed energy λ_0.

Example 5.11. For the density matrix ρ from Example 5.6 we get the current

$$j_{\varrho(v)}(\lambda) = T(v)(\lambda)\left(f(\lambda-\epsilon_a) - f(\lambda-\epsilon_b)\right), \qquad \lambda \in (v_a,\infty),$$

where

$$T(v)(\lambda) := \frac{q_b(\lambda)}{q_a(\lambda)}|S_{ba}(\lambda)|^2 = \frac{q_a(\lambda)}{q_b(\lambda)}|S_{ab}(\lambda)|^2$$

is the so-called transmission coefficient. Note that if $\epsilon_a = \epsilon_b$, then $j_{\varrho(v)}(\lambda) = 0$, i.e. in particular for any density matrix as in Example 5.5 the current is zero.

Proposition 5.12. *If*

$$\int_{v_a}^{\infty} d\lambda\, \mathrm{tr}_{\mathbb{C}^2}(\rho(\lambda)) < \infty,$$

then the total current is bounded and the bound does not depend on v:

$$|j_{\varrho(v)}| \leq \frac{1}{2\pi\hbar}\int_{v_a}^{\infty} d\lambda\, \mathrm{tr}_{\mathbb{C}^2}(\rho(\lambda)).$$

Proof. Since $\|(P_a S_v(\lambda)^* P_b - P_b S_v(\lambda)^* P_a) S_v(\lambda)\|_{\mathfrak{h}(\lambda)} \leq 1$ for $\lambda \in (v_a,\infty)$ we immediately get from (5.18) and Lemma 5.9

$$|j_{\varrho(v)}| \leq \frac{1}{2\pi\hbar}\int_{v_a}^{\infty} d\lambda\; \mathrm{tr}_{\mathbb{C}^2}(\rho(\lambda)).$$

□

6 Carrier density operator

In this section we define the nonlinear carrier density operator which associates the potential seen by particles to their density and prove that the density depends continuously on the potential. Following [BKNR] the carrier density operator $\mathcal{N}_{\widehat{\rho}} : \mathsf{L}^\infty_{\mathbb{R}} \longrightarrow \mathsf{L}^1_{\mathbb{R}}$, is defined by

$$\mathcal{N}_{\widehat{\rho}}(v) := u_{\varrho(v)}, \qquad v \in \mathsf{D}(\mathcal{N}_{\widehat{\rho}}) := \mathsf{L}^\infty_{\mathbb{R}}, \tag{6.1}$$

where $u_{\varrho(v)}$ is the carrier density from Definition 5.3,

Remark 6.1. If we assume instead of (5.8) the slightly stronger condition

$$\operatorname*{esssup}_{\lambda\in(v_b,\infty)} \|\rho_{ac}(\lambda)\|_{\mathfrak{B}(\mathfrak{h}(\lambda))}(1+\lambda^2) < \infty,$$

then one can prove that the particle density operator $\mathcal{N}_{\widehat{\rho}}(\cdot)$ is not only well defined as an operator from $\mathsf{L}^\infty_\mathbb{R}$ into $\mathsf{L}^1_\mathbb{R}$, but takes its values in $\mathsf{W}^{1,2}_\mathbb{R}$.

By means of Proposition 2.6, Proposition 2.8, and Lemma 5.7 one obtains

Lemma 6.2. *If $v \in \mathsf{L}^\infty_\mathbb{R}$, then*

$$\|\mathcal{N}_{\widehat{\rho}}(v)\|_{\mathsf{L}^1} \le C_p\left(1 + \frac{\sqrt{2\|m\|_{\mathsf{L}^\infty}}(b-a)}{\pi\hbar}\sqrt{\|v\|_{\mathsf{L}^\infty} + |v_b|}\right) + C_{ac}\left(3 + \left(8 + 4\sqrt{\|m\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar}\right)\sqrt{1 + \|v\|_{\mathsf{L}^\infty}.}\right).$$

We are now going to prove that the particle density operator is continuous. For doing this we need some technical lemmata.

Lemma 6.3. *Assume $(v_n)_{n\in\mathbb{N}} \subset \mathsf{L}^\infty_\mathbb{R}$ and $v \in \mathsf{L}^\infty_\mathbb{R}$. If $v_n \xrightarrow{\mathsf{L}^\infty} v$ as $n \to \infty$, then*

$$\lim_{n\to\infty} \|(K_{v_n} - z)^{-1} - (K_v - z)^{-1}\|_{\mathfrak{B}_1(\mathcal{K})} = 0,$$

for all z in the resolvent set of K_v.

Proof. By [K, Theorem IV.1.16] $K_{v_n} - z$ is boundedly invertible for z in the resolvent set of K_v, if $\|v - v_n\|_{\mathsf{L}^\infty} < \left(\|(K_v - z)^{-1}\|_{\mathfrak{B}(\mathcal{K})}\right)^{-1}$. Hence, z is also in the resolvent set of K_{v_n} for sufficiently large n. Furthermore, there is

$$\|(K_{v_n} - z)^{-1}\|_{\mathfrak{B}(\mathcal{K})} \le \frac{\|(K_v - z)^{-1}\|_{\mathfrak{B}(\mathcal{K})}}{1 - \|v_n - v\|_{\mathsf{L}^\infty}\|(K_v - z)^{-1}\|_{\mathfrak{B}(\mathcal{K})}}.$$

Since $P^\mathcal{K}_\mathcal{H}(K_v - z)^{-1}$ is trace class one gets

$$\|(K_{v_n} - z)^{-1} - (K_v - z)^{-1}\|_{\mathfrak{B}_1(\mathcal{K})} \le \|(K_{v_n} - z)^{-1}\|_{\mathfrak{B}(\mathcal{K})}\|v_n - v\|_{\mathsf{L}^\infty}\|P^\mathcal{K}_\mathcal{H}(K_v - z)^{-1}\|_{\mathfrak{B}_1(\mathcal{K})}$$

which completes the proof. □

Lemma 6.4. *Assume $v \in \mathsf{L}^\infty_\mathbb{R}$, $(v_n)_{n\in\mathbb{N}} \subseteq \mathsf{L}^\infty_\mathbb{R}$. Let $\lambda_1(v), \ldots, \lambda_{N(v)}(v)$ and $\lambda_1(v_n), \ldots, \lambda_{N(v_n)}(v_n)$ be the eigenvalues of K_v and K_{v_n}, respectively. If $v_n \xrightarrow{\mathsf{L}^\infty} v$ as $n \to \infty$, then we have $N(v) = N(v_n)$ for sufficiently large n and*

$$\lim_{n\to\infty} \lambda_k(v_n) = \lambda_k(v), \quad \lim_{n\to\infty} \|P(\lambda_j(v_n)) - P(\lambda_j(v))\|_{\mathfrak{B}(\mathcal{K})} = 0, \quad k = 1, \cdots, N(v),$$

where $P(\lambda_k(v_n))$, $P(\lambda_k(v))$, denote the projection onto the eigenspaces of K_{v_n}, K_v corresponding to the eigenvalue $\lambda_k(v_n)$, $\lambda_k(v)$, $k = 1, \cdot, N(v)$, respectively.

The proof follows immediately from Lemma 6.3 and [K, Theorem IV.3.16].

Lemma 6.5. *If* $v \in \mathsf{L}^\infty_\mathbb{R}$, $(v_n)_{n\in\mathbb{N}} \subseteq \mathsf{L}^\infty_\mathbb{R}$ *with* $v_n \xrightarrow{\mathsf{L}^\infty} v$, *then*

$$\begin{aligned} \operatorname*{s-lim}_{n\to\infty} W_\pm(K_{v_n}, K_{v_0}) &= W_\pm(K_v, K_{v_0}), \\ \operatorname*{s-lim}_{n\to\infty} W^*_\pm(K_{v_n}, K_{v_0}) &= W^*_\pm(K_v, K_{v_0}), \end{aligned} \tag{6.2}$$

where K_{v_0} *is the operator* (2.3) *referring to the constant potential* $v \equiv v_0$, *see also Corollary 4.2.*

Proof. Lemma 6.3 and [K, Theorem X.4.15] provide

$$\operatorname*{s-lim}_{n\to\infty} W_\pm((K_{v_n}+\mu)^{-1}, (K_{v_0}+\mu)^{-1}) = W_\pm((K_v+\mu)^{-1}, (K_{v_0}+\mu)^{-1})$$

for a sufficiently large $\mu \in \mathbb{R}$. Taking into account the invariance principle, see for example [BW], we obtain the first assertion, the second one follows in the same manner. □

Theorem 6.6. *Assume* $v \in \mathsf{L}^\infty_\mathbb{R}$ *and* $(v_n)_{n\in\mathbb{N}} \subset \mathsf{L}^\infty_\mathbb{R}$. *If* $v_n \xrightarrow{\mathsf{L}^\infty} v$, *then*

$$\mathcal{N}_{\widehat{\rho}}(v_n) \xrightarrow{\mathsf{L}^1} \mathcal{N}_{\widehat{\rho}}(v) \quad \text{and} \quad j_{\varrho(v_n)} \longrightarrow j_{\varrho(v)} \qquad \text{as } n \to \infty,$$

i.e. the carrier density operator is a continuous operator from $\mathsf{L}^\infty_\mathbb{R}$ *to* $\mathsf{L}^1_\mathbb{R}$ *and the current density operator is continuous from* $\mathsf{L}^\infty_\mathbb{R}$ *to* $\mathbb{R}$.

Proof. According to Lemma 5.7 there is

$$\int_a^b dx\ ((\mathcal{N}_{\widehat{\rho}}(v_n))(x) - (\mathcal{N}_{\widehat{\rho}}(v))(x))\, h(x) = \operatorname{tr}((\varrho(v_n) - \varrho(v))M(h)), \tag{6.3}$$

for every real-valued $h \in \mathsf{L}^\infty$. Using the decomposition (5.5) for the steady states $\varrho(v_n)$ and $\varrho(v)$ we get

$$\operatorname{tr}((\varrho(v_n) - \varrho(v))M(h)) = \operatorname{tr}((\varrho_p(v_n) - \varrho_p(v))M(h)) + \operatorname{tr}((\varrho_{ac}(v_n) - \varrho_{ac}(v))M(h)), \tag{6.4}$$

where $\varrho_{ac}(v)$, $\varrho_{ac}(v_n)$ and $\varrho_p(v)$, $\varrho_p(v_n)$ are given by (5.6) and (5.7), respectively. We will first show that the first addend in (6.4) tends to zero as $n \to \infty$. By Lemma 6.4 we have that $\dim(\operatorname{ran}(\varrho_p(v_n))) = \dim(\operatorname{ran}(\varrho_p(v))) =: N < \infty$, for sufficiently large n. Hence, it suffices to show that $\|\varrho_p(v_n) - \varrho_p(v)\|_{\mathfrak{B}(\mathcal{K})} \to 0$ as $n \to \infty$. We have by the definition of $\varrho_p(v_n)$ and $\varrho_p(v)$, see (5.7),

$$\begin{aligned} &\|\varrho_p(v_n) - \varrho_p(v)\|_{\mathfrak{B}(\mathcal{K})} \\ &\quad \le \sum_{j=1}^N \Big(|\rho_p(\lambda_j(v_n)) - \rho_p(\lambda_j(v))| + |\rho_p(\lambda_j(v))|\ \|P(\lambda_j(v_n)) - P(\lambda_j(v))\|_{\mathfrak{B}(\mathcal{K})} \Big). \end{aligned} \tag{6.5}$$

Since $\rho_p \in \mathsf{C}^{\mathsf{b}}_{\mathbb{R}}(-\infty, v_b)$, see (5.1), we get by Lemma 6.4 and (6.5) that $\varrho_p(v_n)$ converges in the norm of $\mathfrak{B}(\mathcal{K})$ to $\varrho_p(v)$ as $n \to \infty$. Hence,

$$\lim_{n\to\infty} \sup_{\|h\|_{L^\infty}\le 1} |\mathrm{tr}((\varrho_p(v_n) - \varrho_p(v))M(h))| \le N \lim_{n\to\infty} \|\varrho_p(v_n) - \varrho_p(v)\|_{\mathfrak{B}(\mathcal{K})} = 0. \tag{6.6}$$

To prove that the second addend in (6.4) tends to zero as $n \to \infty$, we set

$$W := W_-(K_v, K_{v_0}) \quad \text{and} \quad W_n := W_-(K_{v_n}, K_{v_0}).$$

By (5.6) we obtain

$$\varrho_{ac}(v_n) - \varrho_{ac}(v) = (W_n - W)\varrho_{ac}(v_0)W_n^* + W\varrho_{ac}(v_0)(W_n^* - W^*).$$

Since $WK_{v_0} = K_vW$, $W_nK_{v_0} = K_{v_n}W_n$, and $\|\varrho_{ac}(v_0)(K_{v_0} \pm i)\| \le C_{ac} < \infty$, see (5.10), we get

$$\begin{aligned}
&|\mathrm{tr}((\varrho_{ac}(v_n) - \varrho_{ac}(v))M(h))| \\
&\quad\le \left|\mathrm{tr}\left(\left((K_{v_n}+i)^{-1}W_n - (K_{v_0}+i)^{-1}W\right)\varrho_{ac}(v_0)(K_{v_0}+i)W_n^*M(h)\right)\right| \\
&\qquad + \left|\mathrm{tr}\left(W(K_{v_0}-i)\varrho_{ac}(v_0)\left(W_n^*(K_{v_n}-i)^{-1} - W^*(K_{v_0}-i)^{-1}\right)M(h)\right)\right|.
\end{aligned}$$

We estimate the terms on the right hand side separately:

$$\begin{aligned}
&\left|\mathrm{tr}\left(((K_{v_n}+i)^{-1}W_n - (K_{v_0}+i)^{-1}W)\varrho_{ac}(v_0)(K_{v_0}+i)W_n^*M(h)\right)\right| \\
&\qquad\le C_{ac}\left\|\left(W_n^*(K_{v_n}-i)^{-1} - W^*(K_{v_0}-i)^{-1}\right)M(h)\right\|_{\mathfrak{B}_1(\mathcal{K})},
\end{aligned}$$

$$\begin{aligned}
&\left|\mathrm{tr}\left(W(K_{v_0}-i)\varrho_{ac}(v_0)(W_n^*(K_{v_n}-i)^{-1} - W^*(K_{v_0}-i)^{-1})M(h)\right)\right| \\
&\quad\le C_{ac}\left\|\left(W_n^*(K_{v_n}-i)^{-1} - W^*(K_{v_0}-i)^{-1}\right)M(h)\right\|_{\mathfrak{B}_1(\mathcal{K})} \\
&\quad\le C_{ac}\left\|(K_{v_n}-i)^{-1} - (K_{v_0}-i)^{-1}\right\|_{\mathfrak{B}_1(\mathcal{K})}\|h\|_{L^\infty} \\
&\qquad + C_{ac}\left\|(W_n^* - W^*)(K_{v_0}-i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\right\|_{\mathfrak{B}_1(\mathcal{K})}\|h\|_{L^\infty}
\end{aligned}$$

and finally obtain

$$\begin{aligned}
|\mathrm{tr}((\varrho_{ac}(v_n) - \varrho_{ac}(v))M(h))| \le 2C_{ac}\|h\|_{L^\infty}\Big(&\left\|(K_{v_n}-i)^{-1} - (K_v-i)^{-1}\right\|_{\mathfrak{B}_1(\mathcal{K})} \\
&+ \left\|(W_n^* - W^*)(K_{v_0}-i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}\right\|_{\mathfrak{B}_1(\mathcal{K})}\Big).
\end{aligned}$$

By Lemma 6.3, Lemma 6.5 and the fact that $(K_{v_0} - i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}$ is trace class one gets

$$\lim_{n\to\infty} \sup_{\|h\|_{L^\infty}\le 1} |\mathrm{tr}((\varrho_{ac}(v_n) - \varrho_{ac}(v))M(h))| = 0. \tag{6.7}$$

Now (6.3), (6.4), (6.6) and (6.7) imply the assertion.

Lemma 6.5 implies by Corollary 4.2 the strong convergence $\widehat{S_{v_n}} \xrightarrow{\mathsf{s}} \widehat{S_v}$. Using the expression (5.21) for $C(v)(\lambda)$ one sees that $j_{\varrho(v_n)} \longrightarrow j_{\varrho(v)}$ as $n \to \infty$. □

7 Quantum transmitting Schrödinger-Poisson system

Let us now consider the quantum transmitting Schrödinger-Poisson system, i.e. the non-linear Poisson equation (1.1) with the carrier density operator from Section 6:

$$-\frac{d}{dx}\epsilon\frac{d}{dx}\varphi = q\left(C + \mathcal{N}^{+}_{\widehat{\rho}_+}(v_+) - \mathcal{N}^{-}_{\widehat{\rho}_-}(v_-)\right) \quad \text{in } (a,b) \tag{7.1}$$

and the mixed boundary conditions

$$\varphi = \varphi_\Gamma \quad \text{on } \Gamma, \qquad -\epsilon\frac{d}{dx}\varphi = k(\varphi - \varphi_\Gamma) \quad \text{on } \{a,b\}\setminus\Gamma, \tag{7.2}$$

where $\Gamma \subseteq \{a,b\}$ is the Dirichlet part of the boundary and the function φ_Γ, defined on $[a,b]$, represents the Dirichlet boundary values given on Γ and the inhomogeneous boundary conditions of third kind on $\{a,b\}\setminus\Gamma$; the function $k \geq 0$ is defined on $\{a,b\}$ and can be seen as the capacity of the boundary; in particular k is zero at an insulating interface, see [G]. We recall from Section 1 that ϵ is the dielectric permittivity function, q is the elementary charge, C is the concentration of ionized dopants. Each of the carrier density operators $\mathcal{N}^{\pm}_{\widehat{\rho}_\pm}(v_\pm)$ is determined by a Buslaev-Fomin operators $K^{\pm}_{v_\pm}$, one for electrons (with index $-$) and for holes (with index $+$). The potential for the electrons and holes is given by

$$v_\pm := w^\pm \pm q\varphi,$$

where $w^\pm$ are given real-valued potentials—the band edge offsets. The thus specified non-linear Poisson equation (7.1), (7.2) will be called the quantum transmitting Schrödinger-Poisson system. In order to define the notion of solutions to this system precisely we introduce the following function spaces: With respect to the (possibly empty) set $\Gamma \subset \{a,b\}$ of Dirichlet points in the boundary conditions on Poisson's equation we define

$$\mathsf{W}^{1,2}_\Gamma := \mathsf{W}^{1,2}_\mathbb{R} \cap \{\psi \,|\, \psi(\Gamma) \subset \{0\}\}.$$

The dual space of $\mathsf{W}^{1,2}_\Gamma$ is denoted by $\mathsf{W}^{-1,2}_\Gamma$ and by $\langle\cdot,\cdot\rangle$ we denote the dual pairing between $\mathsf{W}^{1,2}_\Gamma$ and $\mathsf{W}^{-1,2}_\Gamma$. The embedding constants from $W^{1,2}_\mathbb{R}$ into $\mathsf{L}^\infty_\mathbb{R}$ is denoted ϵ_∞ and the embedding constant from $\mathsf{L}^1_\mathbb{R}$ into $\mathsf{W}^{-1,2}_\Gamma$ is denoted by ϵ_1.

7.1 Assumptions

Throughout this section we make the following assumptions on the data of the problem:

A1. The effective masses $m_\pm$ are positive and obey $m_\pm$, $\frac{1}{m_\pm} \in \mathsf{L}^\infty_\mathbb{R}$. The constants $m^\pm_a$, $m^\pm_b \in \mathbb{R}$ are positive.

A2. The real constants $v^\pm_a$, $v^\pm_b$ obey $v^\pm_a > v^\pm_b$.

A3. The external potentials $w^\pm$ belong to $\mathsf{L}^\infty_\mathbb{R}$.

A4. The functions $\rho_\pm(\cdot) = \rho_p^\pm(\cdot) \oplus \rho_{ac}^\pm(\cdot)$, with

$$\rho_p^\pm(\cdot) \in \mathsf{C}^{\mathsf{b}}_{\mathbb{R}}(-\infty, v_b^\pm) \quad \text{and} \quad \rho_{ac}^\pm(\cdot) \in \mathsf{L}^\infty((v_b^\pm, \infty), \mathfrak{B}(\mathfrak{h}_\pm(\lambda)), \nu_{ac}),$$

see (5.1), where $\mathfrak{h}_\pm(\lambda)$ are given by (3.24) with v_b, v_a replaced by $v_b^\pm$, $v_a^\pm$. Furthermore, the $\rho_\pm(\cdot)$ satisfy (5.2) and (5.8).

A5. The doping profile C, see (7.1), belongs to the function space $\mathsf{W}_\Gamma^{-1,2}$.

A6. The dielectric permittivity function ϵ is positive and obeys ϵ, $\frac{1}{\epsilon} \in \mathsf{L}^\infty_{\mathbb{R}}$. We set $\tilde{\epsilon} := \max\{1, \|\frac{1}{\epsilon}\|_{\mathsf{L}^\infty}\}$.

A7. The set $\Gamma \subset \{a, b\}$ is not empty or at least one of the numbers $k(x)$, $x \in \{a, b\} \setminus \Gamma$, is strictly positive.

A8. The function φ_Γ is from the space $\mathsf{W}^{1,2}_{\mathbb{R}}$.

To each Buslaev-Fomin operator $K^\pm_{v_\pm}$, see (2.3), we associate a QTB family $\{H^\pm_{v_\pm}(z)\}_{z\in\mathbb{C}_+}$ according to Definition 2.2. The functions $\rho_\pm(\cdot)$ define by (5.4) steady states $\varrho_\pm(v)$, i.e. non-negative selfadjoint operators which commute with $K^\pm_{v_\pm}$. The carrier densities $u_{\varrho_\pm(v)}$ for the electrons and holes are determined by Definition 5.3. The corresponding carrier density operators (6.1) are denoted by $\mathcal{N}^\pm_{\widehat{\rho}_\pm}(v)$.

7.2 Definition of solutions

The linear Poisson operator $\mathcal{P} : \mathsf{W}^{1,2}_{\mathbb{R}} \longrightarrow \mathsf{W}_\Gamma^{-1,2}$ is defined by

$$\langle \mathcal{P}\upsilon, \varsigma\rangle = \int_a^b dx\, \epsilon(x)\upsilon'(x)\varsigma'(x) + \sum_{x\in\{a,b\}\setminus\Gamma} k(x)\upsilon(x)\varsigma(x),$$

$$\text{for all } \varsigma \in \mathsf{W}^{1,2}_\Gamma,\ \upsilon \in \mathsf{D}(\mathcal{P}) = \mathsf{W}^{1,2}_{\mathbb{R}}.$$

The restriction of $\mathcal{P}$ to $\mathsf{W}^{1,2}_\Gamma$ will be denoted by $\mathcal{P}_0$. We note that the inverse of $\mathcal{P}_0$ exists; its norm does not exceed $\tilde{\epsilon}(1 + \gamma_k)$, see [BKNR], where

$$\gamma_k := \sup_{0\neq\psi\in W^{1,2}_\Gamma} \frac{\|\psi\|^2_{\mathsf{L}^2}}{\|\psi'\|^2_{\mathsf{L}^2} + \sum_{x\in\{a,b\}\setminus\Gamma} k(x)|\psi(x)|^2}$$

which is finite since the case of purely homogeneous Neumann boundary conditions is excluded by assumption **A7**. We denote by $\widetilde{\varphi}_\Gamma$ the bounded linear form

$$\upsilon \longmapsto \int_a^b dx\, \epsilon(x)\varphi_\Gamma'(x)\upsilon'(x), \qquad \upsilon \in \mathsf{D}(\widetilde{\varphi}_\Gamma) = \mathsf{W}^{1,2}_\Gamma.$$

Definition 7.1. If $u^\pm \in \mathsf{L}^1_{\mathbb{R}}$, then $\varphi \in \mathsf{W}^{1,2}_{\mathbb{R}}$ is a solution of Poisson's equation

$$-\frac{d}{dx}\epsilon\frac{d}{dx}\varphi = q\left(C + u^+ - u^-\right) \quad \text{in } (a,b)$$

with the boundary conditions (7.2) iff $\varphi - \varphi_\Gamma \in \mathsf{W}^{1,2}_\Gamma$ satisfies

$$\mathcal{P}_0(\varphi - \varphi_\Gamma) = D + q\,E_1 u^+ - q\,E_1 u^-, \tag{7.3}$$

where $D := qC - \tilde{\varphi}_\Gamma$ and E_1 denotes the embedding operator from L^1 into $\mathsf{W}^{-1,2}_\Gamma$.

Definition 7.2. $(\varphi, u^+, u^-) \in \mathsf{W}^{1,2}_{\mathbb{R}} \times \mathsf{L}^1_{\mathbb{R}} \times \mathsf{L}^1_{\mathbb{R}}$ is a solution of the quantum transmitting Schrödinger-Poisson system if φ satisfies Poisson's equation in the sense of Definition 7.1 with

$$u^+ = u^+_{\varrho_+(w^+ + qE_\infty\varphi)} \quad \text{and} \quad u^- = u^-_{\varrho_-(w^- - qE_\infty\varphi)},$$

where E_∞ denotes the embedding operator from $\mathsf{W}^{1,2}_{\mathbb{R}}$ into $\mathsf{L}^\infty_{\mathbb{R}}$.

7.3 Existence of solutions

Following [KR] we define a mapping whose fixed points determine the solutions of the quantum transmitting Schrödinger-Poisson system. To that end we first introduce the mapping $\mathcal{J} : \mathsf{L}^1_{\mathbb{R}} \times \mathsf{L}^1_{\mathbb{R}} \longrightarrow \mathsf{W}^{1,2}_{\mathbb{R}}$ which assigns to a couple of densities $(u^+, u^-) \in \mathsf{L}^1_{\mathbb{R}} \times \mathsf{L}^1_{\mathbb{R}}$ the solution of Poisson's equation:

$$\mathcal{J}(u^+, u^-) = \mathcal{P}_0^{-1}\left(D + qE_1(u^+ - u^-)\right) + \varphi_\Gamma. \tag{7.4}$$

Obviously, the map $\mathcal{J}$ is continuous. Now we define $\Psi : \mathsf{L}^\infty_{\mathbb{R}} \longrightarrow \mathsf{W}^{1,2}_{\mathbb{R}}$ by

$$\Psi : v \mapsto \left(\mathcal{N}^+_{\widehat{\rho}_+}(w^+ + qv), \mathcal{N}^-_{\widehat{\rho}_-}(w^- - qv)\right) \mapsto \mathcal{J}\left(\mathcal{N}^+_{\widehat{\rho}_+}(w^+ + qv), \mathcal{N}^-_{\widehat{\rho}_-}(w^- - qv)\right).$$

Since the carrier density operators $\mathcal{N}^\pm_{\widehat{\rho}_\pm}$ are continuous, see Theorem 6.6, we get that Ψ is continuous. Finally we define $\Psi_\infty : \mathsf{L}^\infty_{\mathbb{R}} \longrightarrow \mathsf{L}^\infty_{\mathbb{R}}$ by

$$\Psi_\infty := E_\infty \Psi.$$

As both Ψ and the embedding operator E_∞ from $\mathsf{W}^{1,2}_{\mathbb{R}}$ into $\mathsf{L}^\infty_{\mathbb{R}}$ are continuous so is Ψ_∞, Moreover, the map Ψ_∞ is compact because E_∞ is compact.

Lemma 7.3. *An element $v \in \mathsf{L}^\infty_{\mathbb{R}}$ is a fixed point of Ψ_∞ if and only if the triple*

$$(\Psi(v), u^+, u^-) = (\Psi(v), u^+_{\varrho_+(w^+ + qv)}, u^-_{\varrho_-(w^- - qv)})$$

is a solution of the quantum transmitting Schrödinger-Poisson system.

The proof follows directly from the definitions.

Definition 7.4. With respect to the data of the problem we define

$$x_0 := \frac{\sigma_1}{2} + \sqrt{\frac{\sigma_1^2}{4} + \sigma_2},$$

as the (unique) positive root of the polynomial $p : x \mapsto x^2 - \sigma_1 x - \sigma_2$, where

$$\sigma_1 := \epsilon_\infty \epsilon_1 \tilde{\epsilon}(1+\gamma_k) q(\sigma_1^+ + \sigma_1^-), \tag{7.5}$$

$$\sigma_2 := \epsilon_\infty \|\varphi_\Gamma\|_{\mathsf{W}^{1,2}} + \epsilon_\infty \tilde{\epsilon}(1+\gamma_k)\left\{\|D\|_{\mathsf{W}^{-1,2}} + q\epsilon_1(\sigma_2^+ + \sigma_2^-)\right\}, \tag{7.6}$$

and

$$\sigma_1^\pm := \sqrt{q} C_{ac}^\pm \left(8 + 4\sqrt{\|m_\pm\|_{\mathsf{L}^\infty}} \frac{(b-a)}{\hbar}\right) + \sqrt{q} C_p^\pm \left(\frac{\sqrt{2\|m_\pm\|_{\mathsf{L}^\infty}}(b-a)}{\pi\hbar}\right), \tag{7.7}$$

$$\begin{aligned} \sigma_2^\pm := & C_{ac}^\pm \left(3 + \left(8 + 4\sqrt{\|m_\pm\|_{\mathsf{L}^\infty}} \frac{(b-a)}{\hbar}\right) \sqrt{1 + \|w^\pm\|_{\mathsf{L}^\infty}}\right) \\ & + C_p^\pm \left(1 + \frac{\sqrt{2\|m_\pm\|_{\mathsf{L}^\infty}(\|w_\pm\|_{\mathsf{L}^\infty} + |v_b|)}(b-a)}{\pi\hbar}\right), \end{aligned} \tag{7.8}$$

with $C_{ac}^\pm$ and $C_p^\pm$ according to (5.8) and (5.9), respectively

Theorem 7.5. *The map $\Psi_\infty : \mathsf{L}^\infty_\mathbb{R} \longrightarrow \mathsf{L}^\infty_\mathbb{R}$ has a fixed point. For any fixed point v of Ψ_∞ there is*

$$\|v\|_{\mathsf{L}^\infty} \le x_0^2, \tag{7.9}$$

where x_0 is according to Definition 7.4.

Proof. By the definition (7.4) of the operator $\mathcal{J}$ we have

$$\begin{aligned} \|\mathcal{J}(u^+, u^-)\|_{\mathsf{W}^{1,2}_\mathbb{R}} & \le \|\varphi_\Gamma\|_{\mathsf{W}^{1,2}_\mathbb{R}} + \tilde{\epsilon}(1+\gamma_k)\|D + qE_1(u^+ - u^-)\|_{\mathsf{W}^{-1,2}_\Gamma} \\ & \le \|\varphi_\Gamma\|_{\mathsf{W}^{1,2}_\mathbb{R}} + \tilde{\epsilon}(1+\gamma_k)\left(\|D\|_{\mathsf{W}^{-1,2}_\Gamma} + \epsilon_1 q\left(\|u^+\|_{\mathsf{L}^1} + \|u^-\|_{\mathsf{L}^1}\right)\right). \end{aligned} \tag{7.10}$$

Since $u^\pm := \mathcal{N}^\pm_{\hat{\rho}_\pm}(v_\pm)$ with $v_\pm = w^\pm \pm qv$ we get from Lemma 6.2:

$$\|u^\pm\|_{\mathsf{L}^1} \le \sigma_1^\pm \sqrt{\|v\|_{\mathsf{L}^\infty}} + \sigma_2^\pm, \tag{7.11}$$

where $\sigma_1^\pm$ and $\sigma_2^\pm$ are given by (7.7) and (7.8). Thus, (7.10), (7.5), and (7.6) provide

$$\|\Psi_\infty(v)\|_{\mathsf{L}^\infty} \le \epsilon_\infty \|\mathcal{J}(\mathcal{N}^+_{\hat{\rho}_+}(v), \mathcal{N}^-_{\hat{\rho}_-}(v))\|_{\mathsf{W}^{1,2}} \le \sigma_1 \|v\|^{1/2}_{\mathsf{L}^\infty} + \sigma_2. \tag{7.12}$$

If x_0 is the unique positive root of the polynomial $p : x \mapsto x^2 - \sigma_1 x - \sigma_2$ and $\|v\|_{\mathsf{L}^\infty} \le x_0^2$, then

$$\|\Psi_\infty(v)\|_{\mathsf{L}^\infty} \le \sigma_1 x_0 + \sigma_2 = x_0^2.$$

Hence, Ψ_∞ maps the ball $\{v \in \mathsf{L}^\infty_\mathbb{R} \,|\, \|v\|_{\mathsf{L}^\infty} \le x_0^2\}$ continuously into itself. Since Ψ_∞ is compact, the image of this ball is precompact in $\mathsf{L}^\infty_\mathbb{R}$. Therefore Schauder's fixed point theorem assures the existence of a fixed point.

Let us now assume the second assertion were false, i.e. we assume that there exists a fixed point v satisfying $\|v\|_{\mathsf{L}^\infty} > x_0^2$. By (7.12) we get

$$(\|v\|^{1/2}_{\mathsf{L}^\infty})^2 = \|v\|_{\mathsf{L}^\infty} = \|\Psi_\infty(v)\|_{\mathsf{L}^\infty} \le \sigma_1 \|v\|^{1/2}_{\mathsf{L}^\infty} + \sigma_2.$$

This is a contradiction to $p(x) > 0$ for $x > x_0$. □

Theorem 7.6. *Under the assumptions* **A1**–**A8** *the quantum transmitting Schrödinger-Poisson system always admits a solution in the sense of Definition 7.2 and any solution* (φ, u^+, u^-) *of the quantum transmitting Schrödinger-Poisson system satisfies the a priori estimate*

$$\|\varphi\|_{\mathsf{L}^\infty} \le x_0^2, \qquad \|u^\pm\|_{\mathsf{L}^1} \le C^\pm_{ac} r_\pm + C^\pm_p s_\pm, \tag{7.13}$$

where x_0 *is given by Definition 7.4 and*

$$r_\pm := 3 + \left(8 + 4\sqrt{\|m_\pm\|_{\mathsf{L}^\infty}}\frac{(b-a)}{\hbar}\right)\left(\sqrt{q}x_0 + \sqrt{1 + \|w^\pm\|_{\mathsf{L}^\infty}}\right),$$

$$s_\pm := 1 + \frac{\sqrt{2\|m_\pm\|_{\mathsf{L}^\infty}}(b-a)}{\pi\hbar}\left(\sqrt{\|w^\pm\|_{\mathsf{L}^\infty} + |v_b|} + \sqrt{q}x_0\right).$$

Proof. The first assertion follows from Lemma 7.3 and Theorem 7.5. The first inequality (7.13) is obtained by (7.9); The second inequality is implied by the first one and Lemma 6.2. □

7.4 Concluding remarks

Open quantum systems like the quantum transmitting Schrödinger-Poisson system were treated in a very general framework by F. Nier in [N1]. In [N1] the density matrix $\varrho(v)$ was assumed to be of the form $\varrho(v) = f(K_v)$, for some smooth function f with compact support. This leads to a zero current, see example 5.11. We have demonstrated that for density matrices of a more general form the QTB family allows to model a non zero current flow through the boundary of the device. This allows a current coupling of a QTB family with a classical drift diffusion model or a kinetic model. However, in coupling the QTB family with an external model for the potential to be seen by Schrödinger's operator one cannot assume anymore that the potential outside the interval (a, b), i.e. v_a, v_b is fixed. Hence, the operator E defined by (2.1) has to be replaced by the operator $\widetilde{E} : \mathsf{C}_\mathbb{R}([a, b]) \longrightarrow \mathsf{C}^\mathsf{b}_\mathbb{R}(\mathbb{R})$ given by

$$\left(\widetilde{E}v\right)(x) := \begin{cases} v(a), & -\infty < x \le a, \\ v(x), & x \in (a, b), \\ v(b), & b \le x < \infty, \end{cases} \qquad v \in \mathsf{D}(\widetilde{E}) = \mathsf{C}_\mathbb{R}([a, b]).$$

The Buslaev-Fomin operators are then defined by

$$\widetilde{K}_v := -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{\hat{m}}\frac{d}{dx} + \widetilde{E}v.$$

Note that in this case the absolutely continuous spectrum depends on the potential v, i.e. $\sigma_{ac}(\tilde{K}_v) = [\min\{v(a), v(b)\}, \infty)$. Furthermore, in general the wave operators

$$W_\pm(\widetilde{K}_w, \widetilde{K}_v) = \operatorname*{s-lim}_{t\to\pm\infty} \exp(it\widetilde{K}_w)\exp(-it\widetilde{K}_v)P_{ac}(\widetilde{K}_v), \quad v, w \in \mathsf{C}_{\mathbb{R}}([a,b])$$

do not exist and therefore we do not have a representation as given in Remark 5.2. Thus, the techniques used in this paper to prove the continuity of the particle density operator, see Theorem 6.6 do not apply in this case.

There is a close relation between the dissipative Schrödinger-Poisson system treated in [BKNR] and the quantum transmitting Schrödinger-Poisson system we have investigated in this paper: As already noted in Remark 5.4 and Remark 5.10 the carrier and current densities of the dissipative and the quantum transmitting Schrödinger-Poisson system coincide for fixed energy $\lambda_0 > v_b$, provided the density matrix of the dissipative system is transformed according to (5.15). Therefore the dissipative Schrödinger-Poisson system can be regarded as a single energy approximation of the quantum transmitting Schrödinger-Poisson system.

We have demonstrated that the quantum transmitting Schrödinger-Poisson system always admits a solution, if the assumptions **A1**–**A8** are satisfied. Moreover, there are a priori estimates for any solution φ and the corresponding carrier densities $u_\pm$. However, uniqueness of solutions has not been settled. We have shown that the QTB family contains all the information, which is needed to determine the carrier and the current density, see Lemma 3.4 and the expression (5.13) for the carrier density and Lemmata 4.3 and 5.9 for the current density. Since the QTB family lives on a bounded domain, an efficient numerical algorithm can be developed to implement the quantum transmitting Schrödinger-Poisson system.

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