Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Scattering matrix, phase shift, spectral shift and trace formula for one-dimensional dissipative Schrödinger-type operators

H. Neidhardt, J. Rehberg

submitted: August 26, 2005

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

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

No. 1045
Berlin 2005

1991 *Mathematics Subject Classification.* 47A20, 47B44, 47A40.

Key words and phrases. dissipative Schrödinger-type operators, Sturm-Liouville operators, self-adjoint dilation, characteristic function, Lax-Phillips scattering theory, scattering matrix, phase shift, spectral shift, trace formula, Birman-Krein formula.

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

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

Abstract

The paper is devoted to Schrödinger operators on bounded intervals of the real axis with dissipative boundary conditions. In the framework of the Lax-Phillips scattering theory the asymptotic behaviour of the phase shift is investigated in detail and its relation to the spectral shift is discussed. In particular, the trace formula and the Birman-Krein formula are verified directly. The results are exploited for dissipative Schrödinger-Poisson systems.

Contents

1 Introduction

Stationary Schrödinger-Poisson systems play an important role for the quantum description of semi-conductors, cf. [27, 28, 29, 34, 35, 36]. The main ingredient of such systems is a Schrödinger operator which defines the carrier densities entering into the Poisson equation. It urns out that as far as the involved Schrödinger operator is defined by self-adjoint boundary conditions the arising current densities are always zero. Hence, carrier transport cannot be modelled by self-adjoint boundary conditions. A natural way to overcome this problem is to replace them by dissipative ones [10, 12, 13, 24, 25] or, more advanced, by families of dissipative operators with spectral parameter dependent dissipative boundary conditions, cf. [9, 11, 15, 16, 19]. In order to handle dissipative Schrödinger-Poisson systems a detailed investigation of dissipative Schrödinger operators and a comprehensive knowledge of their properties is highly desirable.

Moreover, besides the physical relevance of dissipative Schrödinger operators there is an intrinsic mathematical interest in such operators since they are examples of non-selfadjoint operators which admit a fairly good investigation. The powerful tool for this is the dilation and model theory for dissipative operators, cf. [18]. With respect to physical applications the self-adjoint dilation of a dissipative Schrödinger operator can be regarded as the Hamiltonian of a closed quantum system in which the dissipative Schrödinger system is embedded. This gives rise to interpret dissipative systems as open ones. There is an rich literature on dissipative Schrödinger operators, their dilations and eigenfunction expansions mainly for Sturm-Liouville operators [2, 3, 5, 7],[38]-[41] but also for Schrödinger operator in higher dimensions, cf. [37]. The investigations are extended to matrix-valued dissipative Sturm-Liouville operators, see [4, 6, 8].

From [18] it s known that dissipative operators are completely described by the characteristic function which is an analytic contraction-valued operator function defined in the lower half-plane. It turns out that the characteristic function of a dissipative operator can be regarded as the scattering matrix of a suitable posed Lax-Phillips scattering theory, cf. [32]. In view of dissipative Schrödinger-Poisson systems the characteristic function is a very important quantity, too. In fact, it is directly related to the current density of such systems, cf. [11, 12, 24], and the asymptotic properties of the so-called phase shift strongly affects the definition of the carrier density. We show this in a forthcoming paper [33]. Current and carrier densities, however, are crucial for Schrödinger-Poisson systems with carrier transport.

In the following we consider Schrödinger-type operators $H[\kappa_a, \kappa_b, V]$ defined by

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

where

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

such that the boundary coefficients obey $\kappa_a, \kappa_b \in \overline{\mathbb{C}_+} := \{z \in \mathbb{C} : \Im\mathrm{m}(z) \geq 0\}$ and the potential $V \in L^\infty(\Omega)$ is real. Throughout the paper we always assume that m is a real function obeying

$$0 \le m + \frac{1}{m} \in L^\infty(\Omega)$$

without mentioning this explicitly in the following. In [26] we have calculated the characteristic function $\Theta[\kappa_a,\kappa_b,V]$, the self-adjoint dilation $K[\kappa_a,\kappa_b,V]$ of $H[\kappa_a,\kappa_b,V]$ as well as the generalized eigenfunctions of $K[\kappa_a,\kappa_b,V]$ for the case $\kappa_a,\kappa_b \in \mathbb{C}_+ := \{z \in \mathbb{C}_+ : \Im\mathrm{m}(z) > 0\}$. Now we are interested in the associated Lax-Phillips scattering theory, the phase and spectral shifts and their asymptotic behaviour.

The paper is organized as follows. In Section 2 we introduce a boundary triplet which allows us appropriately to describe self-adjoint and maximal dissipative Schrödinger-type operators used in the following. In particular, we verify in this way some properties of Schrödinger-type operators not proven in [26] and introduce the characteristic function quite different from [26] in terms of that boundary triplet. In Section 3 we give a short introduction to the Lax-Phillips scattering theory for Schrödinger-type operators. Section 4 is devoted to the phase shift of the Lax-Phillips scattering theory; in particular, asymptotic estimates of the phase shift are verified. Finally, in Section 5 we introduce the spectral shift for the pair $\{H[\kappa_a,\kappa_b,V], H_D[V]\}$ where $H_D[V]$ is the the self-adjoint operator generated by $l[V]$ with Dirichlet boundary conditions. The existence of the spectral shift follows from an abstract result proven in [1].

Notation: Hilbert spaces are denoted by Gothic letters, for instance $\mathfrak{H} = L^2(\Omega)$, the dilation space $\mathfrak{K}$, etc, where $L^p(\Omega)$, $1 \le p \le \infty$, denoted the usual Banach spaces of summable functions on $\Omega \subseteq \mathbb{R}$. If we have in mind real functions, we write $L^p_{\mathbb{R}}(\Omega)$. By $W^{l,p}(\Omega)$, $p \ge 1$, $l \ge 1$, we denote the standard Sobolev spaces. The norm of a Banach space $\mathfrak{X}$ is denoted by $\|\cdot\|_{\mathfrak{X}}$ or simply by $\|\cdot\|$. The scalar product of a Hilbert space $\mathfrak{H}$ is denoted by $(\cdot,\cdot)_{\mathfrak{H}}$ or simply by $(\cdot,\cdot)$. In the special case of the Hilbert space $\mathbb{C}^2$ we use the notation $\langle\cdot,\cdot\rangle$ for the scalar product. The set of bounded operators on some Banach space $\mathfrak{X}$ is denoted by $\mathcal{B}(\mathfrak{X})$. For a densely defined linear operator $A : \mathfrak{X} \longrightarrow \mathfrak{X}$ we denote by A^*, spec(A) and res(A) its adjoint operator, the spectrum and resolvent set, respectively.

2 Dissipative Schrödinger-type operators

2.1 Boundary triplets, Weyl function and γ-field

We note that the operators $H[\kappa_a,\kappa_b,V]$, $\kappa_a,\kappa_b \in \overline{\mathbb{C}_+}$, and $H_D[V]$ can be regarded as dissipative or self-adjoint extensions of one and the same closed symmetric operator $S[V]$,

$$\begin{aligned} (S[V]g)(x) &:= (l[V]g)(x), \quad g \in \mathrm{dom}(S[V]),\\ \mathrm{dom}(S[V]) &= \left\{ g \in W^{1,2}(\Omega) : \begin{array}{c} \frac{1}{m}g' \in W^{1,2} \\ g(b) = \frac{1}{2m(b)}g'(b) = 0 \\ g(a) = \frac{1}{2m(a)}g'(a) = 0 \end{array} \right\} \end{aligned} \tag{2.1}$$

which has the deficiency indices $(2,2)$. The adjoint operator $S[V]^*$ is given by

$$\begin{aligned} (S[V]^*g)(x) &:= (l[V]g)(x), \quad g \in \mathrm{dom}(S[V]^*),\\ \mathrm{dom}(S[V]^*) &= \left\{ g \in W^{1,2}(\Omega) : \tfrac{1}{m}g' \in W^{1,2} \right\}. \end{aligned}$$

It is straightforward to verify that $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$ performs a boundary triplet for $S[V]^*$, for definition see [23] and references therein, where $\Gamma_0, \Gamma_1 : \mathrm{dom}(S[V]^*) \to \mathbb{C}^2$ are linear operators, given by

$$\Gamma_0 g := \begin{pmatrix} g(b) \\ -g(a) \end{pmatrix} \quad \text{and} \quad \Gamma_1 g := -\frac{1}{2} \begin{pmatrix} \frac{1}{m(b)} g'(b) \\ \frac{1}{m(a)} g'(a) \end{pmatrix}. \tag{2.2}$$

That is, one has to show that Green's identity

$$(S[V]^* f, g) - (f, S[V]^* g) = \langle \Gamma_1 f, \Gamma_0 g \rangle - \langle \Gamma_0 f, \Gamma_1 g \rangle, \quad f, g \in \mathrm{dom}(S[V]^*),$$

is satisfied and the operator $\Gamma : \mathfrak{H} \longrightarrow \mathbb{C}^2 \oplus \mathbb{C}^2$,

$$\Gamma f := \Gamma_0 f \oplus \Gamma_1 f, \quad f \in \mathrm{dom}(\Gamma) := \mathrm{dom}(S[V]^*),$$

is surjective, which can be easily seen. We note that the selfadjoint extension $H_D[V] := S[V]^* \restriction \ker(\Gamma_0)$ corresponds to the Dirichlet boundary conditions, that is,

$$\mathrm{dom}(H_D[V]) = \left\{ g \in W^{1,2}(\Omega) : \frac{1}{m} g' \in W^{1,2}(\Omega),\ f(a) = f(b) = 0 \right\}.$$

Let B a dissipative or self-adjoint operator on the Hilbert space $\mathbb{C}^2$. By

$$H_B[V] := S[V]^* \restriction \ker(\Gamma_1 - B\Gamma_0)$$

one defines a maximal dissipative or self-adjoint extension of the symmetric operator $S[V]$. Setting

$$\kappa := \begin{pmatrix} \kappa_b & 0 \\ 0 & \kappa_a \end{pmatrix}, \quad \kappa_a, \kappa_b \in \overline{\mathbb{C}_+},$$

we find that $H_{-\kappa}[V] = H[\kappa_a, \kappa_b, V]$.

The defect subspace of $S[V]$ at the point $\overline{z} \in \mathbb{C}$ is denoted by $\mathcal{N}_z[V]$, i.e., $\mathcal{N}_z[V] := \ker(S[V]^* - z)$, $z \in \mathbb{C}_+$. For every $z \in \mathrm{res}(H_D[V])$ we set

$$\gamma[V](z) := (\Gamma_0 \restriction \mathcal{N}_z[V])^{-1} \quad \text{and} \quad M[V](z) := \Gamma_1 \gamma[V](z).$$

The functions $\mathrm{res}(H_D[V]) \ni z \longrightarrow \gamma[V](z)$ and $\mathrm{res}(H_D[V]) \ni z \longrightarrow M[V](z)$ are called the γ-field and the Weyl function corresponding to $S[V]$ and the boundary triplet $\{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$. We note that the Weyl function is a Nevanlinna function, that is, a holomorphic operator-valued function in $\mathbb{C}_+$ and $\mathbb{C}_-$ such that $\Im\mathrm{m}(M[V](z)) \geq 0$ for $z \in \mathbb{C}_+$, and

$$M[V](z)^* = M[V](\overline{z}), \quad z \in \mathrm{res}(H_D[V]).$$

In the present case the Weyl function is meromorphic in $\mathbb{C}$ with poles on $\mathbb{R}$ which coincide with the eigenvalues of $H_D[V]$.

For any dissipative or self-adjoint operator B on $\mathbb{C}^2$ the so-called Krein's formula

$$(H_B[V] - z)^{-1} = (H_D[V] - z)^{-1} + \gamma(z)(B - M[V](z))^{-1}\gamma(\overline{z})^*, \quad z \in \mathbb{C}_+,$$

holds, cf. [20]. In particular, we have

$$(H[\kappa_a, \kappa_b, V] - z)^{-1} = (H_D[V] - z)^{-1} - \gamma(z)(\kappa + M[V](z))^{-1}\gamma(\overline{z})^*, \quad z \in \mathbb{C}_+. \tag{2.3}$$

The Schrödinger-type operator $H[\kappa_a, \kappa_b, V]$ is maximal dissipative if either $\kappa_a \in \mathbb{C}_+$ or $\kappa_b \in \mathbb{C}_+$. In both cases the operator is completely non-selfadjoint, see [25]. In accordance with [26] we consider only the case $\kappa_a, \kappa_b \in \mathbb{C}_+$ in the following. The spectrum of $H[\kappa_a, \kappa_b, V]$ consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity. Since the operator $H[\kappa_a, \kappa_b, V]$ is completely non-selfadjoint, its eigenvalues are non-real. The extension $H[q_a, q_b, V]$, $q_a, q_b \in \mathbb{R}$, of S is self-adjoint and semi-bounded from below.

Lemma 2.1 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \overline{\mathbb{C}_+}$, then*

$$\lim_{\substack{|\kappa_a| \to \infty \\ |\kappa_b| \to \infty}} \left\| (H[\kappa_a, \kappa_b, V] - z)^{-1} - (H_D[V] - z)^{-1} \right\|_{\mathcal{B}(\mathfrak{H})} = 0 \tag{2.4}$$

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

Proof. We note that the γ-field $\gamma[V](z)$ as well as the Weyl function $M[V](z)$ are independent from $\kappa_a, \kappa_b \in \overline{\mathbb{C}_+}$. Using Krein's formula (2.3) we immediately verify the relation (2.4). □

2.2 Characteristic function

If B is dissipative operator, then in accordance with [21] the characteristic function $\Theta_{H_B[V]}(z)$, $z \in \mathbb{C}_-$, of the maximal dissipative operator $H_B[V]$ is given by

$$\Theta_{H_B[V]}(z) = \left(I_{\mathbb{C}^2} - 2i\sqrt{-\Im\mathrm{m}(B)}(B^* - M[V](z))^{-1}\sqrt{-\Im\mathrm{m}(B)} \right) \restriction \mathrm{ran}(\Im\mathrm{m}(B)), \quad z \in \mathbb{C}_-,$$

where $\Im\mathrm{m}(B) := \frac{1}{2i}(B - B^*)$. The characteristic function is analytic and its values are contractions, if $z \in \mathbb{C}_-$. In the present case the characteristic function admits a meromorphic continuation to $\overline{\mathbb{C}_+}$ for any dissipative operator B. The characteristic function entirely characterizes the non-selfadjoint part of the maximal dissipative operator $H_B[V]$, cf. [18].

In the following we use the representations

$$\kappa_a = q_a + i\frac{\alpha_a^2}{2} \quad \text{and} \quad \kappa_b = q_b + i\frac{\alpha_b^2}{2},$$

where $q_a, q_b \in \mathbb{R}$ and $\alpha_a, \alpha_b > 0$. If $B = -\kappa$, then

$$-\Im\mathrm{m}(B) = \frac{1}{2i}(\kappa - \kappa^*) = \frac{1}{2}\begin{pmatrix} \alpha_b^2 & 0 \\ 0 & \alpha_a^2 \end{pmatrix}.$$

Hence we obtain

$$\sqrt{-\Im\mathrm{m}(B)} = \frac{1}{\sqrt{2}}\alpha, \quad \alpha := \begin{pmatrix} \alpha_b & 0 \\ 0 & \alpha_a \end{pmatrix}.$$

Setting $\Theta[\kappa_a, \kappa_b, V](z) := \Theta_{H_{-\kappa}}[V](z)$, $z \in \mathbb{C}_-$, and using the definition (2.2) we get

$$\Theta[\kappa_a, \kappa_b, V](z) = I_{\mathbb{C}^2} + i\alpha(\kappa^* + M[V](z))^{-1}\alpha, \quad z \in \mathbb{C}_-. \tag{2.5}$$

Since the spectrum of $H[\kappa_a,\kappa_b,V]$ is non-real the characteristic function $\Theta[\kappa_a,\kappa_b,V](\cdot)$ is well-defined on $\mathbb{R}$ and, moreover, holomorphic in a neighbourhood of $\mathbb{R}$. Furthermore, a straightforward computation shows that $\Theta[\kappa_a,\kappa_b,V](\lambda)$ is unitary for of $\lambda\in\mathbb{R}$. Since the maximal dissipative operator $H[\kappa_a,\kappa_b,V]$ is completely non-selfadjoint for $\kappa_a,\kappa_b\in\mathbb{C}_+$, the characteristic function $\Theta[\kappa_a,\kappa_b,V](\cdot)$ completely characterizes $H[\kappa_a,\kappa_b,V]$.

The characteristic function of the operator $H[\kappa_a,\kappa_b,V]$ can be represented by the operator $H[\kappa_a,\kappa_b,V]$ itself and α_a,α_b. Indeed, multiplying Krein's formula on the left by Γ_0 we obtain

$$G[\kappa_a,\kappa_b,V](z) := \Gamma_0(H[\kappa_a,\kappa_b,V]-z)^{-1} = -(\kappa+M[V](z))^{-1}\gamma(\overline{z})^*,\quad z\in\mathbb{C}_+.$$

Taking the adjoint we get

$$G[\kappa_a,\kappa_b,V](z)^* = -\gamma(\overline{z})(\kappa^*+M[V](z)^*)^{-1},\quad z\in\mathbb{C}_+. \tag{2.6}$$

Multiplying again this equation on the left by Γ_0 we find

$$\Gamma_0 G[\kappa_a,\kappa_b,V](z)^* = -(\kappa^*+M[V](z)^*)^{-1},\quad z\in\mathbb{C}_+.$$

Since $M[V](z)^* = M[V](\overline{z})$, $z\in\mathrm{res}(H_D[V])$, we finally get

$$\Gamma_0 G[\kappa_a,\kappa_b,V](\overline{z})^* = -(\kappa^*+M[V](z))^{-1},\quad z\in\mathbb{C}_-.$$

Inserting this expression into (2.5) one obtains

$$\Theta[\kappa_a,\kappa_b,V](z) = I_{\mathbb{C}^2} - i\alpha\Gamma_0 G[\kappa_a,\kappa_b,V](\overline{z})^*\alpha,\quad z\in\mathbb{C}_-.$$

In [26] the operator-valued function $T[\kappa_a,\kappa_b,V](z):\mathfrak{H}\longrightarrow\mathbb{C}^2$,

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

was introduced for $z\in\mathrm{res}(H[\kappa_a,\kappa_b,V])$. We note that

$$T[\kappa_a,\kappa_b,V](z) = \alpha\Gamma_0(H[\kappa_a,\kappa_b,V]-z)^{-1} = \alpha G[\kappa_a,\kappa_b,V](z),\quad z\in\mathbb{C}_+.$$

Hence the adjoint operator $T[\kappa_a,\kappa_b,V](z)^*:\mathbb{C}^2\longrightarrow L^2(\Omega)$ exists and admits the representation

$$T[\kappa_a,\kappa_b,V](z)^* = G[\kappa_a,\kappa_b,V](z)^*\alpha,\quad z\in\mathbb{C}_+.$$

Taking into account (2.6) we find

$$\mathrm{ran}(T[\kappa_a,\kappa_b,V](z)^*)\subseteq\mathcal{N}_{\overline{z}}[V]\subseteq W^{1,2}(\Omega),\quad z\in\mathbb{C}_+.$$

In [26] the operator $\widehat{\alpha}:L^2(\Omega)\longrightarrow\mathbb{C}$,

$$\widehat{\alpha}f = \begin{pmatrix}\alpha_b f(b)\\ -\alpha_a f(a)\end{pmatrix},\quad f\in\mathrm{dom}(\widehat{\alpha}) := C(\bar{\Omega}), \tag{2.7}$$

was introduced. Since

$$\widehat{\alpha}f = \alpha\Gamma_0 f,\quad f\in\mathrm{dom}(S[V]^*)\subseteq W^{1,2}(\Omega),$$

the characteristic function $\Theta[\kappa_a,\kappa_b,V](\cdot)$ admits the representation

$$\Theta[\kappa_a,\kappa_b,V](z) = I_{\mathbb{C}^2} - i\widehat{\alpha}T[\kappa_a,\kappa_b,V](\overline{z})^*,\quad z\in\mathbb{C}_-, \tag{2.8}$$

which coincides with the representation of the characteristic function of [26]. Using the representation (2.8) we prove the following lemma.

Lemma 2.2 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then the characteristic function $\Theta[\kappa_a,\kappa_b,V](\cdot)$ is holomorphic in a neighbourhood of $\mathbb{R}$ and obeys*

$$\lim_{\lambda\to-\infty} \|\Theta[\kappa_a,\kappa_b,V](\lambda) - I_{\mathbb{C}^2}\|_{\mathcal{B}(\mathbb{C}^2)} = 0. \tag{2.9}$$

Proof. For simplicity we set $H[V] := H[q_a,q_b,V]$. Obviously, we have

$$H[V] := H[0] + V, \quad V \in L^\infty_{\mathbb{R}}(\Omega).$$

We note that $\inf\operatorname{spec}(H[V]) =: \gamma_V$ is finite. Let us introduce the operator

$$U[V](\lambda) := \widehat{\alpha}(H[V]-\lambda)^{-1/2}, \quad \lambda < \gamma_V,$$

where $\widehat{\alpha}$ is defined by (2.7). A straightforward computation shows that the representation

$$T[V](\lambda) = U[V](\lambda)\left(I - \frac{i}{2}U[V](\lambda)^*U[V](\lambda)\right)^{-1}(H[V]-\lambda)^{-1/2}$$

is valid for $\lambda < \gamma_V$. Hence the characteristic function admits the representation

$$\Theta[\kappa_a,\kappa_b,V](\lambda) = I - iU[V](\lambda)\left(I + \frac{i}{2}U[V](\lambda)^*U[V](\lambda)\right)^{-1}U[V](\lambda)^*$$

for $\lambda < \gamma_V$. Using the representation

$$U[V](\lambda) = U[V](\lambda_0)D[V](\lambda), \quad D[V](\lambda) := (H[V]-\lambda_0)^{1/2}(H[V]-\lambda)^{-1/2},$$

$\lambda_0, \lambda < \gamma_V$, we have

$$\begin{aligned}&\Theta[\kappa_a,\kappa_b,V](\lambda) = \\ &\quad I_{\mathbb{C}^2} - iU[V](\lambda_0)D[V](\lambda)\left(I + \frac{i}{2}U[V](\lambda)^*U[V](\lambda)\right)^{-1}D[V](\lambda)U[V](\lambda_0)^*\end{aligned}$$

for $\lambda_0, \lambda < \gamma_V$. Since $s-\lim_{\lambda\to-\infty} D[V](\lambda) = 0$ we obtain $s-\lim_{\lambda\to-\infty}\Theta[V](\lambda) = I_{\mathbb{C}^2}$ which yields immediately the operator-norm convergence of (2.9). $\square$

3 Dilation and Lax-Phillips scattering

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

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K[\kappa_a,\kappa_b,V]-z)^{-1}\restriction\mathfrak{H} = (H[\kappa_a,\kappa_b,V]-z)^{-1}, \quad \Im\mathrm{m}(z) > 0, \tag{3.1}$$

see [18]. The operator $K[\kappa_a,\kappa_b,V]$ is called a self-adjoint dilation of the maximal dissipative operator $H[\kappa_a,\kappa_b,V]$. Obviously, from the condition (3.1) one gets

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

If the condition

$$\operatorname{clospan}_{z\in\mathbb{C}\setminus\mathbb{R}}(K[\kappa_a,\kappa_b,V]-z)^{-1}\mathfrak{H} = \mathfrak{K}$$

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

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

and

$$(K[\kappa_a,\kappa_b,V]\vec{f})(\mathbf{x}) = -i\frac{d}{dx_-}f_-(x_-)\oplus(l[V]f)(x)\oplus -i\frac{d}{dx_+}f_+(x_+), \tag{3.2}$$

$\mathbf{x}:=(x_-,x,x_+)$, for $\vec{f}:=\vec{f}_-\oplus f\oplus\vec{f}_+\in\mathrm{dom}(K[\kappa_a,\kappa_b,V])$ where

$$\vec{f}_- := \begin{pmatrix} f^b_-(x_-)\\ f^a_-(x_-)\end{pmatrix} \qquad \vec{f}_+ := \begin{pmatrix} f^b_+(x_+)\\ f^a_+(x_+)\end{pmatrix}$$

and

$$\mathrm{dom}(K[\kappa_a,\kappa_b,V]) := \left\{\begin{array}{c} \vec{f}\in W^{1,2}(\mathbb{R}_-,\mathbb{C}^2)\oplus W^{1,2}(\Omega)\oplus W^{1,2}(\mathbb{R}_+,\mathbb{C}^2):\\ \frac{1}{m}f'\in W^{1,2}(\Omega)\\ \frac{1}{2m(b)}f'(b)-\kappa_b f(b)=\alpha_b f^b_-(0)\\ \frac{1}{2m(a)}f'(a)+\kappa_a f(a)=\alpha_a f^a_-(0)\\ \frac{1}{2m(b)}f'(b)-\overline{\kappa_b}f(b)=\alpha_b f^b_+(0)\\ \frac{1}{2m(b)}f'(a)+\overline{\kappa_a}f(b)=\alpha_a f^a_+(0)\end{array}\right\} \tag{3.3}$$

For more details the reader is referred to [26]. Obviously, the closed symmetric operator $L[V]$,

$$\begin{array}{rcl}(L[V]\vec{f})(\mathbf{x}) &:=& -i\frac{d}{dx_-}\vec{f}_-(x_-)\oplus(S[V]f)(x)\oplus -i\frac{d}{dx_+}\vec{f}_+(x_+)\\ \vec{f}\in\mathrm{dom}(L[V]) &:=& W^{1,2}_0(\mathbb{R}_-,\mathbb{C}^2)\oplus\mathrm{dom}(S[V])\oplus W^{1,2}_0(\mathbb{R}_+,\mathbb{C}^2)\end{array}$$

is a symmetric restriction of $K[\kappa_a,\kappa_b,V]$, where

$$W^{1,2}_0(\mathbb{R}_\pm,\mathbb{C}^2) := \{\vec{f}_\pm\in W^{1,2}(\mathbb{R},\mathbb{C}^2):\vec{f}_\pm(0)=0\}.$$

The deficiency indices of $L[V]$ are $(4,4)$. The domain of the adjoint operator $L[V]^*$ is given by

$$\mathrm{dom}(L[V]^*) := W^{1,2}(\mathbb{R}_-,\mathbb{C}^2)\oplus\mathrm{dom}(S[V]^*)\oplus W^{1,2}(\mathbb{R}_+,\mathbb{C}^2).$$

Another self-adjoint extension of $L[V]$ is defined by $K_D[V]$,

$$\begin{array}{rcl}(K_D[V]\vec{f})(\mathbf{x}) &:=& -i\frac{d}{dx_-}\vec{f}_-(x_-)\oplus(H_D[V]f)(x)\oplus -i\frac{d}{dx_+}\vec{f}_+(x_+),\\ \vec{f}\in\mathrm{dom}(K_D[V]) &:=& \{\vec{f}\in\mathrm{dom}(L[V]^*):\vec{f}_-(0)=\vec{f}_+(0)\}\ .\end{array} \tag{3.4}$$

If we introduce the differentiation operator K_0

$$\begin{array}{rcl}(K_0\vec{f}_0)(x) &:=& -i\frac{d}{dx}\vec{f}_0(x),\quad x\in\mathbb{R},\\ \vec{f}_0 &\in& \mathrm{dom}(K_0):=W^{1,2}(\mathbb{R},\mathbb{C}^2)\end{array}$$

and using the decomposition

$$\mathfrak{K} = L^2(\Omega) \oplus \mathfrak{K}_0, \quad \mathfrak{K}_0 := L^2(\mathbb{R}, \mathbb{C}^2), \tag{3.5}$$

then the operator $K_D[V]$ admits the representation

$$K_D[V] = H_D[V] \oplus K_0. \tag{3.6}$$

The wave operators $W_\pm[\kappa_a, \kappa_b, V]$,

$$W_\pm[\kappa_a, \kappa_b, V] := s - \lim_{t\to\pm\infty} e^{itK[\kappa_a,\kappa_b,V]} e^{-itK_D[V]} P^{ac}(K_D[V])$$

can be identified with the Lax-Phillips wave operators, cf. [14, 32], because the absolutely continuous subspace $\mathfrak{K}^{ac}(K_D[V])$ of $K_D[V]$ coincides with $\mathfrak{K}_0$. We note that the absolutely continuous part $K^{ac}_D[V]$ of $K_D[V]$ coincides with K_0. The wave operators exist by the Lax-Phillips scattering theory and are complete, cf. [32]. However, in our special situation there is an additional reason for the existence and completeness of the wave operators. Since $K[\kappa_a, \kappa_b, V]$ and $K_D[V]$ are self-adjoint extensions of one and the same closed symmetric operator $L[V]$ with deficiency indices $(4, 4)$ its turns out that the resolvent difference of $K[\kappa_a, \kappa_b, V]$ and $K_D[V]$ is a four dimensional operator. Hence the wave operator exist and are complete by the trace class existence theorem, cf. [14, 30].

The Lax-Phillips scattering operator $S_{LP}[\kappa_a, \kappa_b, V]$ is defined by

$$S_{LP}[\kappa_a, \kappa_b, V] := W_+[\kappa_a, \kappa_b, V]^* W_-[\kappa_a, \kappa_b, V].$$

It acts only on the subspace $\mathfrak{K}_0$ and is unitary there. Further, the Lax-Phillips scattering operator commutes with $K_D[V]$, in particular, with $0 \oplus K_0$. The Fourier transform $F : L^2(\mathbb{R}, \mathbb{C}^2) \longrightarrow L^2(\mathbb{R}, \mathbb{C}^2)$,

$$(F\vec{f}_0)(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx e^{-i\lambda x} \vec{f}_0(x), \quad \vec{f}_0 \in L^2(\mathbb{R}, \mathbb{C}^2),$$

defines a unitary operator such that FK_0F^* coincides with the multiplication operator M,

$$\begin{aligned} &(M\vec{f})(\lambda) := \lambda \vec{f}(\lambda), \quad \lambda \in \mathbb{R}, \\ &\vec{f} \in \mathrm{dom}(M) := \{\vec{f} \in L^2(\mathbb{R}, \mathbb{C}^2) : \lambda \vec{f}(\lambda) \in L^2(\mathbb{R}, \mathbb{C}^2). \end{aligned}$$

Since Lax-Phillips scattering operator $S_{LP}[\kappa_a, \kappa_b, V]$ commutes with K_0 the transformed operator $FS_{LP}[\kappa_a, \kappa_b, V]F^*$ commutes with M. Hence there is a measurable family $\{S_{LP}[\kappa_a, \kappa_b, V](\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators on $\mathbb{C}^2$ such that the $FS_{LP}[\kappa_a, \kappa_b, V]F^*$ coincides with the multiplication operator induced by $\{S_{LP}[\kappa_a, \kappa_b, V](\lambda)\}_{\lambda\in\mathbb{R}}$. The family $\{S_{LP}[\kappa_a, \kappa_b, V](\lambda)\}_{\lambda\in\mathbb{R}}$ is called the Lax-Phillips scattering matrix. One of the main results of the Lax-Phillips scattering theory is that

$$S_{LP}[\kappa_a, \kappa_b, V](\lambda) = \Theta[\kappa_a, \kappa_b, V](\lambda)^*$$

holds for a.e. $\lambda \in \mathbb{R}$, see also [24].

4 Phase shift

The phase shift $\omega[\kappa_a,\kappa_b,V](\cdot):\mathbb{R}\longrightarrow\mathbb{R}$ is defined by

$$e^{-2\pi i\omega[\kappa_a,\kappa_b,V](\lambda)} := \det(S_{LP}[\kappa_a,\kappa_b,V](\lambda)), \quad \lambda\in\mathbb{R}, \tag{4.1}$$

which is equivalent to

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

Notice that the phase shift is determined modulo $\mathbb{Z}$. To eliminate this non-uniqueness of the definition we demand in the following that $\omega[\kappa_a,\kappa_b,V](\lambda)$ is continuous in $\lambda\in\mathbb{R}$ and obeys

$$\lim_{\lambda\to-\infty}\omega[\kappa_a,\kappa_b,V](\lambda)=0 \tag{4.2}$$

which is in accordance with Lemma 2.2.

Lemma 4.1 *If $V\in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a,\kappa_b\in\mathbb{C}_+$, then the phase shift $\omega[\kappa_a,\kappa_b,V](\cdot)$ is holomorphic in a neighbourhood of $\mathbb{R}$ and satisfies*

$$\omega'[\kappa_a,\kappa_b,V](\lambda) := \frac{d}{d\lambda}\omega[\kappa_a,\kappa_b,V](\lambda) = -\frac{1}{2\pi}\mathrm{tr}(T[\kappa_a,\kappa_b,V](\lambda)T[\kappa_a,\kappa_b,V](\lambda)^*) \le 0$$

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

Proof. For brevity we set $H := H[\kappa_a,\kappa_b,V]$, $T(\lambda) := T[\kappa_a,\kappa_b,V](\lambda)$, $T_*(\lambda) := T_*[\kappa_a,\kappa_b,V](\lambda) := \widehat{\alpha}(H[\kappa_a,\kappa_b,V]^*-\lambda)^{-1}$ and $\Theta(\lambda) := \Theta[\kappa_a,\kappa_b,V](\lambda)$ as well as $\omega(\lambda) := \omega[\kappa_a,\kappa_b,V](\lambda)$. Since the characteristic function $\Theta(\lambda)$ is holomorphic in a neighbourhood of $\mathbb{R}$ one gets that the phase shift $\omega(\lambda)$ is also holomorphic there. By

$$T(\lambda)T(\lambda)^* = \alpha\left((H-\lambda)^{-1}-(H^*-\lambda)^{-1}\right)T(\lambda)^* + T_*(\lambda)T(\lambda)^*,$$

$\lambda\in\mathbb{R}$, and Lemma 3.1 of [26] we find

$$T(\lambda)T(\lambda)^* = i\alpha T_*(\lambda)^*T_*(\lambda)T(\lambda)^* + T_*(\lambda)T(\lambda)^*, \quad \lambda\in\mathbb{R},$$

or

$$T(\lambda)T(\lambda)^* = \{I+i\alpha T_*(\lambda)^*\}T_*(\lambda)T(\lambda)^*, \quad \lambda\in\mathbb{R}.$$

Using Formula (3.39) of [26] we obtain

$$T(\lambda)T(\lambda)^* = \Theta(\lambda)^*T_*(\lambda)T(\lambda)^*, \quad \lambda\in\mathbb{R}.$$

Using (2.8), a straightforward computation shows

$$\frac{\partial}{\partial\lambda}\Theta(\lambda) = -iT_*(\lambda)T(\lambda)^*, \quad \lambda\in\mathbb{R},$$

which gives

$$T(\lambda)T(\lambda)^* = i\Theta(\lambda)^*\frac{\partial}{\partial\lambda}\Theta(\lambda), \quad \lambda\in\mathbb{R}.$$

Taking into account formula (IV.1.14) of [22] we obtain

$$0 \le \mathrm{tr}(T(\lambda)T(\lambda)^*) = i\,\mathrm{tr}(\Theta(\lambda)^* \frac{\partial}{\partial\lambda}\Theta(\lambda)) = i\,\frac{d}{d\lambda}\ln\left(\det(\Theta(\lambda))\right) = -2\pi\frac{d}{d\lambda}\omega(\lambda)$$

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

Lemma 4.1 shows that the phase shift is a non-increasing function. Since $\lim_{\lambda\to-\infty}\omega[\kappa_a,\kappa_b,V](\lambda) = 0$ the phase function is non-positive. In order to estimate the growth of $-\omega[\kappa_a,\kappa_b,V](\cdot)$ let us investigate the counting function

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

To estimate $\Phi[\kappa_a,\kappa_b,V](\lambda)$ we consider the eigenvalue problem

$$\Theta[\kappa_a,\kappa_b,V](\lambda)\vec{x} = \mu\vec{x}, \quad \mu \in \mathbb{T}, \quad \vec{x} \in \mathbb{C}^2,$$

for each fixed $\lambda \in \mathbb{R}$. To treat this problem we introduce the family $\{H_\theta[V]\}_{\theta\in(0,2\pi)}$,

$$H_\theta[V] := H[q_a(\theta), q_b(\theta), V] \quad \text{and} \quad H_0[V] := H_D[V]$$

where the boundary coefficients are given by

$$q_b(\theta) := q_b - \frac{\alpha_b^2\cot(\theta/2)}{2} \quad \text{and} \quad q_a(\theta) := q_a - \frac{\alpha_a^2\cot(\theta/2)}{2}.$$

The spectrum $\mathrm{spec}(H_\theta[V])$ consists of simple eigenvalues $\mathrm{spec}(H_\theta[V]) = \{\lambda_k[V](\theta)\}_{k\in\mathbb{N}}$, $-\infty < \lambda_1[V](\theta) < \lambda_2[V](\theta) < \ldots$.

Lemma 4.2 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then $H_\theta[V] \ge H_{\theta'}[V]$ for $0 \le \theta \le \theta' < 2\pi$.*

Proof. The sesquilinear form $\mathfrak{t}_\theta[V]$ corresponding to $H_\theta[V]$ is given by $\mathrm{dom}(\mathfrak{t}_\theta[V]) = W^{1,2}(\Omega)$,

$$\mathfrak{t}_\theta[V](f,g) = \tag{4.3}$$
$$-q_a(\theta)f(a)\overline{g(a)} - q_b(\theta)f(b)\overline{g(b)} + \int_a^b dx\,\frac{1}{2m(x)}f'(x)\overline{g'(x)} + V(x)f(x)\overline{g(x)},$$

$f,g \in \mathrm{dom}(\mathfrak{t}_\theta[V]) = W^{1,2}(\Omega)$, $\theta \in (0,2\pi)$. Since $q_a(\theta') \le q_a(\theta)$ and $q_b(\theta') \le q_b(\theta)$ for $\theta' < \theta$ we easily obtain $\mathfrak{t}_\theta[V] \le \mathfrak{t}_{\theta'}[V]$. If $\theta' = 0$, then $\mathrm{dom}(t_0[V]) = W^{1,2}_0(\Omega) \subseteq W^{1,2}(\Omega) = \mathrm{dom}(\mathfrak{t}_\theta[V])$ and

$$\mathfrak{t}_\theta[V](f,f) \le \mathfrak{t}_0[V](f,f), \quad f \in \mathrm{dom}(\mathfrak{t}_0[V]), \quad \theta \in (0,2\pi)$$

which completes the proof. $\square$

The min-max principle gives the following

Corollary 4.3 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then the eigenvalue curves $\lambda_n[V](\cdot)$ of $H_\theta[V]$ satisfy*

$$\lambda_n[V](\theta') \le \lambda_n[V](\theta), \quad 0 \le \theta \le \theta' < 2\pi, \quad n \in \mathbb{N}.$$

Let us show that in fact the monotonicity of the eigenvalue curves is strict:

Lemma 4.4 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$\lambda_n[V](\theta') < \lambda_n[V](\theta), \quad 0 \le \theta < \theta' < 2\pi, \quad n \in \mathbb{N}.$$

Proof. We note that $\{H_\theta := H_\theta[V]\}_{\theta\in(0,2\pi)}$ is not only a monotone family but also an analytic one of self-adjoint operators of type (B), cf. [30, Section VII.4.2]. This yields that the eigenvalues of $\lambda_n(\theta) := \lambda_n[V](\theta)$ depend analytically on $\theta \in (0, 2\pi)$. Assuming now that there is a $k \in \mathbb{N}$ such that $\lambda_k(\theta') = \lambda_k(\theta'')$ for some $0 < \theta' < \theta'' < 2\pi$. In this case we get $\lambda_k(\theta') = \lambda_k(\theta) = \lambda_k(\theta'')$ for $\theta \in [\theta', \theta'']$. Since $\lambda_k(\theta)$ is analytic we find $\lambda_k(\theta) = \lambda_k(0)$, $\theta \in (0, 2\pi)$, that is, $\lambda_k(\theta)$ is constant and equals the Dirichlet eigenvalue $\lambda_k(0)$.

Next we show that if for some $k \in \mathbb{N}$ we have $\lambda_k(\theta) = \lambda_k(0)$, $\theta \in (0, 2\pi)$, then for each $j \in 1, 2, \ldots, k$ one has $\lambda_j(\theta) = \lambda_j(0)$, $\theta \in (0, 2\pi)$. Indeed, let us assume that there is a $\theta \in (0, 2\pi)$ such that $\lambda_{k-1}(\theta) < \lambda_{k-1}(0)$. In this case there is a neighbourhood $\mathcal{U} := (\lambda_{k-1}(\theta), \lambda_k(0))$ of $\lambda_{k-1}(0)$ which contains no eigenvalue of $H_{\theta'}$ for $\theta' \in (\theta, 2\pi)$. However, this is impossible by Lemma 2.1. In fact, if θ' is sufficiently close to 2π, then the neighbourhood $\mathcal{U}$ has to contain an eigenvalue of $H_{\theta'}$. Hence the assumption $\lambda_{k-1}(\theta) < \lambda_{k-1}(0)$ was false which yields $\lambda_{k-1}(\theta) = \lambda_{k-1}(0)$ for $\theta \in (0, 2\pi)$. By induction we get that $\lambda_j(\theta) = \lambda_j(0)$, $\theta \in (0, 2\pi)$, holds for each $j = 1, 2, \ldots, k$.

In particular, this holds for the lowest eigenvalue $\lambda_1(\theta) = \lambda_1(0)$, $\theta \in (0, 2\pi)$, which is given by

$$\lambda_1(\theta) := \inf\{\mathfrak{t}_\theta[V](f, f) : \ f \in W^{1,2}(\Omega), \quad \|f\|_{L^2(\Omega)} = 1\}, \quad \theta \in (0, 2\pi).$$

But (4.3) implies $\lim_{\theta\uparrow 2\pi} \lambda_1(\theta) = -\infty$ which contradicts the conclusion that $\lambda_1(\theta)$ remains unchanged for $\theta \in (0, 2\pi)$. □

Our next aim is to determine $\lim_{\theta\downarrow 0} \lambda_n[V](\theta)$ and $\lim_{\theta\uparrow 2\pi} \lambda_k[V](\theta)$.

Lemma 4.5 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then the eigenvalue curves satisfy*

$$\lim_{\theta\downarrow 0} \lambda_n[V](\theta) = \lambda_n[V](0), \quad n \in \mathbb{N}, \tag{4.4}$$

and

$$\lim_{\theta\uparrow 2\pi} \lambda_n[V](\theta) = \lambda_{n-2}[V](0), \quad n \in \mathbb{N}, \tag{4.5}$$

where $\lambda_{-1}[V](0) := \lambda_0[V](0) := -\infty$.

Proof. The family $\{H_\theta[V]\}_{\theta\in(0,\pi)}$ is operator norm continuous in the resolvent sense. In particular, this yields that the eigenvalues $\lambda_k[V](\theta)$, $k \in \mathbb{N}$, are continuous in $\theta \in (0, 2\pi)$. Moreover, since $\lim_{\theta\downarrow 0} q_a(\theta) = \lim_{\theta\downarrow 0} q_b(\theta) = \infty$ and $\lim_{\theta\uparrow 2\pi} q_a(\theta) = \lim_{\theta\uparrow 2\pi} q_b(\theta) = \infty$ we get by Lemma 2.1

$$\lim_{\theta\downarrow 0} \|(H_\theta[V] - i)^{-1} - (H_D[V] - i)^{-1}\|_{\mathcal{B}(\mathfrak{H})} = \lim_{\theta\uparrow 2\pi} \|(H_\theta[V] - i)^{-1} - (H_D[V] - i)^{-1}\|_{\mathcal{B}(\mathfrak{H})} = 0.$$

An application of Lemma 4.2 implies (4.4). It remains to show (4.5). First, by monotonicity the limits $\lim_{\theta\uparrow 2\pi} \lambda_k[V](\theta)$, $k \in \mathbb{N}$, exist, too. We introduce the intervals

$$\Delta_1 := (-\infty, \lambda_1[V](0)) \quad \text{and} \quad \Delta_n := (\lambda_{n-1}[V](0), \lambda_n[V](0)), \quad n = 2, 3, \ldots ,$$

that is, the sequence of spectral gaps of the Dirichlet operator $H_D[V]$. Further, we consider the symmetric operator $\widehat{S}[V]$ defined by

$$\begin{aligned} \widehat{S}[V]g &:= l[V]g, \quad g \in \mathrm{dom}(\widehat{S}[V]), \\ \mathrm{dom}(\widehat{S}[V]) &:= \left\{ g \in W^{1,2}(\Omega) : \begin{array}{l} \frac{1}{m}g' \in W^{1,2}(\Omega),\ g(a) = 0, \\ \frac{1}{2m(b)}g'(b) = g(b) = 0 \end{array} \right\}. \end{aligned}$$

The closed symmetric operator $\widehat{S}[V]$ has the deficiency indices $(1,1)$. Obviously we have $S[V] \le \widehat{S}[V] \le H_D[V]$ where $S[V]$ is defined by (2.1). By $\widehat{H}_\theta[V]$, $\theta \in (0,2\pi)$, we denote the self-adjoint operator

$$\begin{aligned} \widehat{H}_\theta[V]g &:= l[V]g, \quad g \in \mathrm{dom}(\widehat{H}_\theta[V]), \\ \mathrm{dom}(\widehat{H}_\theta[V]) &:= \left\{ g \in W^{1,2}(\Omega) : \begin{array}{l} \frac{1}{m(x)}g'(x) \in W^{1,2},\ \ g(a) = 0, \\ \frac{1}{2m(b)}g'(b) = q_b(\theta)g(b) \end{array} , \right\} \end{aligned}$$

and we set $\widehat{H}_0[V] := H_D[V]$. Moreover, similar to Lemma 4.2 the family $\{\widehat{H}_\theta[V]\}_{\theta\in(0,2\pi)}$ is non-increasing, i.e.

$$\widehat{H}_{\theta'}[V] \le \widehat{H}_\theta[V], \quad 0 \le \theta \le \theta' < 2\pi,$$

and analytic in sense of type B, cf. [30, Sect. VII.4.2]. Denoting by $\{\widehat{\lambda}_k[V](\theta)\}_{k\in\mathbb{N}}$ the eigenvalues of $\widehat{H}_\theta[V]$ we get similarly to Lemma 4.4 that

$$\widehat{\lambda}_k[V](\theta') < \widehat{\lambda}_k[V](\theta), \quad k \in \mathbb{N}, \quad 0 \le \theta < \theta' < 2\pi. \tag{4.6}$$

Since $H_D[V]$ is a self-adjoint extension of $\widehat{S}[V]$ the open intervals Δ_k are gaps for $\widehat{S}[V]$. Since $\widehat{S}[V]$ has deficiency indices $(1,1)$ the self-adjoint extension $\widehat{H}_\theta[V]$ of $\widehat{S}[V]$ has at most one eigenvalue in each gap Δ_k. Taking into account (4.6) we find

$$\widehat{\lambda}_k[V](\theta) \in \Delta_k, \quad k \in \mathbb{N}, \quad \theta \in (0,2\pi).$$

We set

$$\widehat{\Delta}_1(\theta) := (-\infty, \widehat{\lambda}_1[V](\theta)), \quad \widehat{\Delta}_k(\theta) := (\widehat{\lambda}_{k-1}[V](\theta), \widehat{\lambda}_k[V](\theta)), \quad k = 2,3,\dots ,$$

$\theta \in (0,2\pi)$. Obviously we have

$$\widehat{\Delta}_k(\theta) \subseteq \Delta_{k-1} \cup \{\lambda_{k-1}[V](0)\} \cup \Delta_k \quad \theta \in (0,2\pi), \quad k \in \mathbb{N}. \tag{4.7}$$

Further, let us introduce the symmetric operator $\widetilde{S}[V]$ defined by

$$\widetilde{S}[V]g := l[V]g, \quad \mathrm{dom}(\widetilde{S}[V]) := \left\{ g \in W^{1,2}(\Omega) : \begin{array}{l} \frac{1}{m}g' \in W^{1,2}(\Omega), \\ \frac{1}{2m(a)}g'(a) = g(a) = 0, \\ \frac{1}{2m(b)}g'(b) = q_b(\theta)g(b) \end{array} \right\},$$

which has the deficiency indices $(1,1)$, too. Obviously, the operator $\widehat{H}_\theta[V]$, $\theta \in [0,2\pi)$, is a self-adjoint extension of $\widetilde{S}[V]$. Therefore, the open intervals $\widehat{\Delta}_k(\theta)$ are spectral gaps of the closed symmetric operator $\widetilde{S}[V]$. Moreover, the operator $H_\theta[V]$, $\theta \in [0,2\pi)$, is a self-adjoint extension of $\widetilde{S}[V]$, too. As above we get

$$\lambda_k[V](\theta) \in \widehat{\Delta}_k(\theta), \quad k \in \mathbb{N}, \quad \theta \in (0,2\pi).$$

Taking into account (4.7) we obtain $\lambda_k[V](\theta) \in \Delta_{k-1} \cup \{\lambda_{k-1}[V](0)\} \cup \Delta_k$. Hence we have either

$$\lim_{\theta \uparrow 2\pi} \lambda_k[V](\theta) = \lambda_{k-1}[V](0) \quad \text{or} \quad \lim_{\theta \uparrow 2\pi} \lambda_k[V](\theta) = \lambda_{k-2}[V](0)$$

for $k = 2, 3, \ldots$. Let us assume that for some $j \geq 2$ we have

$$\lim_{\theta \uparrow 2\pi} \lambda_j[V](\theta) = \lambda_{j-1}[V](0).$$

In this case, we find that $\lim_{\theta \uparrow 2\pi} \lambda_{j-1}[V](\theta) = \lambda_{j-3}[V](0)$ is impossible. Indeed, if θ is sufficiently close to 2π, then there is neighbourhood of $\lambda_{j-2}[V](0)$ which does not contain an eigenvalue of $H_\theta[V]$. However, this contradicts Lemma 2.1. Therefore, we obtain that $\lim_{\theta \uparrow 2\pi} \lambda_k[V](\theta) = \lambda_{k-1}[V](0)$, $k = 2, 3, \ldots, j-1$. Furthermore, one gets that $\lim_{\theta \uparrow 2\pi} \lambda_{j+1}[V](\theta) = \lambda_{j-1}[V](0)$ is also impossible. In fact, for each sufficiently small neighbourhood of $\lambda_{j-1}[V](0)$ there is a sufficiently large $\theta \in (0, 2\pi)$ such that this neighbourhood contains two eigenvalues of $H_\theta[V]$ which contradicts again Lemma 2.1. Hence $\lim_{\theta \uparrow 2\pi} \lambda_k[V](\theta) = \lambda_{k-1}[V](0)$, $k = j+1, j+2, \ldots$. Therefore, we find $\lim_{\theta \uparrow 2\pi} \lambda_k[V](\theta) = \lambda_{k-1}[V](0)$ for $k \in \mathbb{N}$. In particular, we have that the interval Δ_1 contains only one eigenvalue of $H_\theta[V]$ for each $\theta \in (0, 2\pi)$. However, this is impossible, too. To show this we introduce the self-adjoint operator h_θ, $\theta \in (0, 2\pi)$,

$$\begin{aligned}
(h_\theta g)(x) &:= -\tau \tfrac{d^2}{dx^2} g(x) + \|V\|_{L^\infty} g(x), \quad g \in \mathrm{dom}(h_\theta), \\
\mathrm{dom}(h_\theta) &:= \left\{ f \in W^{2,2}(\Omega) : \begin{array}{rcl} \tau f'(a) &=& -q_a(\theta) f(a) \\ \tau f'(b) &=& q_b(\theta) f(b) \end{array} \right\}
\end{aligned}$$

and $\tau := \|1/2m\|_{L^\infty}$. Obviously, we have $H_\theta[V] \leq h_\theta$, $\theta \in (0, 2\pi)$, which yields $\lambda_k[V](\theta) \leq \mu_k(\theta)$, $k \in \mathbb{N}$, for $\theta \in (0, 2\pi)$, where $\{\mu_k(\theta)\}_{k \in \mathbb{N}}$ are the eigenvalues of h_θ. An involved but straightforward computation shows that the first two eigenvalues $\mu_1(\theta)$ and $\mu_2(\theta)$ of h_θ tend to $-\infty$ as $\theta \uparrow 2\pi$. Hence the first two eigenvalues $\lambda_1[V](\theta)$ and $\lambda_2[V](\theta)$ tend also to $-\infty$ as $\theta \uparrow 2\pi$ which shows that for sufficiently large $\theta \in (0, 2\pi)$ one has $\lambda_1[V](\theta) \in \Delta_1$ and $\lambda_2[V](\theta) \in \Delta_1$. $\square$

Next we show that the eigenvalues of the characteristic function $\Theta[\kappa_a, \kappa_b, V](\lambda)$ are intrinsically connected with the eigenvalues of the family $\{H_\theta[V]\}_{\theta \in [0, 2\pi)}$.

Lemma 4.6 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then*

$$\mu = e^{i\theta} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda)) \Longleftrightarrow \lambda \in \mathrm{spec}(H_\theta[V]), \quad \theta \in [0, 2\pi), \quad \lambda \in \mathbb{R}.$$

Proof. Multiplying the relation (2.8) on the left by $T[\kappa_a, \kappa_b, V](\lambda)^*$ we find

$$T[\kappa_a, \kappa_b, V](\lambda)^* \xi - iT[\kappa_a, \kappa_b, V](\lambda)^* \alpha T[\kappa_a, \kappa_b, V](\lambda)^* \xi = \mu T[\kappa_a, \kappa_b, V](\lambda)^* \xi.$$

Setting $g := T[\kappa_a, \kappa_b, V](\lambda)^* \xi \in W^{1,2}(\Omega)$ we obtain

$$g - iT[\kappa_a, \kappa_b, V](\lambda)^* \alpha g = \mu g \quad \text{or} \quad T[\kappa_a, \kappa_b, V](\lambda)^* \alpha g = i(\mu - 1) g.$$

Let $h \in L^2(\Omega)$. Then

$$\langle \alpha g, T[\kappa_a, \kappa_b, V](\lambda) h \rangle = i(\mu - 1)(g, h)$$

where we recall that $\langle\cdot,\cdot\rangle$ denotes the scalar product of $\mathbb{C}^2$. Setting $f := (H[\kappa_a,\kappa_b,V]-\lambda)^{-1}h \in \mathrm{dom}(H[\kappa_a,\kappa_b,V])$ we get

$$\langle \alpha g, \alpha f\rangle = i(\mu-1)(g,(H[\kappa_a,\kappa_b,V]-\lambda)f). \tag{4.8}$$

One has

$$(g,(H[\kappa_a,\kappa_b,V]-\lambda)f) = \int_a^b dx\, g(x)\overline{((l[V]f)(x)-\lambda f(x))}.$$

Since $(l[V]-\lambda)g = 0$ we find

$$\begin{aligned}(g,(H[\kappa_a,\kappa_b,V]-\lambda)f) &=\\ -g(b)\frac{1}{2m(b)}\overline{f'(b)} + g(a)\frac{1}{2m(a)}\overline{f'(a)} &+ \frac{1}{2m(b)}g'(b)\overline{f(b)} - \frac{1}{2m(a)}g'(a)\overline{f(a)}.\end{aligned}$$

Since $f\in \mathrm{dom}(H[\kappa_a,\kappa_b,V]))$ we get that

$$\begin{aligned}(g,(H[\kappa_a,\kappa_b,V]-\lambda)f) &=\\ -g(b)\overline{\kappa_b}\overline{f(b)} - g(a)\overline{\kappa_a}\overline{f(a)} &+ \frac{1}{2m(b)}g'(b)\overline{f(b)} - \frac{1}{2m(a)}g'(a)\overline{f(a)}\end{aligned}$$

which yields

$$\begin{aligned}(g,(H[\kappa_a,\kappa_b,V]-\lambda)f) &=\\ \left\{\frac{1}{2m(b)}g'(b) - \overline{\kappa_b}g(b)\right\}\overline{f(b)} &+ \left\{-\frac{1}{2m(a)}g'(a) - \overline{\kappa_a}g(a)\right\}\overline{f(a)}.\end{aligned}$$

Taking into account (4.8) one gets that the element g has to satisfy the boundary conditions

$$\begin{aligned}\alpha_b^2 g(b) &= i(\mu-1)\left\{\tfrac{1}{2m(b)}g'(b) - \overline{\kappa_b}g(b)\right\},\\ \alpha_a^2 g(a) &= i(\mu-1)\left\{-\tfrac{1}{2m(a)}g'(a) - \overline{\kappa_a}g(a)\right\}\end{aligned}$$

which implies

$$\frac{1}{2m(b)}g'(b) = q_b(\theta)g(b), \quad \text{and} \quad \frac{1}{2m(a)}g'(a) = -q_a(\theta)g(a), \quad \theta\in(0,2\pi),$$

for $\mu\neq 1$. If $\mu = 1$, then $g(a) = g(b) = 0$. Hence, $g\in\mathrm{dom}(H_D[V])$ and $\lambda\in\mathrm{spec}(H_D[V]) = \mathrm{spec}(H_0[V])$, i.e $\theta = 0$.

Conversely, if $\lambda\in\mathrm{spec}(H_\theta[V])$, $\theta\in[0,2\pi)$, then the eigenfunction g, $H_\theta[V]g = \lambda g$, satisfies the equation

$$T[V]^*(\lambda)\alpha g = i(\mu-1)g$$

or

$$(I - iT[V]^*(\lambda)\alpha)g = \mu g.$$

Multiplying on the left by α we obtain

$$(I - i\alpha T[V]^*(\lambda))\alpha g = \mu\alpha g.$$

Setting $\xi := \alpha g$ and using (2.8) we complete the proof. □

Lemma 4.7 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then we have*

$$\{\lambda \in \mathbb{R} : \det(\Theta[\kappa_a, \kappa_b, V](\lambda)) = 1\} = \bigcup_{\theta \in (0,\pi)} \mathrm{spec}(H_\theta[V]) \cap \mathrm{spec}(H_{2\pi-\theta}[V]). \tag{4.9}$$

Proof. At first we note that $\det(\Theta[\kappa_a, \kappa_b, V](\lambda)) = 1$ if and only if $\mu = e^{i\theta} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda))$ and $\overline{\mu} = e^{i(2\pi-\theta)} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda))$, $\theta \in [0, 2\pi)$. It remains to show that the cases $\theta = 0$ and $\theta = \pi$ are impossible: indeed, if $\theta = 0$, then $\mu = 1$. In this case the eigenvalue $\mu = 1$ of $\Theta[\kappa_a, \kappa_b, V](\lambda)$ has the multiplicity two. Hence, there are two mutually orthogonal eigenvectors $\xi_1, \xi_2 \in \mathbb{C}^2$ such that that $\Theta[\kappa_a, \kappa_b, V](\lambda)\xi_i = \xi_i$, $i = 1, 2$. We set

$$g_i := T[\kappa_a, \kappa_b, V](\lambda)^* \xi_i \in W^{1,2}(\Omega), \quad i = 1, 2.$$

Both functions g_i are eigenfunctions of $H_D[V]$ with the eigenvalue λ. Since the spectrum of $H_D[V]$ is simple there are constants $C_i \in \mathbb{C}$ such that $C_1 g_1 + C_2 g_2 = 0$. Hence

$$T[\kappa_a, \kappa_b, V](\lambda)^* \{C_1 \xi_1 + C_2 \xi_2\} = 0.$$

For each $h \in L^2(\Omega)$ we have

$$(C_1 \xi_1 + C_2 \xi_2, T[\kappa_a, \kappa_b, V](\lambda) h) = 0.$$

Since $\mathrm{ran}(T[\kappa_a, \kappa_b, V](\lambda)) = \mathbb{C}^2$ we find $C_1 \xi_1 + C_2 \xi_2 = 0$ which is impossible. The same holds for $\theta = \pi$ which yields $\mu = -1$. By Lemma 4.6 we have $\mu = e^{i\theta} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda))$ if and only if $\lambda \in \mathrm{spec}(H_\theta[V])$ and $\overline{\mu} = e^{i(2\pi-\theta)} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda))$ if and only if $\lambda \in \mathrm{spec}(H_{2\pi-\theta}[V])$. Hence

$$\mu = e^{i\theta}, \overline{\mu} = e^{i(2\pi-\theta)} \in \mathrm{spec}(\Theta[\kappa_a, \kappa_b, V](\lambda)) \Longleftrightarrow \lambda \in \mathrm{spec}(H_\theta[V]) \cap \mathrm{spec}(H_{2\pi-\theta}[V])$$

which proves (4.9). $\square$

Let us introduce the spectral distribution function

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

Theorem 4.8 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then*

$$N_D[V](\lambda) \le \Phi[\kappa_a, \kappa_b, V](\lambda) \le N_D[V](\lambda) + 1, \quad \lambda \in \mathbb{R}. \tag{4.10}$$

Proof. Let us consider the sets

$$\Lambda_n := \Delta_n \cap \bigcup_{\theta \in (0,\pi)} \mathrm{spec}(H_\theta[V]) \cap \mathrm{spec}(H_{2\pi-\theta}[V]), \quad n \in \mathbb{N}.$$

By Lemma 4.7 one has

$$\{\lambda \in \mathbb{R} : \det(\Theta[\kappa_a, \kappa_b, V](\lambda)) = 1\} = \bigcup_{n \in \mathbb{N}} \Lambda_n.$$

By Proposition 4.5 only the eigenvalues $\lambda_n[V](\theta)$, $\lambda_{n+1}[V](\theta)$, $\theta \in (0, 2\pi)$, belong to the interval Δ_n, other eigenvalues cannot. Further, by Proposition 4.5 we have

$$\lim_{\theta \downarrow 0} \lambda_n[V](\theta) = \lambda_n[V](0) \quad \text{and} \quad \lim_{\theta \downarrow 0} \lambda_{n+1}[V](2\pi - \theta) = \lambda_{n-1}[V](0), \quad n \in \mathbb{N}.$$

Since $\lambda_n[V](\theta)$ is decreasing and $\lambda_{n+1}[V](2\pi-\theta)$ is increasing in $\theta \in (0,2\pi)$, there is at most one $\theta \in (0,\pi)$ such that $\lambda_{n+1}[V](2\pi-\theta) = \lambda_n[V](\theta)$ which yields $\mathrm{card}\{\Lambda_n\} \le 1$. Moreover, we have

$$\lambda_{n-1}[V](0) < \lambda_{n+1}[V](\theta) < \lambda_{n+1}[V](\pi), \quad \theta \in (\pi, 2\pi),$$

and

$$\lambda_n[V](\pi) < \lambda_n[V](\theta) < \lambda_n[V](0), \quad \theta \in (0,\pi),$$

as well as $\lambda_n[V](\pi) < \lambda_{n+1}[V](\pi)$. Hence there is at least one $\theta \in (0,\pi)$ such that $\lambda_{n+1}[V](2\pi-\theta) = \lambda_n[V](\theta)$ which shows $\mathrm{card}\{\Lambda_n\} \ge 1$. Therefore $\mathrm{card}\{\Lambda_n\} = 1$ which implies immediately (4.10). □

Corollary 4.9 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then*

$$0 \le -\omega[\kappa_a,\kappa_b,V](\lambda) \le 2 + \frac{1}{\pi}\sqrt{2\|m\|_{L^\infty}|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+}, \quad \lambda \in \mathbb{R}, \tag{4.11}$$

where $(\lambda + \|V_-\|_{L^\infty})_+ := \frac{1}{2}\left(\lambda + \|V_-\|_{L^\infty} + |\lambda + \|V_-\|_{L^\infty}|\right) \ge 0.$

Proof. Obviously, we have

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

Using Theorem 4.8 we find

$$-\omega[\kappa_a,\kappa_b,V](\lambda) \le 2 + N_D[V](\lambda), \quad \lambda \in \mathbb{R}.$$

Further, we note that $h_D \le H_D[V]$,

$$\begin{array}{rcl} (h_D g)(x) & := & -\frac{1}{2\|m\|_{L^\infty}}\frac{d^2}{dx^2} g(x) - \|V_-\|_{L^\infty} g(x), \\ g & \in & \mathrm{dom}(h_D) := \{f \in W^{2,2}(\Omega) : f(a) = f(b) = 0\}. \end{array}$$

The spectral distribution function $n_D(\cdot)$ of h_D can be estimated by

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

Since $N_D[V](\lambda) \le n_D(\lambda)$, $\lambda \in \mathbb{R}$, one gets (4.11). □

5 Spectral shift and trace formula

Since $H[\kappa_a,\kappa_b,V]$ and $H_D[V]$ are extensions of one and the same closed symmetric operator $S[V]$ with deficiency indices $(2,2)$ the resolvent difference obeys

$$(H[\kappa_a,\kappa_b,V] - z)^{-1} - (H_D[V] - z)^{-1} \in \mathcal{L}_1(\mathfrak{H}), \quad z \in \mathbb{C}_+.$$

In fact, the difference is a two dimensional operator.

Theorem 5.1 *If $V \in L^\infty(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then there is a real function $\xi[\kappa_a,\kappa_b,V](\cdot) \in L^1(\mathbb{R},(1+\lambda^2)^{-1}d\lambda)$ such that the trace formula*

$$\operatorname{tr}\left((H[\kappa_a,\kappa_b,V]-z)^{-1} - (H_D[V]-z)^{-1}\right) = -\int_{\mathbb{R}} (\lambda-z)^{-2}\xi[\kappa_a,\kappa_b,V](\lambda)d\lambda \qquad (5.1)$$

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

Proof. Using formulas (3.13) of [26] we find that

$$\begin{aligned}&-iT[\kappa_a,\kappa_b,V](i)^*T[\kappa_a,\kappa_b,V](i) =\\ &\quad (H[\kappa_a,\kappa_b,V]^*+i)^{-1} - (H[\kappa_a,\kappa_b,V]-i)^{-1} +\\ &\quad 2i(H[\kappa_a,\kappa_b,V]^*+i)^{-1}(H[\kappa_a,\kappa_b,V]-i)^{-1}\end{aligned}$$

which shows that Condition (4.2) of Theorem 4.1 of [1] is satisfied. Since $H_D[V]$ is self-adjoint Condition (4.3) of [1] also holds. Applying Theorem 4.1 of [1] we complete the proof. □

A real function $\xi[\kappa_a,\kappa_b,V](\lambda) \in L^1(\mathbb{R},(1+\lambda^2)d\lambda)$ is called the spectral shift of the pair $\{H[\kappa_a,\kappa_b,V], H_D[V]\}$ if the trace formula (5.1) is satisfied

Considering the pair $\{K[\kappa_a,\kappa_b,V], K_D[V]\}$ one gets that

$$(K[\kappa_a,\kappa_b,V]-z)^{-1} - (K_D[V]-z)^{-1} \in \mathcal{L}_1(\mathfrak{H})$$

for $z \in \mathbb{C}\setminus\mathbb{R}$. This follows from the fact that $K[\kappa_a,\kappa_b,V]$ and $K_D[V]$ are self-adjoint extensions of the same closed symmetric operator $L[V]$ which has deficiency indices $(4,4)$. Using again Theorem 4.1 of [1] we find that the pair $\{K[\kappa_a,\kappa_b,V], K_D[V]\}$ admits a spectral shift $\eta[\kappa_a,\kappa_b,V](\cdot) \in L^1(\mathbb{R},(1+\lambda^2)^{-1}d\lambda)$, too. The trace formula then takes the form

$$\operatorname{tr}\left((K[\kappa_a,\kappa_b,V]-z)^{-1} - (K_D[V]-z)^{-1}\right) = -\int_{\mathbb{R}} (\lambda-z)^{-2}\eta[\kappa_a,\kappa_b,V](\lambda)d\lambda, \quad z \in \mathbb{C}\setminus\mathbb{R}.$$

Let us clarify the relation between $\xi[\kappa_a,\kappa_b,V](\cdot)$ and $\eta[\kappa_a,\kappa_b,V](\cdot)$.

Lemma 5.2 *Assume $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a,\kappa_b \in \mathbb{C}_+$. Then*

$$\operatorname{tr}\left((K[\kappa_a,\kappa_b,V]-z)^{-1} - (K_D[V]-z)^{-1}\right) = \operatorname{tr}\left((H[\kappa_a,\kappa_b,V]-z)^{-1} - (H_D[V]-z)^{-1}\right)$$

for $z \in \mathbb{C}_+$. Consequently, any spectral shift $\xi[\kappa_a,\kappa_b,V](\cdot) \in L^1(\mathbb{R},(1+\lambda^2)^{-1}d\lambda)$ of the pair $\{H[\kappa_a,\kappa_b,V], H_D[V]\}$ is a spectral shift of the pair $\{K[\kappa_a,\kappa_b,V], K_D[V]\}$ and vice versa.

Proof. Using the terminology of Ch. 3 and taking into account (3.5) and (3.6) we find that

$$\begin{aligned}&((K_D[V]-z)^{-1}\vec{f})(\mathbf{x}) = \qquad (5.2)\\ &\quad i\int_{-\infty}^{x_-} dy\; e^{i(x_--y)z}\vec{f}_-(y) \oplus (H_D[V]-z)^{-1}f(x) \oplus\\ &\quad i\int_0^{x_+} dy\; e^{i(x_+-y)z}\vec{f}_+(y) + i\int_{-\infty}^0 dy\; e^{i(x_+-y)z}\vec{f}_-(y),\end{aligned}$$

$\vec{f} = \vec{f}_- \oplus f \oplus \vec{f}_+$ and $z \in \mathbb{C}_+$. From Theorem 4.2 of [27] one gets the representation

$$\begin{aligned}
&((K[\kappa_a,\kappa_b,V] - z)^{-1}\vec{f})(\mathbf{x}) = \\
&\quad i\int_{-\infty}^{x_-} dy\; e^{i(x_- - y)z}\vec{f}_-(y) \oplus \\
&\quad (H[\kappa_a,\kappa_b,V] - z)^{-1}f(x) + iT_*[\kappa_a,\kappa_b,V](\overline{z})^*\int_{-\infty}^{0} dy\; e^{-iyz}\vec{f}_-(y) \oplus \\
&\quad i\int_{0}^{x_+} dy\; e^{i(x_+ - y)z}\vec{f}_+(y) + ie^{izx_+}T[\kappa_a,\kappa_b,V](z)f + \\
&\quad i\Theta[\kappa_a,\kappa_b,V](\overline{z})^*\int_{-\infty}^{0} dy\; e^{i(x_+ - y)z}\vec{f}_-(y),
\end{aligned} \tag{5.3}$$

$\vec{f} = \vec{f}_- \oplus f \oplus \vec{f}_+$ and $z \in \mathbb{C}_+$. Denoting by $P_\pm$ the orthogonal projections form $\mathfrak{K}$ onto the subspaces $L^2(\mathbb{R}_\pm, \mathbb{C}^2)$ one easily obtains from (5.2) and (5.3) that

$$P_\pm\left((K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right)P_\pm = 0 \tag{5.4}$$

for $z \in \mathbb{C}_+$. Using the representation

$$\begin{aligned}
&\operatorname{tr}\left((K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right) = \\
&\quad \operatorname{tr}\left(P_-\left\{(K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right\}P_-\right) + \\
&\quad \operatorname{tr}\left(P^{\mathfrak{K}}_{\mathfrak{H}}\left\{(K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right\}P^{\mathfrak{K}}_{\mathfrak{H}}\right) + \\
&\quad \operatorname{tr}\left(P_+\left\{(K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right\}P_+\right)
\end{aligned}$$

and taking into account (5.4) we get

$$\begin{aligned}
&\operatorname{tr}\left((K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right) = \\
&\quad \operatorname{tr}\left(P^{\mathfrak{K}}_{\mathfrak{H}}\left\{(K[\kappa_a,\kappa_b,V] - z)^{-1} - (K_D[V] - z)^{-1}\right\}P^{\mathfrak{K}}_{\mathfrak{H}}\right)
\end{aligned}$$

for $z \in \mathbb{C}_+$. Using that $K[\kappa_a,\kappa_b,V]$ is a self-adjoint dilation of the maximal dissipative operator $H[\kappa_a,\kappa_b,V]$ we have thus proved (5.2). The second assertion follows directly from the first. □

Lemma 5.3 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a,\kappa_b \in \mathbb{C}_+$, then*

$$\frac{d}{d\lambda}(E_{K[\kappa_a,\kappa_b,V]}(\lambda)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}} = \frac{1}{2\pi}\langle T[\kappa_a,\kappa_b,V](\lambda)f, T[\kappa_a,\kappa_b,V](\lambda)g\rangle_{\mathbb{C}^2} \tag{5.5}$$

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

Proof. We note that

$$\begin{aligned}
&\frac{d}{d\lambda}(E_{K[\kappa_a,\kappa_b,V]}(\lambda)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}} = \\
&\quad \frac{1}{2\pi i}\lim_{\epsilon\downarrow 0}\Big\{((K[\kappa_a,\kappa_b,V] - \lambda - i\epsilon)^{-1})P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}} - \\
&\quad ((K[\kappa_a,\kappa_b,V] - \lambda + i\epsilon)^{-1})P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}}\Big\}
\end{aligned}$$

for a.e. $\lambda \in \mathbb{R}$. Since $K[\kappa_a, \kappa_b, V]$ is a dilation of $H[\kappa_a, \kappa_b, V]$ we find

$$\begin{aligned}
&\frac{d}{d\lambda}(E_{K[\kappa_a,\kappa_b,V]}(\lambda)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}} = \\
&\qquad \frac{1}{2\pi i}\lim_{\epsilon\downarrow 0}\left\{((H[\kappa_a,\kappa_b,V] - \lambda - i\epsilon)^{-1})f, g)_{\mathfrak{H}} - ((H[\kappa_a,\kappa_b,V]^* - \lambda + i\epsilon)^{-1})f, g)_{\mathfrak{H}}\right\}
\end{aligned}$$

which yields

$$\begin{aligned}
&\frac{d}{d\lambda}(E_{K[\kappa_a,\kappa_b,V]}(\lambda)P^{\mathfrak{K}}_{\mathfrak{H}}\vec{f}, P^{\mathfrak{K}}_{\mathfrak{H}}\vec{g})_{\mathfrak{K}} = \\
&\qquad \frac{1}{2\pi i}\left\{((H[\kappa_a,\kappa_b,V] - \lambda)^{-1})f, g)_{\mathfrak{H}} - ((H[\kappa_a,\kappa_b,V]^* - \lambda)^{-1})f, g)_{\mathfrak{H}}\right\}
\end{aligned} \tag{5.6}$$

where we have used that the spectrum of $H[\kappa_a, \kappa_b, V]$ is non-real. Finally, Lemma 3.1 of [26] states the coincidence of the right hand sides of (5.6) and (5.5), what completes the proof. □

Theorem 5.4 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$, then*

$$\xi_0[\kappa_a,\kappa_b,V](\lambda) := \omega[\kappa_a,\kappa_b,V](\lambda) + N_D[V](\lambda), \quad \lambda \in \mathbb{R}, \tag{5.7}$$

defines a spectral shift of the pair $\{H[\kappa_a, \kappa_b, V], H_D[V]\}$ and, hence, of the pair $\{K[\kappa_a, \kappa_b, V], K_D[V]\}$.

Proof. Using that $K[\kappa_a, \kappa_b, V]$ is a dilation of $H[\kappa_a, \kappa_b, V]$ we get

$$((H[\kappa_a,\kappa_b,V] - z)^{-1}f, f) = \int_{\mathbb{R}} (\lambda - z)^{-1}\, d(E_{K[\kappa_a,\kappa_b,V]}(\lambda)f, f),$$

$f \in \mathfrak{H}$, for $z \in \mathbb{C}_+$. Since $K[\kappa_a, \kappa_b, V]$ is absolutely continuous we obtain

$$((H[\kappa_a,\kappa_b,V] - z)^{-1}f, f) = \int_{\mathbb{R}} (\lambda - z)^{-1}\frac{d}{d\lambda}(E_{K[\kappa_a,\kappa_b,V]}(\lambda)f, f)\, d\lambda,$$

$f \in \mathfrak{H}$, for $z \in \mathbb{C}_+$. Using Lemma 5.3 we find

$$((H[\kappa_a,\kappa_b,V] - z)^{-1}f, f) = \frac{1}{2\pi}\int_{\mathbb{R}} (\lambda - z)^{-1}(T[\kappa_a,\kappa_b,V](\lambda)f, T[\kappa_a,\kappa_b,V](\lambda)f)\, d\lambda, \tag{5.8}$$

$f \in \mathfrak{H}$, for $z \in \mathbb{C}_+$. Further, we have

$$((H_D[V] - z)^{-1}f, f) = \int_{\mathbb{R}} (\lambda - z)^{-1}\, d(E_{H_D[V]}(\lambda)f, f), \tag{5.9}$$

$f \in \mathfrak{H}$, for $z \in \mathbb{C}_+$. We note that

$$\begin{aligned}
&\operatorname{tr}\left((H[\kappa_a,\kappa_b,V] - z)^{-1} - (H_D[V] - z)^{-1}\right) = \\
&\qquad \sum_{n\in\mathbb{N}}\left(\left((H[\kappa_a,\kappa_b,V] - z)^{-1} - (H_D[V] - z)^{-1}\right)f_n, f_n\right)
\end{aligned} \tag{5.10}$$

where $\{f_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $\mathfrak{H}$. Inserting (5.8) and (5.9) into (5.10) we get

$$\begin{aligned}
&\operatorname{tr}\left((H[\kappa_a,\kappa_b,V]-z)^{-1}-(H_D[V]-z)^{-1}\right)= \\
&\sum_{n\in\mathbb{N}}\Big\{\frac{1}{2\pi}\int_{\mathbb{R}}(\lambda-z)^{-1}(T[\kappa_a,\kappa_b,V](\lambda)f_n,T[\kappa_a,\kappa_b,V](\lambda)f_n)\,d\lambda- \\
&\int_{\mathbb{R}}(\lambda-z)^{-1}\,d(E_{H_D[V]}(\lambda)f_n,f_n)\Big\}
\end{aligned}$$

which leads to the relation

$$\begin{aligned}
&\operatorname{tr}\left((H[\kappa_a,\kappa_b,V]-z)^{-1}-(H_D[V]-z)^{-1}\right)= \\
&\quad\frac{1}{2\pi}\int_{\mathbb{R}}(\lambda-z)^{-1}\operatorname{tr}(T[\kappa_a,\kappa_b,V](\lambda)^*T[\kappa_a,\kappa_b,V](\lambda))\,d\lambda- \\
&\quad\int_{\mathbb{R}}(\lambda-z)^{-1}\,d\operatorname{tr}(E_{H_D[V]}(\lambda)).
\end{aligned}$$

Since

$$N_D[V](\lambda)=\operatorname{tr}(E_{H_D[V]}(\lambda)),\quad \lambda\in\mathbb{R},$$

one has

$$\int_{\mathbb{R}}(\lambda-z)^{-1}\,d\operatorname{tr}(E_{H_D[V]}(\lambda))=\int_{\mathbb{R}}(\lambda-z)^{-1}d\,N_D[V](\lambda).$$

Integrating by parts and using that $N_D(\lambda)$ behaves like the square root of λ at $+\infty$ we get

$$\int_{\mathbb{R}}(\lambda-z)^{-1}\,d\operatorname{tr}(E_{H_D[V]}(\lambda))=\int_{\mathbb{R}}(\lambda-z)^{-2}N_D[V](\lambda)\,d\lambda.$$

Similarly, by Lemma 4.1 we get

$$\begin{aligned}
&\frac{1}{2\pi}\int_{\mathbb{R}}(\lambda-z)^{-1}\operatorname{tr}(T[\kappa_a,\kappa_b,V](\lambda)^*T[\kappa_a,\kappa_b,V](\lambda))\,d\lambda= \\
&\quad\frac{1}{2\pi}\int_{\mathbb{R}}(\lambda-z)^{-1}\operatorname{tr}(T[\kappa_a,\kappa_b,V](\lambda)T[\kappa_a,\kappa_b,V](\lambda)^*)\,d\lambda= \\
&\quad-\int_{\mathbb{R}}(\lambda-z)^{-1}\omega'[\kappa_a,\kappa_b,V](\lambda)\,d\lambda.
\end{aligned}$$

Again, integrating by parts and taking into account Theorem 4.8 we obtain

$$\frac{1}{2\pi}\int_{\mathbb{R}}(\lambda-z)^{-1}\operatorname{tr}(T[\kappa_a,\kappa_b,V](\lambda)^*T[\kappa_a,\kappa_b,V](\lambda))\,d\lambda=-\int_{\mathbb{R}}(\lambda-z)^{-2}\omega[\kappa_a,\kappa_b,V](\lambda)\,d\lambda$$

Summing up we find

$$\begin{aligned}
&\operatorname{tr}\left((H[\kappa_a,\kappa_b,V]-z)^{-1}-(H_D[V]-z)^{-1}\right)= \\
&\quad-\int_{\mathbb{R}}(\lambda-z)^{-2}\left\{\omega[\kappa_a,\kappa_b,V](\lambda)+N_D[V](\lambda)\right\}\,d\lambda
\end{aligned}$$

for $z\in\mathbb{C}_+$ which proves (5.7). $\square$

Corollary 5.5 *If $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \mathbb{C}$, then the spectral shift $\xi_0[\kappa_a, \kappa_b, V](\lambda)$ of the pair $\{H[\kappa_a, \kappa_b, V], H_D[V]\}$ obeys*

$$\lim_{\lambda \to -\infty} \xi_0[\kappa_a, \kappa_b, V](\lambda) = 0 \tag{5.11}$$

and

$$-2 \le \xi_0[\kappa_a, \kappa_b, V](\lambda) \le 0, \quad \lambda \in \mathbb{R}. \tag{5.12}$$

Proof. The relation (5.11) follows from (4.2). To verify (5.12) we note that by definition one has

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

Taking into account Theorem 5.4 we find

$$\Phi[\kappa_a, \kappa_b, V](\lambda) - N_D[V](\lambda) \le -\xi_0[\kappa_a, \kappa_b, V](\lambda) \le \Phi[\kappa_a, \kappa_b, V](\lambda) + 1 - N_D[V](\lambda), \quad \lambda \in \mathbb{R}.$$

Finally, using Theorem 4.8 we have

$$0 \le -\xi_0[\kappa_a, \kappa_b, V](\lambda) \le 2, \quad \lambda \in \mathbb{R},$$

which yields (5.12). □

Remark 5.6 We note that a weaker version of Corollary 5.5 can be obtained using abstract results on the spectral shift. Indeed, let us introduce the Cayley transforms

$$U := (i - K[\kappa_a, \kappa_b, V])(i + K[\kappa_a, \kappa_b, V])^{-1}$$

and

$$U_D := (i - K_D[\kappa_a, \kappa_b, V])(i + K_D[\kappa_a, \kappa_b, V])^{-1}$$

where $K[\kappa_a, \kappa_b, V]$ and $K_D[\kappa_a, \kappa_b, V]$ are given by (3.2)-(3.3) and (3.4). We note that $U - U_D$ is a four dimensional operator. This follows from the fact $K[\kappa_a, \kappa_b, V]$ and $K_D[V]$ are self-adjoint extension of the symmetric operator $L[V]$ which has deficiency indices $(4, 4)$. Since $\xi_0[\kappa_a, \kappa_b, V](\lambda)$ obeys the trace formula (5.1) one gets by a straightforward computation that

$$\eta_0(t) := \xi_0[\kappa_a, \kappa_b, V](\tan(t/2)), \quad t = (-\pi, \pi),$$

obeys the trace formula

$$\mathrm{tr}((U - \zeta)^{-1} - (U_D - \zeta)^{-1}) = -i \int_{-\pi}^{\pi} \frac{\eta_0(t)}{(e^{it} - \zeta)^2} \, e^{it} \, dt, \quad |\zeta| \ne 1,$$

for the pair $\{U, U_D\}$. The function $\eta_0(\cdot)$ is called a spectral shift of the pair $\{U, U_D\}$. Any function $\eta(t) := \eta_0(t) + c$, $t \in (-\pi, \pi]$, $c \in \mathbb{R}$, is, of course, a spectral shift of the pair $\{U, U_D\}$, too. Conversely, any spectral shift of the pair $\{U, U_D\}$ differs from $\eta_0(\cdot)$ by a real constant. Among all spectral shifts there is a special normalized one $\eta_n(\cdot)$ obeying

$$i \int_{-\pi}^{\pi} \eta_n(t) dt = \mathrm{tr}(\ln_0(U_D^{-1} U))$$

where $\ln_0(\cdot)$ is a suitably chosen branch of $\ln(\cdot)$, see [31, 42]. Notice that there is a real constant c_n such that

$$\eta_n(t) = \eta_0(t) + c_n, \quad t \in (-\pi, \pi].$$

Since $U-U_D$ is a four-dimensional operator one gets from [31] that $|\eta_n(t)| \leq 4$, $t \in (-\pi,\pi]$. By $\lim_{t\to-\pi}\eta_0(t) = 0$ we obtain that $|c_n| \leq 4$. Hence, we find $|\eta_0(t)| \leq 8$, $t \in (-\pi,\pi]$, which yields

$$|\xi_0[\kappa_a,\kappa_b,V](\lambda)| \leq 8, \quad \lambda \in \mathbb{R}. \tag{5.13}$$

We note that (5.13) is weaker than (5.12), however, the proof relies only on abstract results on the spectral shift.

Remark 5.7 The result (5.13) immediately implies that

$$N_D[V](\lambda) - 8 \leq \omega[\kappa_a,\kappa_b,V](\lambda) \leq N_D[V](\lambda) + 8, \quad \lambda \in \mathbb{R}.$$

Remark 5.8 From (4.1) and (5.7) we get

$$\det(S_{LP}[\kappa_a,\kappa_b,V](\lambda)) = e^{-2\pi i \xi_0[\kappa_a,\kappa_b,V](\lambda)} \tag{5.14}$$

for a.e. $\lambda \in \mathbb{R}$. However, formula (5.14) is the well-known Birman-Krein formula for the pair $\{K[\kappa_a,\kappa_b,V], K_D[V]\}$ which relates the spectral shift to the scattering matrix, cf. [17, 42].

Acknowledgement

The financial support of DFG (Grant RE 1480/2-1) is gratefully acknowledged.

References

[1] V. M. Adamjan, H. Neidhardt, *On the summability of the spectral shift function for pair of contractions and dissipative operators* J. Oper. Theory **24** (1990), no. 1, 187–205.

[2] B. P. Allakhverdiev, *On dissipative extensions of the symmetric Schrödinger operator in Weyl's limit-circle case* Dokl. Akad. Nauk SSSR **293** (1987), 777-781.

[3] B. P. Allakhverdiev, F. G. Maksudov, *On the theory of the characteristic function and spectral analysis of a dissipative Schrödinger operator* Dokl. Akad. Nauk SSSR **303** (1988), no.6, 1307-1309.

[4] B. P. Allakhverdiev, *Schrödinger type dissipative operator with a matrix potential*, in Spectral theory of operators and its applications No.9, 11-41, "Élm", Baku, 1989.

[5] B. P. Allakhverdiev, *On dilation theory and spectral analysis of dissipative Schrödinger operators in Weyl's limit-circle case* Izv. Akad. Nauk SSSR, Ser. Mat. **54** (1990), No.2, 242-257.

[6] B. P. Allakhverdiev, *On the theory of non-selfadjoint operators of Schrödinger type with a matrix potential* Izv. Ross. Akad. Nauk, Ser. Mat. **56** (1993), No. 2, 193-205.

[7] B. P. Allakhverdiev, A. Canoglu, S*pectral analysis of dissipative Schrödinger operators* Proc. R. Soc. Edinb., Sect. A, Math **127** (1997), no. 6, 1113-1121.

[8] B. P. Allakhverdiev, S. Saltan, *Spectral Analysis of non-self-adjoint Schrödinger operators with a matrix potential* J. Math. Anal. Appl. **303** (2005), 208-219.

[9] M. Baro, N. Ben Abdallah, P. Degond, A. A. El Ayyadi, *1D coupled Schrödinger drift-diffusion model including collisions* J. Comput. Phys. **203** (2005), no. 1, 129–153.

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

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

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

[13] M. Baro, H. Neidhardt, J. Rehberg, *Current coupling of drift-diffusion models and dissipative Schrödinger-Poisson systems: Dissipative hybrid models* to appear in SIAM J. Math. Anal. WIAS-preprint No. 946 (2004), Berlin, http://www.wias-berlin.de/publications/preprints/946/ .

[14] H. Baumgärtel, M. Wollenberg, *Mathematical scattering theory* Akademie-Verlag, Berlin 1983.

[15] N. Ben Abdallah, *On a multidimensional Schrödinger-Poisson scattering model for semiconductors* J. Math. Phys. **41** (2000), no. 7, 4241–4261.

[16] N. Ben Abdallah, P. Degond, P. A. Markowich, *On a one-dimensional Schrödinger-Poisson scattering model* Z. Angew. Math. Phys. **48** (1997), No. 1, 135-155.

[17] M. Š. Birman, M. G. Kreĭn, *On the theory of wave operators and scattering operators* Dokl. Akad. Nauk SSSR **144** (1962), 475-478.

[18] C. Foias, B. Sz.-Nagy, B, *Harmonic analysis of operators on Hilbert spaces* North-Holland Publishing Company, Amsterdam-London 1970.

[19] W. R. Frensley, *Boundary conditions for open quantum systems driven far from equilibrium* Rev. Mod. Phys. 62 (1990), 745-791.

[20] V. A. Derkach, M. M. Malamud, *Generalized Resolvents and the Boundary Value Problems for Hermitian Operators with Gaps* J. Funct. Anal. **95** (1991), 1-95.

[21] V. A. Derkach, M. M. Malamud, *Characteristic functions of almost solvable extensions of Hermitian operators* Ukr. Math. J. **44** (1992) , No.4, 379-401.

[22] I. C. Gohberg, M. G. Kreĭn, *Introduction to the theory of linear non-selfadjoint operators* Translations of Mathematical Monographs, Vol. 18 , American Mathematical Society, Providence, R.I. 1969.

[23] V. I. Gorbachuk, M. L. Gorbachuk, *Boundary value problems for operator differential equations*, Kluwer Academic Publishers Group, Dordrecht, 1991.

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

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

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

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

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

[29] H.-Ch. Kaiser, J. Rehberg, *About a stationary Schrödinger-Poisson system with Kohn-Sham potential in a bounded two- or three-dimensional domain* Nonlinear Anal. **41** (2000), no. 1-2, 33–72.

[30] T. Kato, *Perturbation theory for linear operators* Springer-Verlag, Berlin-Heidelberg-New York 1966.

[31] M. .G. Kreĭn, *On perturbation determinants and a trace formula for unitary and self-adjoint operators* Dokl. Akad. Nauk SSSR **144** (1962), 268–271.

[32] P. Lax, R. S. Phillips, *Scattering theory*, Academic Press, New York-London 1967.

[33] H. Neidhardt, J. Rehberg, *Uniqueness for dissipative Schrödinger-Poisson systems* submitted, WIAS-preprint No. 1044 (2005), Berlin, http://www.wias-berlin.de/publications/preprints/1044/ .

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

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

[36] F. Nier, *Schrödinger-Poisson systems in dimension $d \leq 3$: the whole-space case* Proc. Roy. Soc. Edinb. Sect. A, Math **123** (1993), no. 6, 1179–1201.

[37] B. S. Pavlov, *Self-adjoint dilation of the dissipative Schrödinger operator and its resolution in terms of eigenfunctions* Math. USSR Sb. **102(144)**, 511-536 (1977).

[38] B. S. Pavlov, *Dilation theory and spectral analysis of non-selfadjoint differential operators* Transl., II. Ser., Am. Math. Soc. **115** (1981), 103-142; translation from Proc. 7th. Winter School, Drogobych 1974, 3-69 (1976).

[39] B. S. Pavlov, *Spectral theory of non-selfadjoint operators* In Proc. Int. Congr. Math., Warszawa 1983, Vol.2, 1011-1025 (1984).

[40] B. S. Pavlov, *Spectral analysis of a dissipative singular Schrödinger operator in terms of a functional model* Partial Differential Equations VIII (M. A. Shubin, ed), Encyclopaedia of Mathematical Science, vol. 65, Springer, Berlin, 1966, 87-153.

[41] B. S. Pavlov, *Irreversibility, Lax-Phillips approach to resonance scattering and spectral analysis of non-selfadjoint operators in Hilbert space* Int. J. Theor. Phys. **38** (1999), no.1, 21-45.

[42] D. R. Yafaev, *Mathematical scattering theory. General theory.* American Mathematical Society, Providence, RI, 1992.