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Macroscopic current induced boundary conditions for Schrödinger–type operators

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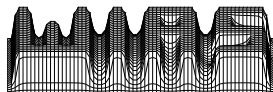
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*Dedicated to Konrad Gröger
— teacher, colleague, friend —
on the occasion of his 65th birthday.*

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Abstract

We describe an embedding of a quantum mechanically described structure into a macroscopic flow. The open quantum system is partly driven by an adjacent macroscopic flow acting on the boundary of the bounded spatial domain designated to quantum mechanics. This leads to an essentially non-selfadjoint Schrödinger-type operator, the spectral properties of which will be investigated.

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1 Introduction

The current continuity equation models macroscopic flow, while quantum mechanics portraits individual states. We aim at an embedding of a quantum mechanically described structure into a macroscopic flow. To that end we regard the quantum system as an open one and describe it by an essentially non-selfadjoint Hamiltonian. The non-symmetric part in the corresponding form is twofold. There is a purely imaginary boundary term providing a coupling to the macroscopic flow, and there is a complex-valued potential, whose imaginary part reflects absorptive and dispersive properties of the substrate. Let the open quantum system be situated in a bounded spatial domain Ω of \mathbb{R}^d , $d \leq 3$. The system is partly driven by an adjacent macroscopic flow acting on the boundary $\partial\Omega$ of Ω . The macroscopic flow is assumed to be of the form

$$J = -U \mathbf{v}, \quad (1.1)$$

where U is the density of the macroscopic transport quantity and \mathbf{v} is the corresponding velocity density. We regard the Schrödinger-type operator

$$H = -\frac{\hbar^2}{2} \nabla \cdot (m^{-1} \nabla) + V \quad \text{on } \Omega \quad (1.2)$$

with a mass tensor m , a complex-valued potential V , and the boundary condition

$$\hbar \nu \cdot m^{-1} \nabla \psi = i \psi \nu \cdot \mathbf{v} \quad \text{on } \partial\Omega, \quad (1.3)$$

where ν denotes the outer unit normal on $\partial\Omega$.

1.1 Remark. The boundary condition (1.3) is motivated by the aim to retain some form of current continuity. Indeed, if the quantum mechanical particle density u and the corresponding current density j are given by

$$u = |\psi|^2, \quad j = \hbar \Im (\bar{\psi} m^{-1} \nabla \psi),$$

respectively, where ψ denotes a non degenerate ground state of the open quantum system, then the boundary condition implies the equality of the normal components of j and J on $\partial\Omega$, if either $u = U$ or $\nu \cdot \mathbf{v} = 0$ on $\partial\Omega$. Indeed, multiplying (1.3) for the state ψ under consideration by $\bar{\psi}$ implies

$$\hbar \bar{\psi} \nu \cdot m^{-1} \nabla \psi = i |\psi|^2 \nu \cdot \mathbf{v} \quad \text{on } \partial\Omega,$$

and taking the imaginary part

$$\hbar \Im (\bar{\psi} \nu \cdot m^{-1} \nabla \psi) = |\psi|^2 \nu \cdot \mathbf{v}$$

leads to the result

$$\nu \cdot j = \nu \cdot \hbar \Im (\overline{\psi} m^{-1} \nabla \psi) = \nu \cdot u \mathbf{v} = \nu \cdot J.$$

N.B. If there is $\nu \cdot \mathbf{v} = 0$ on some part of the boundary of Ω , then $\nu \cdot m^{-1} \nabla \psi = 0$ on this part of the boundary, hence $\nu \cdot J = \nu \cdot j = 0$.

Schrödinger-type operators with Robin boundary conditions have been investigated since long. The interest has mainly focused on selfadjoint operators. In contrast, we are interested in the non-selfadjoint case in spatial dimensions $d = 1, 2, 3$. First results concerning the one dimensional case can be found in Najmark [29]. The non-selfadjoint one dimensional Sturm–Liouville problem has been treated by Marchenko [25]. This problem corresponds to $m = \text{const.}$ in our context, while we are interested in non-smooth mass tensors m and Schrödinger potentials V .

The point of this paper is that the boundary condition (1.3) cannot be implemented by using the usual boundary integral within the weak formulation, but has to be defined by a more subtle form approach, due to the deficient regularity of the adjacent macroscopic flow. In view of this we will give a weak formulation of the boundary condition (1.3) making use of $\nu \cdot \mathbf{v}$ as a distribution which is concentrated on the boundary of Ω , such that the boundary term is still form subordinated to the main part of Schrödinger’s operator.

The abstract framework for the rigorous definition and spectral analysis of the Schrödinger-type operator (1.2), (1.3) is the form perturbation method with a symmetric principal part and a non-symmetric part which is form subordinated to it, cf. Kato [24, chapter VI]. This approach has been further developed by Markus/Matsaev [27], Agranovich [2] and Grinshpun [13], [14], [15], [16]. In addition to the examples given in these papers we are able to verify the abstract conditions on form perturbations for our extremely non-smooth situation. Thus, the statements of Grinshpun [13] and Agranovich [2] apply, providing the spectral asymptotics and an Abel basis of root vectors for the Schrödinger-type operator (1.2), (1.3). In the one dimensional case our weak formulation reduces to the usual one, and one obtains a Riesz basis of root vectors.

We will pay special attention to the case of a dissipative Schrödinger-type operator (1.2), (1.3), which can be regarded as a pseudo-Hamiltonian (cf. [6, 4.1]) and has a (minimal) selfadjoint extension. Dissipative Schrödinger-type operators have been extensively studied by Pavlov [30], [31], [32]. If the Schrödinger-type operator (1.2), (1.3) is dissipative, then it turns out that the distribution $\nu \cdot \mathbf{v}$ defining the boundary condition in fact has to be a positive Radon measure.

2 The Schrödinger–type operator

First we introduce some notations and formulate the assumptions on the spatial domain Ω occupied by the open quantum system and on the adjacent macroscopic flow (1.1).

In the sequel $\Omega \subset \mathbb{R}^d$, $d \leq 3$ will be a bounded domain with a Lipschitz boundary. If p is from $[1, \infty[$, then $L^p = L^p(\Omega)$ is the space of complex-valued, Lebesgue measurable, p -integrable functions on Ω , and $W^{s,p} = W^{s,p}(\Omega)$, $s > 0$ are the usual Sobolev spaces on Ω , cf. e.g. [17, 1.3.1.1]. The L^p – $L^{p'}$ duality shall be given by the extended L^2 duality

$$(\psi_1, \psi_2) = \int_{\Omega} \psi_1(x) \overline{\psi_2(x)} dx. \quad (2.1)$$

$L^\infty = L^\infty(\Omega)$ is the space of Lebesgue measurable, essentially bounded functions on Ω , and $C = C(\overline{\Omega})$ is the space of up to the boundary continuous functions on Ω . The spaces $L^p(\partial\Omega)$ and $W^{s,p}(\partial\Omega)$ refer to the surface measure on $\partial\Omega$. Throughout this paper $\mathcal{B}(X; Y)$ denotes the space of bounded linear operators from X to Y , X and Y being Banach spaces. We abbreviate $\mathcal{B}(X) = \mathcal{B}(X; X)$. Sometimes we will write $\|\cdot\|$ short for $\|\cdot\|_{\mathcal{B}(X; Y)}$. If X is a separable Hilbert space, then $\mathcal{B}_t(X) \subset \mathcal{B}(X)$ is the class of t -summable operators, $1 \leq t < \infty$, cf. e.g. [8, Chapter III]

2.1 Assumption. Let \mathcal{U} be an open bounded set from \mathbb{R}^d with a Lipschitz boundary such that $\overline{\Omega} \subset \mathcal{U}$. Thus, $\mathcal{U} \stackrel{\text{def}}{=} \mathcal{U} \setminus \overline{\Omega}$ is a bounded open set from \mathbb{R}^d with a Lipschitz boundary. We assume

$$\mathbf{v} \in L^p(\mathcal{U}; \mathbb{R}^d), \quad \nabla \cdot \mathbf{v} \in L^{\tilde{p}}(\mathcal{U}), \quad (2.2)$$

where

$$p > d \quad \text{and} \quad \tilde{p} \geq \begin{cases} 1 & \text{if } d = 1, \\ 2p/(p+2) & \text{if } d = 2, \\ 3p/(p+3) & \text{if } d = 3. \end{cases} \quad (2.3)$$

In particular (2.2) implies

$$\mathbf{v} \in W^{1, \tilde{p}}(\mathcal{U}; \mathbb{R}) \hookrightarrow C(\overline{\mathcal{U}}; \mathbb{R}) \quad \text{if } d = 1. \quad (2.4)$$

2.2 Definition. Let $\Delta(x, \overline{\Omega})$ be a regularizing distance for the closure of Ω such that

$$\text{dist}(x, \overline{\Omega})/2 \leq \Delta(x, \overline{\Omega}) \leq 3 \text{dist}(x, \overline{\Omega})/2 \quad \forall x \in \mathbb{R}^d \setminus \overline{\Omega},$$

cf. e.g. Stein [36, VI.2.1 and VI.5.3], and let ϵ_0 be a strictly positive constant such that

$$6\epsilon_0 \leq \text{dist}(\mathbb{R}^d \setminus \mathcal{U}, \overline{\Omega}).$$

For $x \in \overline{\mathcal{U}}$ we define the function

$$\omega(x) \stackrel{\text{def}}{=} \begin{cases} 0 & \text{if } 2\epsilon_0 \leq \Delta(x, \overline{\Omega}), \\ \exp(1 + \epsilon_0/(\Delta(x, \overline{\Omega}) - 2\epsilon_0)) & \text{if } \epsilon_0 < \Delta(x, \overline{\Omega}) < 2\epsilon_0, \\ 1 & \text{otherwise.} \end{cases} \quad (2.5)$$

2.3 Definition. Let p' be the adjoint number to p from Assumption 2.1.

$d > 1$: In the two and three dimensional case we denote by

$$\gamma : W^{1,p'}(\mathcal{U}) \longrightarrow W^{1-1/p',p'}(\partial\mathcal{U}) \quad (2.6)$$

the usual continuous trace mapping onto the boundary of \mathcal{U} , cf. e.g. [17, 1.5.1.3]. Further, let

$$\gamma^{-1} : W^{1-1/p',p'}(\partial\mathcal{U}) \longrightarrow W^{1,p'}(\mathcal{U}) \quad (2.7)$$

be a continuous right inverse of γ , cf. e.g. Grisvard [17, 1.5].

$d = 1$: In the one dimensional case, $\Omega = (x_1, x_2)$, there is

$$W^{1,p'}(\mathcal{U}) \hookrightarrow C(\overline{\mathcal{U}}),$$

and we denote by γ the continuous “inner” trace mapping

$$\gamma f = \{f(x_1), f(x_2)\} \in \mathbb{C}^2 \quad f \in C(\overline{\mathcal{U}})$$

from $C(\overline{\mathcal{U}})$ onto \mathbb{C}^2 , equipped with the maximum norm

$$\|\{c_1, c_2\}\|_{\mathbb{C}^2} = \max_{j=1,2} |c_j|.$$

γ^{-1} denotes the continuous right inverse

$$\gamma^{-1}\{c_1, c_2\}(x) = \begin{cases} c_1 & \text{if } x \leq x_1, \\ c_2 & \text{if } x \geq x_2. \end{cases}$$

of γ . Obviously there is

$$\|\gamma^{-1}\|_{\mathcal{B}(\mathbb{C}^2; C(\overline{\mathcal{U}}))} = \|\gamma\|_{\mathcal{B}(C(\overline{\mathcal{U}}); \mathbb{C}^2)} = 1. \quad (2.8)$$

2.4 Definition. We define $W_{\partial\Omega}^{1,r}(\mathcal{U})$ as the closure in $W^{1,r}(\mathcal{U})$ of the set

$$C_{\partial\Omega}^{\infty}(\mathcal{U}) \stackrel{\text{def}}{=} \{f|_{\mathcal{U}} : f \in C_0^{\infty}(\mathbb{R}^d), \text{supp}(f) \cap \partial\Omega = \emptyset\}. \quad (2.9)$$

2.5 Lemma. *If \mathbf{v} , \mathcal{U} and ω are according to Assumption 2.1 and Definition 2.2, then the linear form*

$$\mathfrak{T} : f \longmapsto \int_{\mathcal{U}} \mathbf{v} \cdot \nabla(\omega f) + \omega f \nabla \cdot \mathbf{v} \, dx \quad (2.10)$$

is continuous on the space $W^{1,p'}(\mathcal{U})$. It annihilates the space $W_{\partial\Omega}^{1,p'}(\mathcal{U})$. We define

$$T \stackrel{\text{def}}{=} \mathfrak{T} \circ \gamma^{-1}.$$

If $d > 1$, then T is a linear, continuous functional on the space $W^{1-1/p',p'}(\partial\Omega)$ and does not depend on the chosen right inverse γ^{-1} from Definition 2.3. In the one dimensional case, $\Omega = (x_1, x_2)$, the two values of \mathbf{v} on the boundary $\partial\Omega$ exist, and

$$\langle T, c \rangle = \sum_{j=1,2} (-1)^j \mathbf{v}(x_j) c_j \quad \forall c = \{c_1, c_2\} \in \mathbb{C}^2.$$

Moreover, the linear forms \mathfrak{T} and T commute with the complex conjugation.

Proof. The continuity of the linear form (2.10) follows immediately from (2.2) and the continuity of the embeddings

$$\begin{aligned} W^{1,p'}(\mathcal{U}) &\hookrightarrow C(\overline{\mathcal{U}}) && \text{if } d = 1, \\ W^{1,p'}(\mathcal{U}) &\hookrightarrow L^{\frac{2p}{p-2}}(\mathcal{U}) && \text{if } d = 2, \\ W^{1,p'}(\mathcal{U}) &\hookrightarrow L^{\frac{3p}{2p-3}}(\mathcal{U}) && \text{if } d = 3. \end{aligned}$$

Moreover, the linear form \mathfrak{T} annihilates the set $C_{\partial\Omega}^{\infty}(\mathcal{U})$, which is dense in $W_{\partial\Omega}^{1,p'}(\mathcal{U})$, cf. Definition 2.4. Because $W_{\partial\Omega}^{1,p'}(\mathcal{U})$ belongs to the kernel of \mathfrak{T} , the distribution T does not depend on the choice of the right inverse γ^{-1} . If $d > 1$, then T defines a continuous linear functional on $W^{1-1/p',p'}(\partial\Omega)$. Indeed,

$$\|T\|_{(W^{1-1/p',p'}(\partial\Omega))^*} \leq \|\mathfrak{T}\|_{(W^{1,p'}(\mathcal{U}))^*} \|\gamma^{-1}\|_{\mathcal{B}(W^{1-1/p',p'}(\partial\Omega); W^{1,p'}(\mathcal{U}))}.$$

In the one dimensional case, the assertion follows from (2.4) and there is

$$\|T\|_{(\mathbb{C}^2)^*} = \|\{-\mathbf{v}(x_1), \mathbf{v}(x_2)\}\|_{(\mathbb{C}^2)^*} = \sum_{j=1,2} |\mathbf{v}(x_j)|. \quad (2.11)$$

□

2.6 Remark. In the two and three dimensional case ($d > 1$), T is in general not a regular distribution. However, if one assumes instead of Assumption 2.1 more regularity of the flow \mathbf{v} , such that the trace of $\nu \cdot \mathbf{v}$ on the boundary $\partial\Omega$ is from a space $L^\tau(\partial\Omega)$, $1 \leq \tau \leq \infty$, then

$$\langle T, f \rangle = \int_{\partial\Omega} \nu \cdot \mathbf{v} f \, d\sigma \quad \forall f \in L^{\tau'}(\partial\Omega), \quad 1/\tau + 1/\tau' = 1, \quad (2.12)$$

and $\nu \cdot \mathbf{v}$ is a continuous linear functional on the space $W^{s,2}(\Omega)$, for

$$s \geq \max \{1/2, (d-1)/\tau + (2-d)/2\}. \quad (2.13)$$

Indeed, applying Hölder's inequality and using the continuity of the embeddings $W^{s,2}(\Omega) \hookrightarrow W^{s-1/2,2}(\partial\Omega)$, cf. e.g. [17, 1.5.1.3], and $W^{s-1/2,2}(\partial\Omega) \hookrightarrow L^{\tau'}(\partial\Omega)$ one obtains for all $f \in W^{s,2}(\Omega)$

$$\left| \int_{\partial\Omega} \nu \cdot \mathbf{v} f \, d\sigma \right| \leq \|\nu \cdot \mathbf{v}\|_{L^\tau(\partial\Omega)} \|f\|_{L^{\tau'}(\partial\Omega)} \leq c \|\nu \cdot \mathbf{v}\|_{L^\tau(\partial\Omega)} \|f\|_{W^{s,2}(\Omega)}, \quad (2.14)$$

where c denotes the embedding constant of $W^{s,2}(\Omega) \hookrightarrow L^{\tau'}(\partial\Omega)$.

2.7 Remark. If the macroscopic flow (1.1) is governed by a reaction–diffusion equation

$$\frac{\partial U}{\partial t} + \nabla \cdot J = R(U, J) \quad (2.15)$$

in the neighbourhood of Ω , then one can prove the required regularity of \mathbf{v} for wide classes of such equations, cf. [11] for the semilinear case, [20] for the quasilinear case, and one can rewrite (2.10) in the following way:

$$\langle \mathfrak{I}, f \rangle = - \int_{\mathcal{V}} J \cdot \nabla \left(\frac{\omega f}{U} \right) + \frac{\omega f}{U} \nabla \cdot J \, dx = \int_{\mathcal{V}} \mathbf{v} \cdot \nabla(\omega f) + \omega f \nabla \cdot \mathbf{v} \, dx.$$

2.8 Remark. If (1.1) represents the electron or hole current in a semiconductor device described by the stationary Van Roosbroeck equations, then one obtains the required regularity of these currents in the two dimensional case from L^∞ -bounds of the corresponding potentials (cf. e.g. [7], [18], [26, Theorem 3.2.1]) by means of a $W^{1,p}$ -estimate for solutions to boundary value problems for second order elliptic differential equations, cf. [19]. — For the two dimensional transient case cf. [21].

By means of the distribution T it is now possible to construct a sesquilinear form, which represents the "boundary part" of the Schrödinger operator.

2.9 Theorem. *Let p be a Sobolev exponent from Assumption 2.1 and p' its adjoint number. Further, let s be a real number such that*

$$2s \geq 1 + d/p, \quad \text{if } d > 1, \quad 2s > 1, \quad \text{if } d = 1. \quad (2.16)$$

Then multiplication

$$(\psi_1 \times \psi_2)(x) = \psi_1(x)\psi_2(x), \quad x \in \partial\Omega \quad (2.17)$$

is a well defined, bilinear and continuous mapping

$$W^{s-1/2,2}(\partial\Omega) \times W^{s-1/2,2}(\partial\Omega) \longrightarrow W^{1-1/p',p'}(\partial\Omega) \quad \text{if } d > 1, \quad (2.18)$$

$$\mathbb{C}^2 \times \mathbb{C}^2 \longrightarrow \mathbb{C}^2 \quad \text{if } d = 1, \quad (2.19)$$

with the norm ι . Let

$$\gamma_s : W^{s,2}(\Omega) \longrightarrow \begin{cases} W^{s-1/2,2}(\partial\Omega) & \text{if } d > 1, \\ \mathbb{C}^2 & \text{if } d = 1, \end{cases} \quad (2.20)$$

be the usual trace mapping, cf. e.g. [17, 1.5.1.2]). Then

$$\mathfrak{t}_{\partial\Omega}[\psi_1, \psi_2] \stackrel{\text{def}}{=} i \langle T, \gamma_s(\psi_1)\gamma_s(\overline{\psi_2}) \rangle, \quad (2.21)$$

is a well defined, sesquilinear and continuous form on $W^{s,2}(\Omega) \times W^{s,2}(\Omega)$. More precisely there is

$$|\mathfrak{t}_{\partial\Omega}[\psi_1, \psi_2]| \leq \iota \|T\| \|\gamma_s\|^2 \|\psi_1\|_{W^{s,2}(\Omega)} \|\psi_2\|_{W^{s,2}(\Omega)}. \quad (2.22)$$

for all $\psi_1 \in W^{s,2}(\Omega)$, $\psi_2 \in W^{s,2}(\Omega)$. In the one dimensional case there is in particular $\iota = \|\gamma_s\| = 1$, and (2.11).

2.10 Remark. The essential point of Theorem 2.9 is that by Assumption 2.1 and (2.16) s may be chosen smaller than 1.

Proof. The proof is obvious for the one dimensional case, $\Omega = (x_1, x_2)$, as $W^{s,2}(\Omega)$ with $s > 1/2$ embeds continuously into $C(\overline{\Omega})$, and the sesquilinear form (2.21) has the following simple structure

$$\mathfrak{t}_{\partial\Omega}[\psi_1, \psi_2] = i \sum_{j=1,2} (-1)^j \mathbf{v}(x_j) \psi_1(x_j) \overline{\psi_2(x_j)}, \quad (2.23)$$

cf. Lemma 2.5.

Let us now regard the two and three dimensional case, $d > 1$. We start with the proof of (2.18). As Ω is a bounded domain in \mathbb{R}^2 or \mathbb{R}^3 with a Lipschitz boundary we may localize $\partial\Omega$ in a way such that the local parts of $\partial\Omega$ are mapped via bi-Lipschitz homeomorphisms onto subsets of $[0, 1]$ or $[0, 1] \times [0, 1]$, respectively. These Lipschitz homeomorphisms transport the Sobolev spaces on local parts of $\partial\Omega$ into spaces of the same Sobolev class on $[0, 1]$ or $[0, 1] \times [0, 1]$. Here the continuity of the multiplication mapping (2.17) follows from [17, 1.4.4.2]. The back transformation also preserves the Sobolev class. Hence one can estimate

$$\begin{aligned} |\mathbf{t}_{\partial\Omega}[\psi_1, \psi_2]| &\leq \|T\| \|\gamma_s \psi_1 \overline{\gamma_s \psi_2}\|_{W^{1-1/p', p'}(\partial\Omega)} \\ &\leq \iota \|T\| \|\gamma_s \psi_1\|_{W^{s-1/2, 2}(\partial\Omega)} \|\gamma_s \psi_2\|_{W^{s-1/2, 2}(\partial\Omega)} \\ &\leq \iota \|T\| \|\gamma_s\|^2 \|\psi_1\|_{W^{s, 2}(\Omega)} \|\psi_2\|_{W^{s, 2}(\Omega)}. \end{aligned}$$

□

2.11 Theorem. *Let $V \in L^q(\Omega)$ be a given complex-valued function, where q is a real number such that*

$$q \geq 1 \quad \text{if } d = 1 \quad \text{and} \quad q > d/2 \quad \text{if } d > 1. \quad (2.24)$$

If $t \geq d/(2q)$, then

$$\mathbf{t}_V[\psi_1, \psi_2] \stackrel{\text{def}}{=} \int_{\Omega} V \psi_1 \overline{\psi_2} \, dx \quad (2.25)$$

is a continuous sesquilinear form on the space $W^{t, 2}(\Omega) \times W^{t, 2}(\Omega)$.

2.12 Remark. The essential point of Theorem 2.11 is that by (2.24) t may be chosen smaller than 1.

Proof. With $r = 2q/(q - 1)$ there is

$$\begin{aligned} |\mathbf{t}_V[\psi_1, \psi_2]| &= \left| \int_{\Omega} V \psi_1 \overline{\psi_2} \, dx \right| \leq \|V\|_{L^q} \|\psi_1\|_{L^r} \|\psi_2\|_{L^r} \\ &\leq c^2 \|V\|_{L^q} \|\psi_1\|_{W^{t, 2}} \|\psi_2\|_{W^{t, 2}}, \end{aligned} \quad (2.26)$$

where c is Sobolev's embedding constant from $W^{t, 2}$ to L^r , and all the function spaces refer to the spatial domain Ω . □

With respect to the spatial domain $\Omega \subset \mathbb{R}^d$ we define the Gagliardo–Nirenberg constant, cf. e.g. Maz'ya [28, 1.4.8/1],

$$\mathfrak{g}_q = \sup_{0 \neq \psi \in W^{1, 2}} \frac{\|\psi\|_{L^{\frac{2q}{q-1}}}}{\|\psi\|_{W^{1, 2}}^{\frac{d}{2q}} \|\psi\|_{L^2}^{1 - \frac{d}{2q}}}, \quad (2.27)$$

where in the case $q = 1$, which is only admissible if $d = 1$, the fraction $2q/(q - 1)$ should be read as ∞ .

2.13 Definition. Let $m \in L^\infty(\Omega; \mathcal{B}(\mathbb{R}^d; \mathbb{R}^d))$ be a function over Ω with positive definite, invertible values such that m^{-1} is also from $L^\infty(\Omega; \mathcal{B}(\mathbb{R}^d; \mathbb{R}^d))$. We introduce

$$\tilde{m} = \max \left\{ 1, \frac{2}{\hbar^2} \|m\|_{L^\infty(\Omega, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))} \right\}. \quad (2.28)$$

We define on the space $W^{1,2}(\Omega) \times W^{1,2}(\Omega)$ the sesquilinear form

$$\mathfrak{t}[\psi_1, \psi_2] \stackrel{\text{def}}{=} \int_{\Omega} \frac{\hbar^2}{2} m(x)^{-1} \nabla \psi_1(x) \cdot \nabla \overline{\psi_2}(x) + \psi_1(x) \overline{\psi_2}(x) dx, \quad (2.29)$$

which is (strictly) positive and closed on $L^2(\Omega)$. Further we introduce the sum of the sesquilinear forms (2.29), (2.25), and (2.21)

$$\mathfrak{t}_{\partial\Omega, V} = \mathfrak{t} + \mathfrak{t}_{\partial\Omega} + \mathfrak{t}_{(V-1)}. \quad (2.30)$$

The quadratic forms corresponding to the sesquilinear forms will be denoted by the same symbol with only one argument.

2.14 Remark. By means of (2.28) one can estimate

$$\|\psi\|_{W^{1,2}(\Omega)}^2 \leq \tilde{m} \mathfrak{t}[\psi]. \quad (2.31)$$

Now we want to define the operator induced by the form $\mathfrak{t}_{\partial\Omega, V}$ on $L^2(\Omega)$. Having this goal in mind, we first state multiplicative and relative form bounds for \mathfrak{t}_V and $\mathfrak{t}_{\partial\Omega}$ with respect to \mathfrak{t} .

2.15 Definition. Let \mathfrak{A} be a densely defined, symmetric closed form bounded from below by 1 acting on a separable complex Hilbert space \mathcal{H} . A sesquilinear form \mathfrak{B} with $\text{dom}(\mathfrak{A}) \subset \text{dom}(\mathfrak{B})$ is s -subordinated to \mathfrak{A} , if

$$|\mathfrak{B}[\psi]| \leq c(\mathfrak{A}[\psi])^s (\|\psi\|_{\mathcal{H}}^2)^{1-s} \quad \forall \psi \in \text{dom}(\mathfrak{A}) \quad (2.32)$$

for some $s < 1$ and $c > 0$.

2.16 Theorem. (*Form subordination of the boundary term*). Let p be according to Assumption 2.1 and

$$d/p + 1/2 \leq s < 1 \quad \text{if } d > 1 \quad \text{and} \quad 1/2 \leq s < 1 \quad \text{if } d = 1.$$

Then the form $\mathfrak{t}_{\partial\Omega}$ is s -subordinated to \mathfrak{t} , i.e., for all $\psi \in W^{1,2}(\Omega)$ there is

$$|\mathfrak{t}_{\partial\Omega}[\psi]| \leq K^2 \tilde{m}^s \iota \|T\| \|\gamma_s\|^2 (\mathfrak{t}[\psi])^s \|\psi\|_{L^2}^{2(1-s)}, \quad (2.33)$$

where K is an interpolation constant between the function spaces $L^2(\Omega)$ and $W^{1,2}(\Omega)$. By applying Young's inequality to (2.33) one arrives at

$$|\mathfrak{t}_{\partial\Omega}[\psi]| \leq \delta \mathfrak{t}[\psi] + (1-s) (\delta/s)^{s/(s-1)} \left(K^2 \tilde{m}^s \iota \|T\| \|\gamma_s\|^2 \right)^{1/(1-s)} \|\psi\|_{L^2}^2 \quad (2.34)$$

for all $\delta > 0$.

Proof. One starts with (2.22) for some $s < 1$ with (2.16), putting $\psi_1 = \psi_2 = \psi$. Thus one obtains

$$|\mathfrak{t}_{\partial\Omega}[\psi]| \leq \iota \|T\| \|\gamma_s\|^2 \|\psi\|_{W^{s,2}}^2 \leq K^2 \iota \|T\| \|\gamma_s\|^2 \|\psi\|_{L^2}^{2(1-s)} \|\psi\|_{W^{1,2}}^{2s},$$

where we have applied complex interpolation between $L^2(\Omega)$ and $W^{1,2}(\Omega)$, cf. [38, 4.3.1 and (2.4.2/11)] (N.B. Ω has a Lipschitz boundary and thus the cone property, cf. e.g. Grisvard [17, 1.2.2]). By means of (2.31) one now arrives at (2.33). It remains to prove the case $d = 1$, $s = 1/2$. According to (2.23) and (2.11) there is for all $\psi \in W^{1,2}(\Omega)$

$$|\mathfrak{t}_{\partial\Omega}[\psi]| \leq \sum_{j=1,2} |\mathbf{v}(x_j)| |\psi(x_j)|^2 \leq \|T\| \|\psi\|_C^2 \leq \|T\| \left(\frac{\|\psi\|_{L^2}^2}{x_2 - x_1} + 2\|\psi'\|_{L^2} \|\psi\|_{L^2} \right).$$

By means of (2.31) one now arrives at (2.33). N.B. In the one dimensional case there is $\iota = \|\gamma_s\| = 1$, cf. Theorem 2.9. \square

2.17 Remark. In the one dimensional case, $\Omega = (x_1, x_2)$, Assumption 2.1 implies that $\mathfrak{t}_{\partial\Omega}$ is 1/2-subordinated to the form \mathfrak{t} . If — in the two and three dimensional case — one assumes in the sense of Remark 2.6 instead of Assumption 2.1 more regularity of the flow \mathbf{v} , such that the trace $\nu \cdot \mathbf{v}$ on the boundary $\partial\Omega$ is from the space $L^\infty(\partial\Omega)$, then one also obtains that the form $\mathfrak{t}_{\partial\Omega}$ is 1/2-subordinated to the form \mathfrak{t} :

$$\begin{aligned} |\mathfrak{t}_{\partial\Omega}[\psi]| &= \left| \int_{\partial\Omega} i (\nu \cdot \mathbf{v}) |\psi|^2 d\sigma \right| \leq M_P \|\nu \cdot \mathbf{v}\|_{L^\infty(\partial\Omega)} \|\psi\|_{L^2} \|\psi\|_{W^{1,2}} \\ &\leq M_P \sqrt{\tilde{m}} \|\nu \cdot \mathbf{v}\|_{L^\infty(\partial\Omega)} \mathfrak{t}[\psi]^{1/2} \|\psi\|_{L^2}, \end{aligned} \quad (2.35)$$

where M_P is the constant from Poincaré's inequality, cf. also (2.31).

2.18 Theorem. (Form subordination of the complex-valued Schrödinger potential). If q is according to (2.24), and $d/(2q) \leq s < 1$, then the form \mathfrak{t}_V is s -subordinated to \mathfrak{t} , i.e., for all $\psi \in W^{1,2}(\Omega)$ there is

$$|\mathfrak{t}_V[\psi]| \leq \|V\|_{L^q} \mathfrak{g}_q^2 \tilde{m}^{d/(2q)} (\mathfrak{t}[\psi])^s (\|\psi\|_{L^2}^2)^{1-s}. \quad (2.36)$$

By applying Young's inequality to (2.36) with $s = d/(2q)$ one arrives at

$$|\mathbf{t}_V[\psi]| \leq \delta \mathbf{t}[\psi] + \left(1 - \frac{d}{2q}\right) \left(\frac{2q}{d}\delta\right)^{\frac{d}{d-2q}} \|V\|_{L^q}^{\frac{2q}{2q-d}} \mathfrak{g}_q^{\frac{4q}{2q-d}} \tilde{m}^{\frac{d}{2q-d}} \|\psi\|_{L^2}^2, \quad (2.37)$$

for any $\delta > 0$.

Proof. It is sufficient to prove (2.36) for $s = d/(2q)$. The corresponding inequality for $d/(2q) < s < 1$ then follows from $\|\psi\|_{L^2}^2 \leq \mathbf{t}[\psi]$. We start the proof of (2.36) with Hölder's inequality:

$$|\mathbf{t}_V[\psi]| \leq \mathbf{t}_{|V|}[\psi] \leq \|V\|_{L^q} \|\psi\|_{L^{2q/(q-1)}}^2$$

then apply the Gagliardo–Nirenberg inequality:

$$\leq \|V\|_{L^q} \mathfrak{g}_q^2 \left(\|\psi\|_{W^{1,2}}^2\right)^{d/(2q)} \|\psi\|_{L^2}^{2-d/q}$$

and make use of (2.31):

$$\leq \|V\|_{L^q} \mathfrak{g}_q^2 \tilde{m}^{d/(2q)} \mathbf{t}[\psi]^{d/(2q)} \|\psi\|_{L^2}^{2-d/q}.$$

Finally, (2.37) follows by means of Young's inequality. \square

2.19 Corollary. *There are estimates corresponding to (2.36) and (2.37) for the sesquilinear forms $\mathbf{t}_{\Re(V)}$ and $\mathbf{t}_{\Im(V)}$. Moreover, there is for all $\psi \in W^{1,2}(\Omega)$*

$$\begin{aligned} (1 - d/(2q)) \mathbf{t}[\psi] + \zeta(V) \|\psi\|_{L^2}^2 &\leq \mathbf{t}[\psi] + \mathbf{t}_{\Re(V)}[\psi] \\ &\leq (1 + d/(2q)) \mathbf{t}[\psi] - \zeta(V) \|\psi\|_{L^2}^2, \end{aligned} \quad (2.38)$$

where

$$\zeta(V) = -(1 - d/(2q)) \|\Re V\|_{L^q}^{2q/(2q-d)} \mathfrak{g}_q^{4q/(2q-d)} \tilde{m}^{d/(2q-d)}, \quad (2.39)$$

cf. [22, Proposition 3.3] for the one dimensional case, and [23, Proposition 3.4] for the two and three dimensional case.

2.20 Theorem. *Under the suppositions of Theorem 2.16 and Theorem 2.18 holds: The form $\mathbf{t}_{\partial\Omega} + \mathbf{t}_{V-1}$ is relatively bounded with respect to the form \mathbf{t} with relative bound zero. Hence, the form $\mathbf{t}_{\partial\Omega, V} = \mathbf{t} + \mathbf{t}_{\partial\Omega} + \mathbf{t}_{(V-1)}$ is closed on $L^2(\Omega)$ and sectorial (cf. e.g. Kato [24, VI.§1.6]). It induces exactly one sectorial operator $H_{\partial\Omega, V}$ on $L^2(\Omega)$, such that*

$$\text{dom}(H_{\partial\Omega, V}) \subset \text{dom}(\mathbf{t}_{\partial\Omega, V}) = W^{1,2}(\Omega) \quad (2.40)$$

$$(H_{\partial\Omega, V} u, u) = \mathbf{t}_{\partial\Omega, V}[u] \quad \forall u \in \text{dom}(H_{\partial\Omega, V}). \quad (2.41)$$

Proof. The relative bound of the form $\mathfrak{t}_{\partial\Omega} + \mathfrak{t}_V$ can be obtained from Theorem 2.16 and Theorem 2.18. $\mathfrak{t}_{\partial\Omega, V}$ is closed and sectorial according to the form perturbation theorem [24, Theorem VI/1.33]. The other statements are easily concluded from the first representation theorem for sectorial forms, cf. e.g. Kato [24, Theorem VI/2.1]. \square

2.21 Corollary. *Under the suppositions of Theorem 2.18 the form \mathfrak{t}_{V-1} is relatively bounded with respect to the form \mathfrak{t} with relative bound zero. Hence, the form $\mathfrak{t} + \mathfrak{t}_{(V-1)}$ is closed on $L^2(\Omega)$ and sectorial. It induces exactly one sectorial operator H_V on $L^2(\Omega)$, such that $\text{dom}(H_V) \subset \text{dom}(\mathfrak{t} + \mathfrak{t}_{(V-1)}) = W^{1,2}(\Omega)$ and $(H_V u, u) = \mathfrak{t}[u] + \mathfrak{t}_{(V-1)}[u]$ for all $u \in \text{dom}(H_V)$. If $V \equiv 0$, then we abbreviate H_0 by H .*

2.22 Remark. It is not possible to define $H_{\partial\Omega, V}$ as an operator sum, because the form $\mathfrak{t}_{\partial\Omega}$ is not closable on $L^2(\Omega)$ and, consequently, does not correspond to an operator. That is why we define $H_{\partial\Omega, V}$ in Theorem 2.20, by means of the representation theorem for sectorial forms.

3 Spectral properties

3.1 Theorem. *For the operator $H_{\partial\Omega, V}$ from Theorem 2.20 it holds:*

i) $H_{\partial\Omega, V}$ is an operator with compact resolvent.

ii) If $\Gamma(\mathfrak{t}_{\partial\Omega, V})$ denotes the numerical range of the form (2.30), then

$$\left\| (H_{\partial\Omega, V} - \lambda)^{-1} \right\| \leq \frac{1}{\text{dist}(\lambda, \Gamma(\mathfrak{t}_{\partial\Omega, V}))} \quad \forall \lambda \in \mathbb{C} \setminus \Gamma(\mathfrak{t}_{\partial\Omega, V}). \quad (3.1)$$

iii) The resolvent of $H_{\partial\Omega, V}$ is a trace class operator in the one dimensional case $\Omega = (x_1, x_2)$ and belongs to the summability class \mathcal{B}_t for any $t > d/2$ in the two and three dimensional case.

iv) Let $N(A, r)$ be the counting function, i.e. the dimension of the Riesz projection of the operator A belonging to the centered r -ball in \mathbb{C} [8, I.§3]. If \mathfrak{v} is according to Assumption 2.1 and V satisfies the supposition of Theorem 2.11, then

$$N(H_{\partial\Omega, V}, r) = N(H, r)(1 + o(1)). \quad (3.2)$$

Proof. *i)* is assured by the compactness of the resolvent of the operator H and a perturbation theorem for forms, cf. e.g. Kato [24, Theorem VI/3.4].

ii) follows from the first representation theorem for forms, cf. e.g. Kato [24, Theorem VI/2.1], the compactness of the resolvent of $H_{\partial\Omega, V}$, and [24, Theorem V/3.2].

iii). The relative \mathfrak{t} -form estimates (2.34) and (2.37) for $\mathfrak{t}_{\partial\Omega}$ and \mathfrak{t}_V , respectively, imply for any $\lambda \in \mathbb{R}$ and any $\delta > 0$

$$|\Im((H_{\partial\Omega,V} + \lambda)\psi, \psi)| \leq |\mathfrak{t}_{\partial\Omega}[\psi]| + |\mathfrak{t}_{\Im(V)}[\psi]| \leq \delta \mathfrak{t}[\psi] + C(\delta) \|\psi\|_{L^2}^2,$$

where $C(\delta)$ does not depend on λ , but on the norm of the distribution T in the space $(W^{1-1/p',p'}(\partial\Omega))^*$ and $\|\Im(V)\|_{L^q}$. On the other hand (2.38) provides

$$\begin{aligned} \Re((H_{\partial\Omega,V} + \lambda)\psi, \psi) &= \mathfrak{t}[\psi] + \mathfrak{t}_{\Re(V)}[\psi] + (\lambda - 1) \|\psi\|_{L^2}^2 \\ &\geq (1 - d/(2q)) \mathfrak{t}[\psi] + (\zeta(V) + \lambda - 1) \|\psi\|_{L^2}^2. \end{aligned} \quad (3.3)$$

Putting $\delta = 1 - d/(2q)$ and $\lambda = C(1 - d/(2q)) + 2 - \zeta(V)$ one obtains

$$\left| \frac{\Im((H_{\partial\Omega,V} + \lambda)\psi, \psi)}{\Re((H_{\partial\Omega,V} + \lambda)\psi, \psi)} \right| < 1, \quad (3.4)$$

i.e. the operator $H_{\partial\Omega,V} + \lambda$ is sectorial with vertex 0 and semi-angle smaller than $\pi/4$, cf. [24, V.§3.10]. Hence, there is a symmetric operator $B \in \mathcal{B}(L^2(\Omega))$ such that $\|B\|_{\mathcal{B}} < 1$ and

$$H_{\partial\Omega,V} + \lambda = G^{1/2}(1 + iB)G^{1/2}, \quad G = H_{\Re(V)} + \lambda + 1, \quad (3.5)$$

cf. [24, Theorem V/3.2]. According to [4, Theorem 3] and [38, 5.6.1. Theorem 1] the resolvent of H belongs to the summability class \mathcal{B}_t for $t = 1$ in the one dimensional case and for any $t > d/2$ in the two and three dimensional case. Thus,

$$\begin{aligned} \|(H_{\partial\Omega,V} + \lambda)^{-1}\|_{\mathcal{B}_t} &\leq \|G^{-1/2}H^{1/2}\|_{\mathcal{B}}^2 \|H^{-1/2}\|_{\mathcal{B}_{2t}}^2 \|(i - B)^{-1}\|_{\mathcal{B}} \\ &= \|G^{-1/2}H^{1/2}\|_{\mathcal{B}}^2 \|H^{-1}\|_{\mathcal{B}_t} \|(i - B)^{-1}\|_{\mathcal{B}}, \end{aligned}$$

where the spaces \mathcal{B} and \mathcal{B}_t refer to the Hilbert space $L^2(\Omega)$. The point i belongs to the resolvent set of B as $\|B\|_{\mathcal{B}} < 1$, and $\|G^{-1/2}H^{1/2}\|_{\mathcal{B}}$ is finite because the right hand side of (3.3) is greater than $(1 - d/(2q))\mathfrak{t}[\psi]$ for our choice of λ , cf. [24, VI.§2.6].

The proof of *iv*) rests upon the following result.

3.2 Proposition. (Grinshpun [13, Theorem 2]). *Let A be a positive selfadjoint operator with compact resolvent acting on a separable complex Hilbert space. Suppose $A \geq 1$. Further, let \mathfrak{A} be the corresponding sesquilinear form and let \mathfrak{B} be a sesquilinear form, which is relatively bounded with respect to \mathfrak{A} with relative bound zero. If the counting function $N(A, \lambda)$ for A satisfies*

$$\lim_{\substack{\lambda \rightarrow \infty \\ \epsilon \rightarrow +0}} \frac{N(A, \lambda(1 + \epsilon))}{N(A, \lambda)} = 1, \quad (3.6)$$

then

$$N(A\dot{+}B, \lambda) = N(A, \lambda) (1 + o(1)), \quad (3.7)$$

where $A\dot{+}B$ is the operator associated to the form sum $\mathfrak{A} + \mathfrak{B}$.

Proposition 3.2 applies to our case with $\mathcal{H} = L^2(\Omega)$, $A = H$, and $\mathfrak{B} = \mathfrak{t}_{\partial\Omega} + \mathfrak{t}_{V-1}$. According to Theorem 2.20 $\mathfrak{t}_{\partial\Omega} + \mathfrak{t}_{V-1}$ is \mathfrak{t} -bounded with relative bound zero. It remains to verify (3.6) for the operator H . Indeed, there is

$$\lim_{\lambda \rightarrow \infty} N(H, \lambda) \lambda^{-d/2} = \text{const.} > 0 \quad (3.8)$$

where the constant depends on the domain Ω and the coefficient function $m(x)^{-1}$, cf. [4, Theorem 3]. \square

3.3 Corollary. *In particular, the second item of Theorem 3.1 implies that the operator $H_{\partial\Omega, V}$ generates an analytic semigroup on $L^2(\Omega)$.*

Apart from the asymptotic distribution of eigenvalues of the Schrödinger-type operator $H_{\partial\Omega, V}$ we are interested in the completeness of root functions of $H_{\partial\Omega, V}$ in $L^2(\Omega)$. The positive answer to that problem is based upon the following result.

3.4 Proposition. *(Agranovich [2]). Let \mathfrak{A} and \mathfrak{B} be densely defined, symmetric sesquilinear forms acting on a separable complex Hilbert space \mathcal{H} . Suppose \mathfrak{A} is closed, bounded from below by 1, and the selfadjoint operator A corresponding to \mathfrak{A} by the first representation theorem [24, VI.§2.1] has compact resolvent and its eigenvalues $\lambda_l = \lambda_l(A)$ obey*

$$\limsup_{l \rightarrow \infty} \lambda_l l^{-r} > 0 \quad (3.9)$$

for some $r > 0$. Further let \mathfrak{B} be s -subordinated to \mathfrak{A} , in the sense of Definition 2.15. In the two cases

$$r(1-s) = 1, \quad r(1-s) < 1, \quad (3.10)$$

there exists a Riesz basis, and an Abel basis of order $\beta > 1/r - (1-s)$ in \mathcal{H} , respectively, consisting of finite dimensional subspaces invariant with respect to $A\dot{+}iB$, i.e., in these two cases it is possible to construct a Riesz basis with brackets, and an Abel basis with brackets in \mathcal{H} , respectively, composed of the root functions of the operator $A\dot{+}iB$ associated to the form sum $\mathfrak{A} + i\mathfrak{B}$.

For the notions of Riesz and Abel basis cf. e.g. Gohberg/Krein [8, chapter VI], Agranovich [1, 6.2.a)], Rozenblum/Shubin/Solomyak [34, §20.1].

Generically, there is $r(1-s) < 1$ in our situation. However, in the spatially one dimensional case, $\Omega = (x_1, x_2)$, one obtains $r(1-s) = 1$, and thus a Riesz basis of root functions. Proposition 3.4 applies to our case with

$$\mathcal{H} = L^2(\Omega), \quad \mathfrak{A} = \Re \mathfrak{t}_{\partial\Omega, V-\zeta(V)} = \mathfrak{t} + \mathfrak{t}_{\Re(V)-\zeta(V)}, \quad \mathfrak{B} = \Im \mathfrak{t}_{\partial\Omega, V-\zeta(V)} = \mathfrak{t}_{\partial\Omega} + \mathfrak{t}_{\Im(V)}.$$

First we prove that the operator $H_{\Re(V)}$ complies to supposition (3.9) in Proposition 3.4.

3.5 Lemma. *The operator $H_{\Re(V)}$ from Corollary 2.21 has compact resolvent and its eigenvalues $\lambda_l = \lambda_l(H_{\Re(V)})$ obey*

$$\limsup_{l \rightarrow \infty} \lambda_l l^{-2/d} = \text{const.} > 0. \quad (3.11)$$

Proof. (2.38) implies for all $\lambda \geq 1 - \zeta(V)$

$$(1 - d/(2q)) \mathfrak{t}[\psi] \leq ((H_{\Re(V)} + 1 - \zeta(V))\psi, \psi) \leq ((H_{\Re(V)} + \lambda)\psi, \psi).$$

Thus, the minimax principle, cf. e.g. [33, XIII.1] provides that (3.11) holds for the eigenvalues of $H_{\Re(V)} + \lambda$, if it holds for the eigenvalues of $(1 - d/(2q))H$. According to [38, 5.6.1. Theorem 1] (3.8) implies (3.11) for the eigenvalues of H . Finally, (3.11) is invariant with respect to any fixed shift λ of the operator. \square

Next we prove that the imaginary part of the form $\mathfrak{t}_{\partial\Omega, V-\zeta(V)}$ is s -subordinated to its real part.

3.6 Lemma. *There is a constant $C_{\partial\Omega, V}$ depending on the norm of the distribution T in the space $(W^{1-1/p', p'}(\partial\Omega))^*$ and $\|\Im(V)\|_{L^q}$, such that*

$$|\Im \mathfrak{t}_{\partial\Omega, V-\zeta(V)}[\psi]| \leq C_{\partial\Omega, V} (\Re \mathfrak{t}_{\partial\Omega, V-\zeta(V)})^s \|\psi\|_{L^2}^{2(1-s)},$$

where s is the maximum of the subordination exponents from Theorem 2.16 and Theorem 2.18, $\zeta(V)$ is the number (2.39), and $\mathfrak{t}_{\partial\Omega, V}$ is the form (2.30).

Proof. According to Theorem 2.16 and Theorem 2.18 the form $\mathfrak{t}_{\partial\Omega} + \mathfrak{t}_{\Im(V)}$ is s -subordinated to the form \mathfrak{t} with an exponent $s < 1$. More precisely, there is a constant C with the stated properties such that

$$|\Im \mathfrak{t}_{\partial\Omega, V-\zeta(V)}[\psi]| \leq |\mathfrak{t}_{\partial\Omega}[\psi]| + |\mathfrak{t}_{\Im(V)}[\psi]| \leq C (\mathfrak{t}[\psi])^s \|\psi\|_{L^2}^{2(1-s)}.$$

Due to (2.38) one may continue this estimate by

$$\begin{aligned} &\leq C (1 - d/2q)^{-s} (\mathfrak{t}[\psi] + \mathfrak{t}_{\mathfrak{R}(V)}[\psi] - \zeta(V) \|\psi\|_{L^2}^2)^s \|\psi\|_{L^2}^{2(1-s)} \\ &\leq C (1 - d/2q)^{-s} (\mathfrak{Rt}_{\partial\Omega, V-\zeta(V)})^s \|\psi\|_{L^2}^{2(1-s)}. \end{aligned}$$

□

3.7 Theorem. *If s is the maximum of the subordination exponents from Theorem 2.16 and Theorem 2.18, then there exists an Abel basis in $L^2(\Omega)$ of order $\beta > d/2 - (1 - s)$, consisting of finite dimensional subspaces invariant with respect to the operator $H_{\partial\Omega, V} - \zeta(V)$. Here $H_{\partial\Omega, V}$ is the operator from Theorem 2.20, and $\zeta(V)$ is the number (2.39). In other words, it is possible to construct an Abel basis with brackets in $L^2(\Omega)$, composed of the root functions of the operator $H_{\partial\Omega, V} - \zeta(V)$.*

Proof. Due to Lemma 3.5, presupposition (3.9) of Proposition 3.4 holds with $r = 2/d$ for the eigenvalues of the operator $H_{\mathfrak{R}V} - \zeta(V)$. According to Lemma 3.6 the form $\mathfrak{St}_{\partial\Omega, V-\zeta(V)}$ is s -subordinated to the form $\mathfrak{Rt}_{\partial\Omega, V-\zeta(V)}$ with an exponent $1/2 < s < 1$, and the form $\mathfrak{Rt}_{\partial\Omega, V-\zeta(V)} = \mathfrak{t} + \mathfrak{t}_{\mathfrak{R}(V)-\zeta(V)}$ is bounded from below by 1, cf. (2.38). Hence, the case $r(1 - s) < 1$ in Proposition 3.4 applies, and there exists an Abel basis in $L^2(\Omega)$ of order $\beta > d/2 - (1 - s)$, consisting of finite dimensional subspaces invariant with respect to the operator $H_{\partial\Omega, V} - \zeta(V)$. N.B. Abel summation depends on the operator. □

3.8 Theorem. *If $d = 1$, then there exists a Riesz basis in $L^2(\Omega)$ consisting of finite dimensional subspaces invariant with respect to the operator $H_{\partial\Omega, V}$ from Theorem 2.20, i.e., it is possible to construct a Riesz basis with brackets in $L^2(\Omega)$, composed of the root functions of the operator $H_{\partial\Omega, V}$.*

Proof. Due to Lemma 3.5, presupposition (3.9) of Proposition 3.4 holds with $r = 2$ for the eigenvalues of the operator $H_{\mathfrak{R}V} - \zeta(V)$. According to Lemma 3.6 the form $\mathfrak{St}_{\partial\Omega, V-\zeta(V)}$ is $1/2$ -subordinated to the form $\mathfrak{Rt}_{\partial\Omega, V-\zeta(V)}$, and the form $\mathfrak{Rt}_{\partial\Omega, V-\zeta(V)} = \mathfrak{t} + \mathfrak{t}_{\mathfrak{R}(V)-\zeta(V)}$ is bounded from below by 1, cf. (2.38). Hence, the case $r(1 - s) = 1$ in Proposition 3.4 applies, and there exists a Riesz basis in $L^2(\Omega)$ consisting of finite dimensional subspaces invariant with respect to the operator $H_{\partial\Omega, V} - \zeta(V)$. These subspaces are also invariant with respect to the operator $H_{\partial\Omega, V}$. Moreover, a Riesz basis with brackets in $L^2(\Omega)$, composed of the root functions of the operator $H_{\partial\Omega, V} - \zeta(V)$, which are also the root functions of the operator $H_{\partial\Omega, V}$, remains a Riesz basis with brackets in $L^2(\Omega)$. □

3.9 Remark. For the one dimensional case, $\Omega = (x_1, x_2)$, with $m \equiv 1$, it is well known, cf. Marchenko [25, Theorem 1.3.2], that the system of eigenfunctions and generalized eigenfunctions of the operator $H_{\partial\Omega, V}$ is complete in $L^2(\Omega)$ and constitutes a basis there. Moreover, in that case the asymptotic distribution of eigenvalues of the operator $H_{\partial\Omega, V}$ can be specified, cf. [25, 1.5 Problem 1].

4 The dissipative case

If the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative, then this has serious implications for the analytical structure of the operator and its spectral properties.

4.1 Definition. Let A be an operator on a complex Hilbert space. A is said to be dissipative, if $\Im((A\psi, \psi)) \geq 0$ for all $\psi \in \text{dom}(A)$. A is maximal dissipative, if there is no proper dissipative extension of A .

4.2 Remark. This concept of dissipativity is commonly used in connection with Schrödinger operators, cf. e.g. Gohberg/Krein [8, V.§1]. A is dissipative, if and only if $-iA$ is accretive in the sense of Kato [24, V.§3.10], and A is maximal dissipative, if and only if A^* is maximal dissipative in the sense of Exner [6, 4.2].

Throughout this section we assume that the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative, i.e.,

$$\Im((H_{\partial\Omega, V}\psi, \psi)) \geq 0 \quad \forall \psi \in \text{dom}(H_{\partial\Omega, V}). \quad (4.1)$$

First we note some implications, the dissipativity of the operator $H_{\partial\Omega, V}$ has for its analytical structure.

4.3 Theorem. *If the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative, then:*

i) *The form $\mathfrak{t}_{\partial\Omega, V}$ is dissipative, i.e.,*

$$\Im(\mathfrak{t}_{\partial\Omega, V}[\psi]) = -\frac{i}{2} \left(\mathfrak{t}_{\partial\Omega, V}[\psi] - \overline{\mathfrak{t}_{\partial\Omega, V}[\psi]} \right) \geq 0 \quad \forall \psi \in W^{1,2}(\Omega) \quad (4.2)$$

and both the forms $\mathfrak{t}_{\partial\Omega}$ and \mathfrak{t}_V are dissipative themselves.

ii) $\Im(V) \geq 0$ *almost everywhere in Ω .*

iii) *The distribution T from Lemma 2.5 is a bounded positive Radon measure $\mu_{\partial\Omega}$ with support on $\partial\Omega$, i.e., $\langle T, f \rangle = \int_{\partial\Omega} f d\mu_{\partial\Omega}$. In particular, in the one*

dimensional case, $\Omega = (x_1, x_2)$, the two values of \mathbf{v} on the boundary $\partial\Omega$ obey

$$(-1)^j \mathbf{v}(x_j) \geq 0 \quad j = 1, 2. \quad (4.3)$$

Proof. *i)* (4.2) follows from (4.1) by density. Also, due to density it suffices to prove the dissipativity of $\mathbf{t}_{\partial\Omega}$ and \mathbf{t}_V on the domain $W^{1,2}(\Omega)$ of the form $\mathbf{t}_{\partial\Omega, V}$. As the form \mathbf{t} , cf. Definition 2.13, is selfadjoint one obtains

$$\begin{aligned} 0 &\leq i \overline{\mathbf{t}_{\partial\Omega, V}[\psi]} - i \mathbf{t}_{\partial\Omega, V}[\psi] = i \overline{\mathbf{t}_{\partial\Omega}[\psi]} - i \mathbf{t}_{\partial\Omega}[\psi] + i \overline{\mathbf{t}_V[\psi]} - i \mathbf{t}_V[\psi] \\ &= 2\langle T, \gamma_1(\psi) \overline{\gamma_1(\psi)} \rangle + 2 \int_{\Omega} \Im(V) |\psi|^2 dx \end{aligned} \quad (4.4)$$

for all $\psi \in W^{1,2}(\Omega)$, cf. Definition 2.13, (2.21), and (2.25). N.B. $\langle T, f \rangle$ is a real number, if f is a real-valued function on $\partial\Omega$. (4.4) yields

$$\Im(\mathbf{t}_V[\psi]) = \int_{\Omega} \Im(V) |\psi|^2 dx \geq 0,$$

for all $C_0^\infty(\Omega)$ -functions ψ , what also proves *ii*).

If the form $\mathbf{t}_{\partial\Omega}$ were not dissipative, then there would be a $\tilde{\psi}$ from $W^{1,2}(\Omega)$ such that

$$\frac{i}{2} \left(\overline{\mathbf{t}_{\partial\Omega}[\tilde{\psi}]} - \mathbf{t}_{\partial\Omega}[\tilde{\psi}] \right) = \langle T, \gamma_1(|\tilde{\psi}|^2) \rangle = K < 0. \quad (4.5)$$

Let $\Delta(x, \mathbb{R}^d \setminus \Omega)$ be a regularizing distance for the set $\mathbb{R}^d \setminus \Omega$, cf. e.g. Stein [36, VI.2.1], by means of which we define

$$f_\epsilon(x) = \begin{cases} 0 & \text{if } \Delta(x, \mathbb{R}^d \setminus \Omega) \geq 2\epsilon, \\ \exp(1 + \epsilon/(\Delta(x, \mathbb{R}^d \setminus \Omega) - 2\epsilon)) & \text{if } \epsilon < \Delta(x, \mathbb{R}^d \setminus \Omega) < 2\epsilon, \\ 1 & \text{otherwise,} \end{cases}$$

for each $\epsilon > 0$ and $x \in \overline{\Omega}$. There is $f_\epsilon \in C^\infty(\overline{\Omega})$, the functions $\psi_\epsilon := \tilde{\psi} f_\epsilon$ belong to the space $W^{1,2}(\Omega)$ and

$$\frac{i}{2} \left(\overline{\mathbf{t}_{\partial\Omega}[\tilde{\psi}]} - \mathbf{t}_{\partial\Omega}[\tilde{\psi}] \right) = \langle T, \gamma_1(|\psi_\epsilon|^2) \rangle = \langle T, \gamma_1(|\tilde{\psi}|^2) \rangle = K < 0 \quad (4.6)$$

for all $\epsilon > 0$, cf. (4.5). By the construction of f_ϵ there is

$$0 \leq \Im(V(x)) |\psi_\epsilon(x)|^2 \leq |V(x)| |\tilde{\psi}(x)|^2 \quad \text{and} \quad \lim_{\epsilon \rightarrow 0} \Im(V(x)) |\psi_\epsilon(x)|^2 = 0$$

for almost all $x \in \Omega$, what implies by Lebesgue's dominance that $\Im(\mathbf{t}_V[\psi_\epsilon])$ tends to zero as $\epsilon \rightarrow 0$. This together with (4.6) is a contradiction to the dissipativity of the form $\mathbf{t}_{\partial\Omega, V}$. Hence, the form $\mathbf{t}_{\partial\Omega}$ is dissipative.

iii) In the one dimensional case, $\Omega = (x_1, x_2)$, one obtains (4.3) from the dissipativity of the form $\mathfrak{t}_{\partial\Omega}$ by regarding the functions

$$\psi_1(x) = \frac{x_2 - x}{x_2 - x_1} \quad \psi_2(x) = \frac{x - x_1}{x_2 - x_1} \quad x \in [x_1, x_2]$$

which, belonging to the domain of $\mathfrak{t}_{\partial\Omega}$, provide, cf. also (2.23),

$$0 \leq \overline{i\mathfrak{t}_{\partial\Omega}[\psi_j]} - i\mathfrak{t}_{\partial\Omega}[\psi_j] = 2(-1)^j \mathfrak{v}(x_j), \quad j = 1, 2.$$

Now, we prove the properties of the distribution T in the two and three dimensional case. First, let ψ be any function from $C_0^\infty(\mathbb{R}^d)$, i.e., $\psi|_\Omega \in W^{1,2}(\Omega) \subset \text{dom}(\mathfrak{t}_{\partial\Omega})$. N.B. As ψ is a continuous function on $\overline{\Omega}$ we use the usual trace mapping. The dissipativity of the form $\mathfrak{t}_{\partial\Omega}$ implies

$$0 \leq \overline{i\mathfrak{t}_{\partial\Omega}[\psi|_\Omega]} - i\mathfrak{t}_{\partial\Omega}[\psi|_\Omega] = 2\langle T, |\psi|_{\partial\Omega}|^2 \rangle. \quad (4.7)$$

With respect to $\psi \in C_0^\infty(\mathbb{R}^d)$ let Θ_ψ be a function from $C_0^\infty(\mathbb{R}^d)$ such that

$$\Theta_\psi|_{\partial\Omega} = 1, \quad \text{supp } \Theta_\psi \subset \left\{ x \in \mathbb{R}^d : |\psi(x)|^2 < 2 \sup_{y \in \partial\Omega} |\psi(y)|^2 \right\}$$

and $\tilde{\psi}$ the $C_0^\infty(\mathbb{R}^d)$ function defined by

$$\tilde{\psi}(x) \stackrel{\text{def}}{=} \Theta_\psi(x) \sqrt{2 \sup_{y \in \partial\Omega} |\psi(y)|^2 - |\psi(x)|^2} \quad x \in \mathbb{R}^d.$$

(4.7) applied to the function $\tilde{\psi}$ now provides

$$\langle T, |\psi|_{\partial\Omega}|^2 \rangle \leq \langle T, 2 \sup_{y \in \partial\Omega} |\psi(y)|^2 \rangle = 2 \| |\psi|_{\partial\Omega}|^2 \|_{C(\partial\Omega)} \langle T, 1_{\partial\Omega} \rangle, \quad (4.8)$$

where $1_{\partial\Omega}$ denotes the function which is constant 1 of the set $\partial\Omega$. The inequalities (4.7) and (4.8) extend to

$$0 \leq \langle T, f|_{\partial\Omega} \rangle \leq \|f|_{\partial\Omega}\|_{C(\partial\Omega)} \langle T, 1_{\partial\Omega} \rangle, \quad (4.9)$$

for functions f from the space $W^{1,r}(\Omega; \mathbb{R}^+)$, $r > \max\{p', d\}$ (cf. Assumption 2.1) because the set

$$\left\{ |\psi|_{\partial\Omega}|^2 : \psi \in C_0^\infty(\mathbb{R}^d) \right\} \quad \text{is dense in } W^{1,r}(\Omega; \mathbb{R}^+), \quad (4.10)$$

and the following embeddings are continuous

$$W^{1,r}(\Omega) \hookrightarrow C(\overline{\Omega}) \hookrightarrow C(\partial\Omega), \quad W^{1,r}(\Omega) \hookrightarrow W^{1-1/p', p'}(\partial\Omega).$$

The last embedding ensures according to Lemma 2.5 that the traces of functions $f \in W^{1,r}(\Omega)$ belong to the domain of the functional T . Now, let $f = f^+ - f^-$ be an arbitrary function from $W^{1,r}(\Omega; \mathbb{R})$, and f^+ , f^- its positive and negative part, respectively. Then $f^\pm \in W^{1,r}(\Omega; \mathbb{R}^+)$, cf. [5, 4.2.2 Theorem 4(iii)], and according to (4.9) there is

$$\begin{aligned} |\langle T, f \upharpoonright_{\partial\Omega} \rangle| &= |\langle T, f_{\partial\Omega}^+ \rangle - \langle T, f_{\partial\Omega}^- \rangle| \\ &\leq (\|f^+ \upharpoonright_{\partial\Omega}\|_{C(\partial\Omega)} + \|f^- \upharpoonright_{\partial\Omega}\|_{C(\partial\Omega)}) \langle T, 1_{\partial\Omega} \rangle \\ &\leq 2 \|f \upharpoonright_{\partial\Omega}\|_{C(\partial\Omega)} \langle T, 1_{\partial\Omega} \rangle. \end{aligned}$$

This inequality naturally extends to

$$|\langle T, f \rangle| \leq 4 \|f\|_{C(\partial\Omega)} \langle T, 1_{\partial\Omega} \rangle. \quad (4.11)$$

for all $\partial\Omega$ -traces f of $W^{1,r}(\Omega)$ functions. According to the Weierstrass approximation theorem the $\partial\Omega$ -traces of $W^{1,r}(\Omega)$ -functions are dense in $C(\partial\Omega)$. Hence, (4.11) extends to all $f \in C(\partial\Omega)$, i.e., T is a distribution of order zero, and thus, a — positive — Radon-measure. \square

4.4 Remark. In the two and three dimensional case the distribution T from is from the space $(W^{1-1/p', p'}(\partial\Omega))^*$, cf. Lemma 2.5 and according to Theorem 4.3 it is a bounded positive Radon measure, if the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative. For a characterization of positive measures, which belong to the dual of Sobolev spaces, cf. [39, 4.7].

4.5 Remark. In the one dimensional case $\Omega = (x_1, x_2)$, the two values of $\nu \cdot \mathbf{v}$ on the boundary $\partial\Omega$ exist, cf. Remark 2.6, and are nonnegative according to Theorem 4.3. If, in the two and three dimensional case ($d > 1$), one assumes in the sense of Remark 2.6 instead of Assumption 2.1 more regularity of the flow \mathbf{v} , such that the trace of $\nu \cdot \mathbf{v}$ on the boundary $\partial\Omega$ is from the space $L^1(\partial\Omega)$, then $\nu \cdot \mathbf{v} \geq 0$ almost everywhere in $\partial\Omega$.

4.6 Theorem. *Let $V \in L^q$ be a complex-valued Schrödinger potential with (2.24) and $\Im(V) \geq 0$ almost everywhere in Ω , and suppose the distribution T from Lemma 2.5 is a (bounded) positive measure with support on $\partial\Omega$, i.e., in the one dimensional case, $\Omega = (x_1, x_2)$, the two values of \mathbf{v} on the boundary $\partial\Omega$ obey (4.3). Then the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative. Even more, $H_{\partial\Omega, V}$ is maximal dissipative, i.e., there is no proper dissipative extension of $H_{\partial\Omega, V}$.*

Proof. Obviously $\Im(V) \geq 0$ a.e. in Ω , implies the dissipativity of the form $\mathfrak{t}_{\mathbf{v}}$ and the assumptions on T ensure the dissipativity of the form $\mathfrak{t}_{\partial\Omega}$. Hence, the

form $t_{\partial\Omega, V}$ and a fortiori the operator $H_{\partial\Omega, V}$ is dissipative. (4.1) says that the numerical range of $H_{\partial\Omega, V}$ is contained in the upper complex half plane. As $H_{\partial\Omega, V}$ is an operator with compact resolvent there are regular points of $H_{\partial\Omega, V}$ in the lower half plane. This implies, cf. e.g. Kato [24, Theorem V/3.2], that the whole lower half plane belongs to the resolvent set of $H_{\partial\Omega, V}$ and there is the resolvent estimate

$$\|(H_{\partial\Omega, V} - \lambda)^{-1}\| \leq 1/|\Im(\lambda)| \quad \forall \lambda \text{ with } \Im(\lambda) < 0. \quad (4.12)$$

Hence, $-iH_{\partial\Omega, V}$ is maximal accretive in the sense of Kato, cf. e.g. Kato [24, V.S3.10], i.e., $H_{\partial\Omega, V}$ is maximal dissipative. \square

4.7 Remark. According to the Lumer–Phillips theorem $iH_{\partial\Omega, V}$ is the infinitesimal generator of a strongly continuous semigroup of contractions on $L^2(\Omega)$, if and only if $H_{\partial\Omega, V}$ is maximal dissipative, and due to Theorem 4.6, if and only if $H_{\partial\Omega, V}$ is dissipative. Thus, if $H_{\partial\Omega, V}$ is dissipative, then it is a pseudo–Hamiltonian, cf. Exner [6, 4.1].

4.8 Remark. Results corresponding to those of this section hold if the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is anti–dissipative, i.e., if $i(H_{\partial\Omega, V}^* - H_{\partial\Omega, V}) \geq 0$ in the sense of forms.

5 The completely dissipative case

According to Theorem 4.6 the operator $H_{\partial\Omega, V}$ is not only dissipative but maximal dissipative. Hence, there is a decomposition of $H_{\partial\Omega, V}$ into a selfadjoint part and a completely dissipative part, cf. e.g. Nagy/Foiaş [37, IV.4. Proposition 4.3] or Exner [6, Theorem 4.2.10]. As $H_{\partial\Omega, V}$ has compact resolvent so has its selfadjoint part. Thus, if $H_{\partial\Omega, V}$ is dissipative and has no real eigenvalues, then $H_{\partial\Omega, V}$ is completely dissipative, i.e. the only subspace on which the semigroup generated by $iH_{\partial\Omega, V}$ is unitary is $\{0\}$, cf. Exner [6, 4.2].

In the following we are looking for sufficient conditions on the Schrödinger potential V and the boundary distribution T , such that the operator $H_{\partial\Omega, V}$ from Theorem 2.20 has no real eigenvalues. We will prove general results in the one dimensional case $\Omega = (x_1, x_2)$, cf. Theorem 5.2, and the two dimensional case, cf. Theorem 5.6, and in the three dimensional case a result for Schrödinger operators with piecewise constant mass tensor, cf. Theorem 5.8.

5.1 Lemma. *If the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative and has an eigenvalue $\lambda \in \mathbb{R}$, then for any eigenfunction ψ corresponding to λ there*

is

$$\mathbf{t}_{\partial\Omega}[\psi, \phi] = \mathbf{t}_{\Im(V)}[\psi, \phi] = \mathbf{t}[\psi, \phi] + \mathbf{t}_{\Re(V)-1-\lambda}[\psi, \phi] = 0 \quad \forall \phi \in W^{1,2}(\Omega), \quad (5.1)$$

i.e., λ is an eigenvalue and ψ a corresponding eigenfunction of the operator $\Re(H_{\partial\Omega, V}) = H_{\Re(V)}$ associated to the form sum $\mathbf{t} + \mathbf{t}_{\Re(V)-1}$. In particular, there is a real-valued eigenfunction ψ of $H_{\partial\Omega, V}$ belonging to λ .

Proof. Let $\lambda \in \mathbb{R}$ be an eigenvalue of $H_{\partial\Omega, V}$ and $\psi \in W^{1,2}(\Omega)$ a corresponding eigenfunction. Testing the eigenvalue equation $H_{\partial\Omega, V}\psi = \lambda\psi$ with $\bar{\psi}$ one gets by taking the imaginary part:

$$\int_{\Omega} \Im(V) |\psi|^2 dx = 0 \quad \text{and} \quad \langle T, \gamma_1(\psi)\gamma_1(\bar{\psi}) \rangle = \int_{\partial\Omega} |\gamma_1(\psi)|^2 d\mu_{\partial\Omega} = 0.$$

N.B. There is $\gamma_1(\bar{\psi}) = \overline{\gamma_1(\psi)}$ and according to Theorem 4.3 both terms are separately nonnegative. By means of Hölder's inequality we now conclude

$$\left| \int_{\partial\Omega} \gamma_1(\psi) \phi \upharpoonright_{\partial\Omega} d\mu_{\partial\Omega} \right| \leq \sqrt{\int_{\partial\Omega} |\gamma_1(\psi)|^2 d\mu_{\partial\Omega}} \sqrt{\int_{\partial\Omega} |\phi \upharpoonright_{\partial\Omega}|^2 d\mu_{\partial\Omega}} = 0$$

for all $\phi \in C(\bar{\Omega})$. Again by Hölder's inequality we get

$$\left| \int_{\Omega} \Im(V) \psi \phi dx \right| \leq \left| \int_{\Omega} \psi \phi d\mu_{\Omega} \right| \leq \sqrt{\int_{\Omega} |\psi|^2 d\mu_{\Omega}} \sqrt{\int_{\Omega} |\phi|^2 d\mu_{\Omega}} = 0$$

for all $\phi \in W^{1,2}(\Omega)$, where $\mu_{\Omega} = \Im(V) dx$. Hence, there is (5.1). Obviously, both the real and the imaginary part of ψ are (real-valued) eigenfunctions belonging to λ . \square

First we regard the one dimensional case.

5.2 Theorem. *If $\Omega = (x_1, x_2)$ and the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative, then $H_{\partial\Omega, V}$ has no real eigenvalues, under at least one of the conditions:*

- i) *The imaginary part $\Im(V)$ of the Schrödinger potential is strictly positive on a set of nonzero Lebesgue measure.*
- ii) *$(-1)^j \mathbf{v}(x_j) > 0$ for $j = 1$ or $j = 2$.*

Proof. Let us assume the opposite. If there were an eigenvalue $\lambda \in \mathbb{R}$ of $H_{\partial\Omega, V}$, then — according to Lemma 5.1 — there would be a real-valued

function $\psi \in W^{1,2}(\Omega)$, such that λ is an eigenvalue and ψ an eigenfunction belonging to λ of the operator $\Re(H_{\partial\Omega,V}) = H_{\Re(V)}$ associated to the form sum $\mathfrak{t} + \mathfrak{t}_{\Re(V-1)}$. $\psi \in W^{1,2}(\Omega)$ implies that ψ is absolutely continuous on $\Omega = (x_1, x_2)$ and strongly differentiable on a set M_d of Lebesgue measure $x_2 - x_1$, cf. e.g. Evans/Gariepy [5, 4.9.1].

If $(-1)^j \mathfrak{v}(x_j) > 0$, then (5.1) implies $\psi(x) = 0$ for $x = x_j$. — If the imaginary part $\Im(V)$ of the Schrödinger potential V is strictly positive on a set M of nonzero Lebesgue measure, then the (continuous) function ψ vanishes on M . According to [3, VI. Theorem 15] all except an enumerable number of points of $M \cap M_d$ are points of condensation of this set. Hence, there is at least one point x among them such that $\psi'(x) = \psi(x) = 0$, and thus $\psi'(x)/\tilde{m}(x) = 0$, where \tilde{m} is a representative of m which is strictly positive on $\Omega = (x_1, x_2)$.

Thus in both cases ψ is a weak solution of

$$-\frac{\hbar^2}{2} \frac{d}{dx} \left(\frac{1}{m} \frac{d\psi}{dx} \right) = (\lambda - V)\psi$$

on the intervals (x_1, x) and (x, x_2) with $\psi(x) = 0$. Now the assertion follows immediately from the following Lemma 5.3. \square

5.3 Lemma. *Let V be from $L^1(\xi, \eta)$ and let ψ be a weak solution of*

$$-\frac{d}{dx} \left(\frac{1}{m} \frac{d\psi}{dx} \right) = V\psi \quad \text{a.e. in } (\xi, \eta),$$

i.e.,

$$\int_{\xi}^{\eta} \frac{1}{m} \psi' \bar{\phi}' - V \psi \bar{\phi} dx = 0 \quad \forall \phi \in W^{1,2}(\xi, \eta).$$

If $\psi(\xi) = 0$, then $\psi \equiv 0$ on (ξ, η) .

Proof. From the presupposition follows, cf. e.g. Kato [24, VI.§2.4 Example 2.16], that ψ'/m is absolutely continuous, and $\psi'/m(\xi) = \psi'/m(\eta) = 0$. The strong derivative of ψ'/m exists Lebesgue a.e. on (ξ, η) , cf. e.g. Evans/Gariepy [5, 4.9.1] and coincides a.e. with $V\psi$. Introducing the function $\chi = \psi'/m$ one obtains for the pair ψ, χ the differential equation

$$\frac{d}{dx} \begin{pmatrix} \psi \\ \chi \end{pmatrix} = \begin{pmatrix} 0 & m \\ V & 0 \end{pmatrix} \begin{pmatrix} \psi \\ \chi \end{pmatrix},$$

including the initial condition $\psi(\xi) = \chi(\xi) = 0$. Integrating this equation provides

$$\begin{pmatrix} \psi \\ \chi \end{pmatrix} (x) = \int_{\xi}^x \begin{pmatrix} 0 & m \\ V & 0 \end{pmatrix} (s) \begin{pmatrix} \psi \\ \chi \end{pmatrix} (s) ds.$$

Choosing $\tau \in (\xi, \eta)$, such that

$$\int_{\xi}^{\tau} \left\| \begin{pmatrix} 0 & m \\ V & 0 \end{pmatrix} (s) \right\|_{\mathcal{B}(\mathbb{C}^2)} ds = \frac{1}{2},$$

one verifies that the map

$$\begin{pmatrix} \psi \\ \chi \end{pmatrix} \mapsto \int_{\xi}^{(\cdot)} \begin{pmatrix} 0 & m \\ V & 0 \end{pmatrix} (s) \begin{pmatrix} \psi \\ \chi \end{pmatrix} (s) ds$$

is a contraction over

$$C([\xi, \tau]; \mathbb{C}^2) \cap \left\{ \begin{pmatrix} \psi \\ \chi \end{pmatrix} : \psi(\xi) = \chi(\xi) = 0 \right\}.$$

Hence, the functions ψ and χ vanish identically on the interval $[\xi, \tau]$. Now, the argument repeats finitely many times, thus, covering the whole interval $[\xi, \eta]$. \square

Next we regard the two and three dimensional case. With respect to the Schrödinger potential V and the boundary distribution T we will impose:

5.4 Assumption. The real part of the Schrödinger potential V is essentially bounded, and there is at least one of the following conditions fulfilled.

i) The imaginary part $\Im(V)$ of the Schrödinger potential V has a representative such that the set $\{x \in \Omega : \Im(V)(x) > 0\}$ has an interior point.

ii) The measure $T = \mu_{\partial\Omega}$ from Theorem 4.3 is such that if

$$\langle T, f \rangle = \int_{\partial\Omega} f d\mu_{\partial\Omega} = 0$$

for a nonnegative continuous function f , then f is zero on an open subset of the boundary $\partial\Omega$.

5.5 Lemma. *Suppose Ω is a bounded two or three dimensional domain with a Lipschitz boundary, and $W \in L^q(\Omega; \mathbb{R})$ is a real-valued Schrödinger potential, where q is according to (2.24). Further, let λ be an eigenvalue and $\psi \in W^{1,2}(\Omega)$ a corresponding real-valued eigenfunction of the operator H_W associated to the form sum $\mathfrak{t} + \mathfrak{t}_{W-1}$. If there is an open subset \mathcal{O} of the boundary $\partial\Omega$ of Ω such that ψ is zero almost everywhere on \mathcal{O} , then there is a bounded domain $\widehat{\Omega} \supsetneq \Omega$ with a Lipschitz boundary such that*

$$\int_{\widehat{\Omega}} \frac{\hbar^2}{2} \widehat{m}(x)^{-1} \nabla \widehat{\psi}(x) \cdot \nabla \overline{\widehat{\phi}}(x) + (\widehat{W}(x) - \lambda) \widehat{\psi}(x) \overline{\widehat{\phi}}(x) dx = 0 \quad \forall \widehat{\phi} \in W^{1,2}(\widehat{\Omega}),$$

where \widehat{W} is the continuation of W by zero outside Ω and

$$\widehat{m}(x) = \begin{cases} \mathbb{I} & \text{if } x \in \widehat{\Omega} \setminus \Omega, \\ m(x) & \text{if } x \in \Omega, \end{cases} \quad \widehat{\psi}(x) = \begin{cases} 0 & \text{if } x \in \widehat{\Omega} \setminus \Omega, \\ \psi(x) & \text{if } x \in \Omega. \end{cases}$$

Moreover, there is $\widehat{\psi} \in W^{1,2}(\widehat{\Omega})$.

Proof. Let x be point from the set \mathcal{O} . As Ω is a domain with a Lipschitz boundary there is an open neighborhood \mathcal{V} of x in \mathbb{R}^d and a bi-Lipschitz transformation L from \mathcal{V} onto the unit ball in \mathbb{R}^d such that

$$L(\mathcal{V} \cap \overline{\Omega}) = \{x \in \mathbb{R}^d : \|x\|_{\mathbb{R}^d} < 1, x_d \leq 0\}.$$

Moreover, there is an open neighborhood $\mathcal{O}_x \subset \mathcal{O}$ of x in $\partial\Omega$ such that $L(\mathcal{O}_x)$ is an open neighborhood of the origin in

$$\{x \in \mathbb{R}^d : \|x\|_{\mathbb{R}^d} < 1, x_d = 0\},$$

i.e. there is a ball E in \mathbb{R}^d around the origin such that

$$E \cap \{x \in \mathbb{R}^d : x_d = 0\} \subsetneq L(\mathcal{O}_x).$$

We define $\widehat{\Omega} = \Omega \cup L^{-1}(E)$ and

$$\widehat{\psi}(x) = \begin{cases} 0 & \text{if } L(x) \in E \cap \{x \in \mathbb{R}^d : x_d > 0\}, \\ \psi(x) & \text{if } x \in \Omega. \end{cases}$$

The set $E \cup L(\mathcal{V})$ is a bounded domain with a Lipschitz boundary. Hence, $\widehat{\Omega}$ has a Lipschitz boundary. — According to [10, Theorem 2.7] $\widehat{\psi}$ belongs to the space $W^{1,2}(\widehat{\Omega})$. \square

5.6 Theorem. *Suppose Ω is a bounded two dimensional domain with a Lipschitz boundary. If the operator $H_{\partial\Omega, \mathcal{V}}$ from Theorem 2.20 is dissipative, then $H_{\partial\Omega, \mathcal{V}}$ has no real eigenvalues, under Assumption 5.4.*

Proof. Let us assume the opposite. If there were an eigenvalue $\lambda \in \mathbb{R}$ of $H_{\partial\Omega, \mathcal{V}}$, then — according to Lemma 5.1 — there would be a real-valued function $\psi \in W^{1,2}(\Omega)$, such that λ is an eigenvalue and ψ an eigenfunction belonging to λ of the operator $\Re(H_{\partial\Omega, \mathcal{V}}) = H_{\Re(\mathcal{V})}$ associated to the form sum $\mathfrak{t} + \mathfrak{t}_{\Re(\mathcal{V}-1)}$. The first item of Assumption 5.4 directly implies that ψ vanishes almost everywhere on an open subset of Ω . The second item of Assumption 5.4 assures that there is a bounded domain $\widehat{\Omega} \supsetneq \Omega$ with a Lipschitz boundary and

a function $\widehat{\psi}$ with the properties stated in Lemma 5.5, where $W = \mathfrak{R}(V)$. In particular $\widehat{\psi}$ is an extension of ψ , belongs to the space $W^{1,2}(\widehat{\Omega})$ and vanishes almost everywhere on an open subset of $\widehat{\Omega}$.

According to elliptic regularity theory cf. Griepentrog/Recke [12], [9, Theorem 4.12] ψ ($\widehat{\psi}$) are up to the boundary Hölder continuous functions on Ω ($\widehat{\Omega}$). Hence, ψ ($\widehat{\psi}$) vanishes identically on an open subset of Ω ($\widehat{\Omega}$), and the unique continuation property, cf. [35] provides that ψ ($\widehat{\psi}$) vanishes identically on Ω ($\widehat{\Omega}$). This contradicts our original assumption. \square

In order to give a precise formulation of our assumptions in the three dimensional case we make the following definition relating domain decomposition to graphs:

5.7 Definition. We say that two disjoint domains Ω_1 and Ω_2 from \mathbb{R}^d are Lipschitz adjacent to each other, if there is a point $x \in \overline{\Omega}_1 \cap \overline{\Omega}_2$, an open neighborhood \mathcal{V} of x in \mathbb{R}^d and a bi-Lipschitz transformation L from \mathcal{V} onto the unit ball in \mathbb{R}^d such that

$$\begin{aligned} L(\mathcal{V} \cap \overline{\Omega}_1) &= \{x \in \mathbb{R}^d : \|x\|_{\mathbb{R}^d} < 1, x_d \leq 0\}, \\ L(\mathcal{V} \cap \overline{\Omega}_2) &= \{x \in \mathbb{R}^d : \|x\|_{\mathbb{R}^d} < 1, x_d \geq 0\}. \end{aligned}$$

$\Omega_j \subset \mathbb{R}^d$, $j = 1, \dots, J$ is said to be a Lipschitz decomposition of $\Omega \subset \mathbb{R}^d$ (or Ω Lipschitz decomposable) if Ω and Ω_j , $j = 1, \dots, J$ are bounded domains with Lipschitz boundary, such that the union of all the Ω_j , $j = 1, \dots, J$ is dense in Ω , and the Ω_j , $j = 1, \dots, J$ are the vertices of a connected graph (i.e. every pair of vertices can be reached by a path) with respect to the above defined adjacency relation.

5.8 Theorem. *Let Ω be a three dimensional Lipschitz decomposable domain in the sense of Definition 5.7. Suppose the mass tensor m from Definition 2.13 is constant m_j on each Ω_j . If the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative, then $H_{\partial\Omega, V}$ has no real eigenvalues, under Assumption 5.4.*

Proof. Let us assume the opposite. If there were an eigenvalue $\lambda \in \mathbb{R}$ of $H_{\partial\Omega, V}$, then — according to Lemma 5.1 — there would be a real-valued function $\psi \in W^{1,2}(\Omega)$, such that λ is an eigenvalue and ψ an eigenfunction belonging to λ of the operator $\mathfrak{R}(H_{\partial\Omega, V}) = H_{\mathfrak{R}(V)}$ associated to the form sum $\mathfrak{t} + \mathfrak{t}_{\mathfrak{R}(V-1)}$.

The first item of Assumption 5.4 directly implies that ψ vanishes almost everywhere on an open subset of at least one of the Ω_j . According to Theorem 2.18 multiplication by $\mathfrak{R}(V)$ is relatively bounded with respect to the

Laplacian with bound zero. Moreover, $\mathfrak{R}(V)$ is essentially bounded on Ω_j , cf. Assumption 5.4. Thus, [33, Theorem XIII.57] provides that ψ vanishes almost everywhere on Ω_j .

The second item of Assumption 5.4 assures that there is a bounded domain $\widehat{\Omega} \supsetneq \Omega$ and a function $\widehat{\psi}$ with the properties stated in Lemma 5.5, where $W = \mathfrak{R}(V)$. In particular $\widehat{\psi}$ is an extension of ψ , belongs to the space $W^{1,2}(\widehat{\Omega})$ and vanishes almost everywhere on Ω_0 , the interior of the set $\widehat{\Omega} \setminus \Omega$. N.B. Ω_0 is adjacent to at least one of the Ω_j , according to the construction in the proof of Lemma 5.5. Thus, Ω_j , $j = 0, \dots, J$ is a Lipschitz decomposition of $\widehat{\Omega}$ in the sense of Definition 5.7.

Now, let us assume that ψ vanishes almost everywhere on some Ω_{j_1} , $0 \leq j_1 \leq J$. There is at least one Ω_{j_2} , $1 \leq j_2 \leq J$, $j_2 \neq j_1$, which is adjacent to Ω_{j_1} in the sense of Definition 5.7. As ψ vanishes on Ω_{j_1} we can replace m_{j_1} by m_{j_2} on Ω_{j_1} without changing the eigenvalue equation. Thus, again [33, Theorem XIII.57] applies and provides that ψ vanishes almost everywhere on $\Omega_{j_1} \cup \Omega_{j_2}$. N.B. The Lipschitz adjacency — in the sense of Definition 5.7 — of Ω_{j_1} and Ω_{j_2} is essential for the application of [33, Theorem XIII.57], cf. the proof of this theorem in [33, Appendix to XIII.13].

By repeating the preceding argument one obtains that ψ vanishes on each Ω_j , $j = 1, \dots, J$, because the Ω_j are the vertices of a connected graph. \square

5.9 Remark. Results corresponding to those of this section hold if the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is anti-dissipative.

6 Conclusion

If the operator $H_{\partial\Omega, V}$ from Theorem 2.20 is dissipative and thus by Theorem 4.6 maximal dissipative, then there exists a minimal selfadjoint extension $K_{\partial\Omega, V}$ of $H_{\partial\Omega, V}$, cf. e.g. Nagy/Foiaş [37, I.4. Theorem 4.1] or Exner [6, Theorem 1.4.1] acting in an enlarged Hilbert space \mathcal{H} . $K_{\partial\Omega, V}$ is the quasi-Hamiltonian referring to $H_{\partial\Omega, V}$, \mathcal{H} is the state Hilbert space for the minimal closed quantum system containing the original open one and $P : \mathcal{H} \rightarrow L^2$ is the corresponding orthoprojector onto the original state Hilbert space. Let $W : L^2 \mapsto L^2$ be a selfadjoint operator, i.e. an observable for the open quantum system. The expectation value of W with respect to a generalized state, i.e. a positive, nuclear operator $\rho \in \mathcal{B}_1(L^2)$, is $\text{tr}(\rho W)$, if ρW is nuclear. If $\rho = Pf(K_{\partial\Omega, V})|_{L^2}$, with some suitable continuous function $f : \mathbb{R} \rightarrow \mathbb{R}$, then

$$\rho = \frac{1}{2\pi i} \text{w-lim}_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} f(\lambda) \left((\lambda - i\epsilon - H_{\partial\Omega, V})^{-1} - (\lambda + i\epsilon - H_{\partial\Omega, V}^*)^{-1} \right) d\lambda, \quad (6.1)$$

cf. e.g. Exner [6, Proposition 4.1.4].

On the other hand, according to Theorem 3.7 there is an Abel basis in $L^2(\Omega)$ of order β consisting of finite dimensional subspaces invariant with respect to the operator $H_{\partial\Omega, V} - \zeta(V)$. Let $\{\Lambda_l\}_0^\infty$ be an enumerable covering of the numerical range of $H_{\partial\Omega, V}$, such that

$$P_{l, \beta}(t) = \frac{1}{2\pi i} \int_{\partial\Lambda_l} e^{-t(\lambda - \zeta(V))^\beta} (\lambda - H_{\partial\Omega, V})^{-1} d\lambda \quad (6.2)$$

are the generalized Riesz projections corresponding to the subspaces of the Abel basis. Then (6.1) implies

$$\rho = \frac{1}{2\pi i} \text{s-lim}_{t \rightarrow +0} \sum_{l=0}^{\infty} \int_{\partial\Lambda_l} f(\lambda - \zeta(V)) e^{-t(\lambda - \zeta(V))^\beta} \left((\lambda - H_{\partial\Omega, V})^{-1} - (\lambda - H_{\partial\Omega, V}^*)^{-1} \right) d\lambda, \quad (6.3)$$

with a holomorphic continuation of the function f into the sector of the complex plane which contains the numerical range of $H_{\partial\Omega, V} - \zeta(V)$.

The expressions of ρ in terms of the operator $H_{\partial\Omega, V}$ allow by suitable choices of f and W to define physical quantities (e.g. densities) related to the (dissipative) open quantum system without explicitly knowing the quasi-Hamiltonian $K_{\partial\Omega, V}$ corresponding to the pseudo-Hamiltonian $H_{\partial\Omega, V}$.

6.1 Problem. If $H_{\partial\Omega, V}$ is not dissipative, then (6.1) and (6.3) still apply. What are the conditions on f and W , such that $\text{tr}(\rho W)$ defines a property of the open — but not necessarily dissipative — quantum system.

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