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Spectral semi-classical analysis of a complex Schrödinger operator in exterior domains

- Y. Almog, Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803, USA,
- D. S. Grebenkov, Laboratoire de Physique de la Matière Condensée, CNRS and Ecole Polytechnique, F-91128 Palaiseau, France, and
 - B. Helffer, Laboratoire de Mathématiques Jean Leray, CNRS and Université de Nantes,
 - 2 rue de la Houssinière, 44322 Nantes Cedex France.

Abstract

Generalizing previous results obtained for the spectrum of the Dirichlet and Neumann realizations in a bounded domain of a Schrödinger operator with a purely imaginary potential $-h^2\Delta + iV$ in the semiclassical limit $h \to 0$ we address the same problem in exterior domains. In particular we obtain the left margin of the spectrum, and the emptiness of the essential part of the spectrum under some additional assumptions.

1 Introduction

Let $\Omega = K^c$, where K is a compact set with smooth boundary in \mathbb{R}^d with $d \geq 1$. Consider the operator

$$\mathcal{A}_h^D = -h^2 \Delta + i V \,, \tag{1.1a}$$

defined on

$$D(\mathcal{A}_{h}^{D}) = \{ u \in H^{2}(\Omega) \cap H_{0}^{1}(\Omega), Vu \in L^{2}(\Omega) \},$$
 (1.1b)

or

$$\mathcal{A}_h^N = -h^2 \Delta + i V \,, \tag{1.2a}$$

defined on

$$D(\mathcal{A}_h^N) = \{ u \in H^2(\Omega), \, Vu \in L^2(\Omega), \, \partial_\nu u = 0 \text{ on } \partial\Omega \},$$
 (1.2b)

where V is a C^{∞} -potential in $\overline{\Omega}$, ν is pointing outwards of Ω . The quadratic forms respectively read

$$u \mapsto q_V^D(u) := h^2 \|\nabla u\|_{\Omega}^2 + i \int_{\Omega} V(x) |u(x)|^2 dx,$$
 (1.3)

where the form domain is

$$\mathcal{V}^{D}(\Omega) = \{ u \in H_0^1(\Omega), |V|^{\frac{1}{2}} u \in L^2(\Omega) \},$$

and

$$u \mapsto q_V^N(u) := h^2 \|\nabla u\|_{\Omega}^2 + i \int_{\Omega} V(x) |u(x)|^2 dx, \qquad (1.4)$$

where the form domain is

$$\mathcal{V}^{N}(\Omega) = \{ u \in H^{1}(\Omega), |V|^{\frac{1}{2}}u \in L^{2}(\Omega) \}.$$

Although the forms are not necessarily coercive when V changes sign, a natural definition, via an extended Lax-Milgram theorem, can be given for \mathcal{A}_h^D or \mathcal{A}_h^N under the condition that there exists C>0 such that

$$|\nabla V(x)| \le C\sqrt{V(x)^2 + 1}, \quad \forall x \in \overline{\Omega}.$$
 (1.5)

We refer to [3, 12, 2] for this point and the characterization of the domain of $\mathcal{A}_h^{\#}$, where the notation # is used for D (Dirichlet) or N (Neumann).

Note that (1.5) is satisfied for $V(x) = x_1$ (Bloch-Torrey equation) which is our main motivating example (see [10]).

In this last case and when $K = \emptyset$, it has been demonstrated that the spectrum is empty [1, 14]. Our aim is now to analyze, when K is not empty, the two following properties

- the emptiness of the essential spectrum, although the resolvent is not compact when $d \geq 2$,
- the non emptiness of the spectrum and the extension of the semi-classical result of Almog-Grebenkov-Helffer [2] concerning the bottom of the real part of the spectrum.

Since the case d=1 was analyzed in [12, 14], we will assume from now on that

$$d > 2. \tag{1.6}$$

The study of the spectrum of the operator (1.1) in bounded domains began in [1] where a lower bound on the left margin of the spectrum has been obtained. In [14] the same lower bound has been obtained using a different technique allowing for resolvent estimates (and consequently semigroup estimates), that are not available in [1]. In [4] an upper bound for the spectrum has been obtained under some rather restrictive assumptions on V. In [2] these assumptions were removed and an upper bound (and a lower bound) for the left margin of the spectrum has been obtained not only for (1.1) but also for (1.2) as well as for the Robin realization and for the transmission problem, continuing and relying on some one-dimensional result obtained in [12] and on the formal derivation of the relevant quasimodes obtained in [11].

The rest of this contribution is arranged as follows: in the next section we list our main results. Section 3 is devoted to the emptiness of the essential spectrum of (1.2) under some conditions on the potential. In some case we confine the essential spectrum to a certain part of the complex plain whereas in other cases we show that it is empty. The methods in Section 3 are equally applicable to (1.1) as well as to the Robin realization and to the transmission problem. In Section 4 we derive the left margin of the spectrum in the semi-classical limit, by using the same method as in [2]. In Section 5 we present some numerical results, and in the last section we emphasize some points which were not addressed within the analysis.

2 Main results

2.1 Analysis of the essential spectrum.

It is clear that there is no essential spectrum when $V \to +\infty$ as $|x| \to +\infty$ but we are motivated by the typical example $V(x) = x_1$ with $d \ge 2$, in which case V can tend to $-\infty$ as well. To treat this example, we need, in addition t (1.5), the following assumption:

Assumption 2.1. There exists R > 0 such that $K \subset B(0,R)$ and a potential V_0 satisfying

1. There exists C > 0 such that, for $\forall x \in \mathbb{R}^d$,

$$\sum_{|\alpha|=2} |\partial_x^{\alpha} V_0(x)| \le C |\nabla V_0|^{2/3}, \qquad (2.1)$$

2. There exists c > 0 such that, for $\forall x \in \mathbb{R}^d$,

$$0 < c \le |\nabla V_0(x)|, \tag{2.2}$$

and such that $V = V_0$ outside of B(0, R).

A necessary condition for V at the boundary of B(0,R) is that $\partial_{\nu}V = 0$ at some point of the boundary. If not, any C^1 extension V_0 of V inside B(0,R) has a critical point in B(0,R).

Under Assumption 2.1, we have:

Theorem 2.2. For $\# \in \{D, N\}$, and under Assumption 2.1, for any $\Lambda \in \mathbb{R}$, there exists $h_0 > 0$ such that for $h \in (0, h_0]$ the operator $\mathcal{A}_h^\#$ has no essential spectrum in $\{z \in \mathbb{C} \mid \operatorname{Re} z \leq \Lambda h^{\frac{2}{3}}\}.$

We now introduce the stronger condition (which is Assumption 2.1 with $V_0 = \mathbf{j}x_1$):

Assumption 2.3. The potential V is given in $\mathbb{R}^d \setminus K$ by

$$V(x) = \mathbf{j} x_1 + \tilde{V},$$

where $\tilde{V} \in C^1(\mathbb{R}^d)$ and satisfies $\tilde{V} \to 0$ as $|x| \to +\infty$.

Theorem 2.4. Under Assumption 2.3, the operator $\mathcal{A}_h^{\#}$ has no essential spectrum.

In other words the spectrum of the operator $\mathcal{A}_h^\#$ is either empty, or discrete. This spectral property of the operator $\mathcal{A}_h^\#$ contrasts with a continuous spectrum of the Laplace operator in the exterior of a compact set. Adding a purely imaginary potential V to the Laplace operator drastically changes its spectral properties. As a consequence, the limiting behavior of the operator $-\Delta + igV$ as $g \to 0$ is singular and violates conventional perturbation approaches that are commonly used in physical literature to deal with this problem (see discussion in [10]). This finding has thus important consequences for the theory of diffusion nuclear magnetic resonance (NMR). In particular, the currently accepted perturbative analysis paradigm has to be fundamentally revised.

Remark 2.5. It is not clear at all whether the spectrum of $-\Delta + i \mathbf{j} x_1$ remains empty if we add to it a potential V such that $(-\Delta + i \mathbf{j} x_1)^{-1}V$ is compact (for example V with compact support). In fact, one may construct a real valued $V \in C^1$ with compact support, such that $\sigma(-d^2/dx^2 + i(x+V)) \neq \emptyset$. However, if we consider the operator $A = -\Delta + i x_1 + i V(x')$ acting on \mathbb{R}^d , where $x' \in \mathbb{R}^{d-1}$ so that $x = (x_1, x')$. Since A is separable in x_1 and x' we may write

$$e^{-t\mathcal{A}} = e^{-t(-\partial^2 x_1 + ix_1)} \otimes e^{-t(-\Delta_{x'} + iV(x'))}.$$

Consequently (see also [2, Section 4]) we have

$$||e^{-tA}|| < Ce^{-t^3/12}$$
.

It follows that $\sigma(A) = \emptyset$. If consider the Dirichlet or Neumann realization of A in Ω , then we may use we may use the same procedure detailed in the proof of Theorem 2.4 to conclude that $\sigma_{ess}(A^{\#}) = \emptyset$.

I have dropped the appendix, but kept the statement that it can be done. We can go one step further and drop the entire statement, but I suggest that we still keep something in that spirit.

Remark 2.6. Let

$$V = a x_1^2 + \tilde{V} ,$$

where $\tilde{V} \in C^1$ satisfies $\tilde{V} \xrightarrow[|x| \to +\infty]{} 0$ and a > 0.

Then (with h = 1)

$$\sigma_{ess}(\mathcal{A}_1^{\#}) = \bigcup_{\substack{r \ge 0 \\ n \in \mathbb{N}}} \{e^{i\pi/4} a^{1/2} (2n-1) + r\}.$$

The proof is very similar to the proof of Theorem 2.4 and is therefore skipped. Note that, in the limit $a \to 0^+$, $\sigma_{ess}(\mathcal{A}_1^{\#})$ tends to the sector $0 \le \arg z \le \pi/4$. This is, once again, not in accordance with the guess that the essential spectrum tends to $\mathbb{R}_+ = \sigma_{ess}(-\Delta)$.

2.2 Semi-classical analysis of the bottom of the spectrum.

We begin by recalling the assumptions made in [14, 4, 2] (sometimes in a stronger form) while obtaining a bound on the left margin of the spectrum of $\mathcal{A}_h^{\#}$ in a bounded domain. In contrast, we consider here a domain which lie in the exterior of a bounded boundary $\partial\Omega$ in \mathbb{R}^d for $d \geq 2$.

First, we assume

Assumption 2.7. $|\nabla V(x)|$ never vanishes in $\overline{\Omega}$.

Note that together with Assumption 2.1 this implies that V satisfies (2.1) and (2.2) in $\overline{\Omega}$.

Let $\partial\Omega_{\perp}$ denote the subset of $\partial\Omega$ where ∇V is orthogonal to $\partial\Omega$:

$$\partial\Omega_{\perp} = \left\{ x \in \partial\Omega^{\#} : \nabla V(x) = (\nabla V(x) \cdot \vec{\nu}(x)) \,\vec{\nu}(x) \right\},\tag{2.3}$$

where $\vec{\nu}(x)$ denotes the outward normal on $\partial\Omega$ at x.

We now recall from [2] the definition of the one-dimensional complex Airy operators. To this end we let $\mathfrak{D}^{\#}$, for $\# \in \{D, N\}$, be defined in the following manner

$$\begin{cases}
\mathfrak{D}^{\#} = \{ u \in H_{loc}^{2}(\overline{\mathbb{R}_{+}}) \mid u(0) = 0 \} & \# = D \\
\mathfrak{D}^{\#} = \{ u \in H_{loc}^{2}(\overline{\mathbb{R}_{+}}) \mid u'(0) = 0 \} & \# = N .
\end{cases}$$
(2.4)

Then, we define the operator

$$\mathcal{L}^{\#}(\mathbf{j}) = -\frac{d^2}{dx^2} + i\,\mathbf{j}\,x\,,$$

whose domain is given by

$$D(\mathcal{L}^{\#}(\mathbf{j})) = H^2(\mathbb{R}^+) \cap L^2(\mathbb{R}^+; |x|^2 dx) \cap \mathfrak{D}^{\#}, \qquad (2.5)$$

and set

$$\lambda^{\#}(\mathbf{j}) = \inf \operatorname{Re} \sigma(\mathcal{L}^{\#}(\mathbf{j})). \tag{2.6}$$

Next, let

$$\Lambda_m^{\#} = \inf_{x \in \partial \Omega_{\perp}} \lambda^{\#}(|\nabla V(x)|). \tag{2.7}$$

In all cases we denote by $S^{\#}$ the set

$$S^{\#} := \{ x \in \partial \Omega_{\perp} : \lambda^{\#}(|\nabla V(x)|) = \Lambda_{m}^{\#} \}.$$
 (2.8)

When $\# \in \{D, N\}$ it can be verified by a dilation argument that, when $\mathbf{j} > 0$,

$$\lambda^{\#}(\mathbf{j}) = \lambda^{\#}(1)\,\mathbf{j}^{2/3}\,.$$
 (2.9)

Hence

$$\Lambda_m^{\#} = \lambda^{\#}(\mathbf{j}_m), \text{ with } \mathbf{j}_m := \inf_{x \in \partial \Omega_{\perp}} (|\nabla V(x)|), \qquad (2.10)$$

and $S^{\#}$ is actually independent of #:

$$S^{\#} = S := \{ x \in \partial \Omega_{\perp} : |\nabla V(x)| = \mathbf{j}_m \}.$$
 (2.11)

We next make the following additional assumption:

Assumption 2.8. At each point x of $S^{\#}$,

$$\alpha(x) = \det D^2 V_{\partial}(x) \neq 0, \qquad (2.12)$$

where V_{∂} denotes the restriction of V to $\partial\Omega$, and $D^{2}V_{\partial}$ denotes its Hessian matrix.

It can be easily verified that (2.12) implies that $S^{\#}$ is finite. Equivalently we may write

$$\alpha(x) = \prod_{i=1}^{d-1} \alpha_i(x) \neq 0,$$
(2.13a)

where $\alpha_1, \ldots, \alpha_{d-1}$ are the eigenvalues of the Hessian matrix $D^2V_{\partial}(x)$:

$$\{\alpha_i\}_{i=1}^{d-1} = \sigma(D^2 V_{\partial}),$$
 (2.13b)

where each eigenvalue is counted according to its multiplicity.

Our main result is

Theorem 2.9. Under Assumptions 2.1, 2.7 and 2.8, we have

$$\lim_{h \to 0} \frac{1}{h^{2/3}} \inf \left\{ \operatorname{Re} \, \sigma(\mathcal{A}_h^D) \right\} = \Lambda_m^D, \qquad \Lambda_m^D = \frac{|a_1|}{2} \mathbf{j}_m^{2/3}, \tag{2.14}$$

where $a_1 < 0$ is the rightmost zero of the Airy function Ai. Moreover, for every $\varepsilon > 0$, there exist $h_{\varepsilon} > 0$ and $C_{\varepsilon} > 0$ such that

$$\forall h \in (0, h_{\varepsilon}), \quad \sup_{\substack{\gamma \le \Lambda_m^D \\ \nu \in \mathbb{R}}} \| (\mathcal{A}_h^D - (\gamma - \varepsilon)h^{2/3} - i\nu)^{-1} \| \le \frac{C_{\varepsilon}}{h^{2/3}}. \tag{2.15}$$

In its first part, this result is essentially a reformulation of the result stated by the first author in [1]. Note that the second part provides, with the aid of the Gearhart-Prüss theorem, an effective bound (with respect to both t and h) of the decay of the associated semi-group as $t \to +\infty$. The theorem holds in particular in the case $V(x) = x_1$ where Ω is the complementary of a disc (and hence S^T consists of two points). Note that $\mathbf{j}_m = 1$ in this case.

Remark 2.10. A similar result can be proved for the Neumann case where (2.14) is replaced by

$$\lim_{h \to 0} \frac{1}{h^{2/3}} \inf \left\{ \operatorname{Re} \, \sigma(\mathcal{A}_h^N) \right\} = \Lambda_m^N, \qquad \Lambda_m^N = \frac{|a_1'|}{2} \mathbf{j}_m^{2/3}, \tag{2.16}$$

where $a_1'<0$ is the rightmost zero of Ai', and (2.15) is replaced by

$$\forall h \in (0, h_{\varepsilon}), \quad \sup_{\substack{\gamma \le \Lambda_m^N \\ \nu \in \mathbb{R}}} \| (\mathcal{A}_h^N - (\gamma - \varepsilon)h^{2/3} - i\nu)^{-1} \| \le \frac{C_{\varepsilon}}{h^{2/3}}. \tag{2.17}$$

One can also treat the Robin case or the transmission case (see [2]).

In the case of the Dirichlet problem, this theorem was obtained in [4, Theorem 1.1] for the interior problem and under the stronger assumption that, at each point x of \mathcal{S}^D , the Hessian of $V_{\partial} := V_{/\partial\Omega^{\#}}$ is positive definite if $\partial_{\nu}V(x) < 0$ or negative definite if $\partial_{\nu}V(x) > 0$, with $\partial_{\nu}V := \nu \cdot \nabla V$. This was extended in [2] to the interior problem without the sign condition of the Hessian. Here we prove this theorem for the exterior problem.

3 Determination of the essential spectrum

3.1 Weyl's theorem for non self-adjoint operators

For an operator which is closed but not self-adjoint, there are many possible definitions for the essential spectrum. We refer the reader to the discussion in [13] or [19] for some particular examples. In the present work, we adopt the following definition

Definition 3.1. Let A be a closed operator. We will say that $\lambda \in \sigma_{ess}(A)$ if one of the following conditions is not satisfied:

- 1. The multiplicity $\alpha(A \lambda)$ of λ is finite.
- 2. The range $R(A \lambda)$ of $(A \lambda)$ is closed.
- 3. The codimension $\beta(A-\lambda)$ of $R(A-\lambda)$ is finite.
- 4. λ is an isolated point of the spectrum.

For bounded selfadjoint operators A and B, Weyl's theorem states that if A - B = W is a compact operator, then $\sigma_{ess}(A) = \sigma_{ess}(B)$.

Once the requirement for self-adjointness is dropped, a similar result can be obtained, though not without difficulties (see [13]). We thus recall the following theorem from [19, corollary 2.2] (see also [5, corollary 11.2.3]).

Theorem 3.2. Let A be a bounded operator and B = A + W. If W is compact, then

$$\sigma_{ess}(B) = \sigma_{ess}(A)$$
.

In the present contribution we obtain the essential spectrum of $(\mathcal{A}_h^\# + 1)^{-1}$, which is clearly a bounded operator in view of the accretiveness of $\mathcal{A}_h^\#$. We follow arguments disseminated in [16] (see also [18]), that are rather standard in the self-adjoint case. The idea is to compare two bounded operators in $\mathcal{L}(L^2(\mathbb{R}^d))$. The proof is divided into two steps.

3.2 The pure Bloch-Torrey case in \mathbb{R}^d

We consider the case where $V(x) = V_0(x)$ and V_0 is given by

$$V_0(x) := \mathbf{j} x_1$$

with $\mathbf{j} \neq 0$ (assuming h = 1) and will apply the result of Subsection 3.1. The first operator is, in $\mathcal{L}(L^2(\mathbb{R}^d))$

$$A = (\mathcal{A}_0 + 1)^{-1},$$

where

$$\mathcal{A}_0 = -\Delta + i V_0.$$

Because $d \geq 2$, A is not compact but nevertheless we have

Lemma 3.3.

$$\sigma(A) = \{0\}. \tag{3.1}$$

Proof

To prove that $\sigma(A) \subseteq \{0\}$ we use the property that

$$\lambda \in \sigma(-\Delta + i V_0(x) + 1) \text{ iff } \lambda^{-1} \in \sigma(A) \setminus \{0\}$$

and similarly

$$\lambda \in \sigma_{ess}(-\Delta + i V_0(x) + 1) \text{ iff } \lambda^{-1} \in \sigma_{ess}(A) \setminus \{0\}.$$

However, it has been established in [1, 2] that the spectrum of $(-\Delta + i V_0 + 1)$ is empty and hence $\sigma(A) \subseteq \{0\}$.

To prove that $0 \in \sigma(A)$ we consider first the one-dimensional operator

$$\mathcal{L} = -\partial_{x_1}^2 + i V_0(x_1) \,,$$

defined on $D(\mathcal{L}) = H^2(\mathbb{R}) \cap L^2(\mathbb{R}; x^2 dx)$.

Since $(\mathcal{L}+1)^{-1}$ is compact, it follows that there exists $\{f_k\}_{k=1}^{+\infty} \subset L^2(\mathbb{R})$ such that $||f_k||_2 = 1$ and $\phi_k \stackrel{def}{=} (\mathcal{L} + 1)^{-1} f_k \to 0$. Let $\psi \in C_0^{\infty}(\mathbb{R}^{d-1})$ satisfy $||\psi||_2 = 1$ and further $g_k(x) = f_k(x_1)\psi(x') - \phi_k(x_1)\Delta_{x'}\psi$.

It can be easily verified that

$$Ag_k = \phi_k \psi \to 0$$
, with $||g_k||_2 \to 1$.

Hence, $0 \in \sigma(A)$ and the lemma is proved.

For a given regular set K with non empty interior, consider in $L^2(\mathbb{R}^d)$ (which is identified with $L^2(K) \oplus L^2(\Omega)$ where K is the interior of K) the operator

$$B := 0 \oplus (\mathcal{A}_{\Omega,V_0}^N + 1)^{-1}$$
.

Again we have,

$$\lambda \in \sigma(\mathcal{A}_{\Omega,V_0}^N + 1) \text{ iff } \lambda^{-1} \in \sigma(B) \setminus \{0\},$$

and similarly

$$\lambda \in \sigma_{ess}(\mathcal{A}_{\Omega,V_0}^N + 1) \text{ iff } \lambda^{-1} \in \sigma_{ess}(B) \setminus \{0\},$$

Hence it remains to prove:

Proposition 3.4.

$$\sigma_{ess}(B) = \sigma_{ess}(A)$$
.

By Weyl's theorem, it is enough to prove.

Proposition 3.5. A - B is a compact operator.

Proof. We follow the proof in [16, p. 578-579] (with suitable changes due to the non self-adjointness of A and B). To this end, we introduce the intermediate operator

$$C := (\mathcal{A}_{\dot{K}, V_0}^D + 1)^{-1} \oplus (\mathcal{A}_{\Omega, V_0}^N + 1)^{-1},$$
(3.2)

where \mathcal{A}_{K,V_0}^D is the Dirichlet realization of $(-\Delta + iV(x))$ in K.

It is clear that C-B is compact, hence it is now enough to obtain the compactness

of the operator C - A. For $f, g \in L^2(\mathbb{R}^d)$, let

$$u = Af$$
, $v = C^*q$.

We then define

$$u_{+} = u_{/\Omega}, \quad u_{-} = u_{/\dot{K}}, \quad v_{+} = v_{/\Omega}, \quad v_{-} = v_{/\dot{K}}.$$

Note that

$$v_{-} = ((\mathcal{A}_{\dot{K},V_0}^D + 1)^*)^{-1}g_{-} = (\mathcal{A}_{\dot{K},-V_0}^D + 1)^{-1}g_{-},$$

and

$$v_+ = ((\mathcal{A}_{\Omega,V_0}^N + 1)^*)^{-1}g_+ = (\mathcal{A}_{\Omega,-V_0}^N + 1)^{-1}g_+.$$

We now write

$$\langle (A-C)f,g\rangle = \langle u, \left((\mathcal{A}_{\dot{K},V_0}^D + 1) \oplus (\mathcal{A}_{\Omega,V_0}^N + 1) \right)^* v \rangle - \langle (\mathcal{A}_0 + 1)u, v \rangle$$

$$= \langle u_+, (-\Delta)v_+ \rangle_{L^2(\Omega)} + \langle u_-, (-\Delta)v_- \rangle_{L^2(\dot{K})}$$

$$- \langle (-\Delta)u_+, v_+ \rangle_{L^2(\Omega)} - \langle (-\Delta)u_-, v_- \rangle_{L^2(\dot{K})}.$$

As v_- satisfies a Dirichlet condition on $\Gamma = \partial K = \partial \Omega$ and v_+ satisfies a Neumann condition we obtain via integration by parts

$$\langle (A - C)f, g \rangle = \int_{\Gamma} \left(u_{-} \overline{\partial_{\nu} v_{-}} - \partial_{\nu} u_{+} \overline{v_{+}} \right) ds.$$
 (3.3)

To complete the proof we notice that by Sobolev embedding and the boundedness of the trace operators we have for some compact \tilde{K} such that $K \subset \dot{\tilde{K}}$ and some constants $C_{\tilde{K}}$, $C'_{\tilde{K}}$

$$\begin{aligned} |\langle (A-C)f,g\rangle| &\leq C_{\tilde{K}} \left(\|u_{+}\|_{H^{3/2}(\dot{\tilde{K}}\backslash K)} + \|u_{-}\|_{H^{3/2}(\dot{K})} \right) \left(\|v_{+}\|_{H^{2}(\dot{\tilde{K}}\backslash K)} + \|v_{-}\|_{H^{2}(\dot{K})} \right) \\ &\leq C_{\tilde{K}}' \|u\|_{H^{3/2}(\dot{\tilde{K}})} \|g\|_{2} \,. \end{aligned}$$

Hence,

$$\|(A-C)f\|_2 \le C'_{\tilde{K}} \|Af\|_{H^{3/2}(\dot{\tilde{K}})}. \tag{3.4}$$

Let $\{f_k\}_{k=1}^{\infty} \subset L^2(\mathbb{R}^d)$ satisfy $||f_k|| \leq 1$ for all $k \in \mathbb{N}$. By the boundedness of A in $\mathcal{L}(L^2(\mathbb{R}^d), H^2(\mathbb{R}^d))$ the sequence $||Af_k||$ is bounded in $H^2(\check{K})$. By Rellich's theorem, the injection of $H^2(\check{K})$ in $H^{\frac{3}{2}}(\check{K})$ is compact. Hence there exists a subsequence $\{f_{k_m}\}_{m=1}^{\infty}$ such that $\{Af_{k_m}\}_{m=1}^{\infty}$ is a Cauchy sequence in $H^{3/2}(\check{K})$. By (3.4) $\{(A-C)f_{k_m}\}_{m=1}^{\infty}$ is a Cauchy sequence in $L^2(\mathbb{R}^d)$ and hence convergent. This completes the proof of Proposition 3.5 and hence also of Proposition 3.4.

Proof of Theorem 2.4. To prove Theorem 2.4 under Assumption 2.3 for the case $\tilde{V} \not\equiv 0$ we write, for some $\lambda \in \mathbb{C}$ with Re $\lambda < 0$

$$(-\Delta + i(V_0 + \tilde{V}) - \lambda)^{-1} = (-\Delta + iV_0 - \lambda)^{-1} [1 - i\tilde{V}(-\Delta + i(V_0 + \tilde{V}) - \lambda)^{-1}].$$

Since both $(-\Delta + i(V_0 + \tilde{V}) - \lambda)^{-1} : L^2(\Omega) \to H^2(\Omega)$ and $(-\Delta + iV_0 - \lambda)^{-1} : L^2(\Omega) \to H^2(\Omega)$ are bounded, and since $\tilde{V} : H^2(\Omega) \to L^2(\Omega)$ is compact (as a matter of fact $\tilde{V} : H^1(\Omega) \to L^2(\Omega)$ is compact as well), it follows by Theorem 3.2 that the essential spectrum of $(-\Delta + i(V_0 + \tilde{V}) - \lambda)^{-1}$ is an empty set. This completes the proof of Theorem 2.4 for the case # = N.

To prove Theorem 2.4 for the case #=D we may follow the same procedure as in Proposition 3.5 to obtain a slightly different compact trace operator, or apply the following simple argument: Let R be sufficiently large so that $K \subset B(0,R)$. Let $\mathcal{A}^D_{B(0,R)\backslash K}$ denote the Dirichlet realization of \mathcal{A} in $B(0,R)\backslash K$. By Proposition 3.5, the operators $(\mathcal{A}^N_{\mathbb{R}^d\backslash B(0,R)}+1)^{-1}\oplus (\mathcal{A}^D_{B(0,R)\backslash K}+1)^{-1}$ and $(\mathcal{A}^D_{\Omega}+1)^{-1}$, both in $\mathcal{L}(L^2(\Omega))$, differ by a compact operator. Hence, as

$$\sigma_{ess} \left((\mathcal{A}^N_{\mathbb{R}^d \setminus B(0,R)} + 1)^{-1} \oplus (A^D_{B(0,R) \setminus K} + 1)^{-1} \right) = \emptyset,$$

we obtain that $\sigma_{ess}((A_{\Omega}^{D}+1)^{-1})=\emptyset$ as well.

Remark 3.6. An essentially identical proof permits the comparison of the essential spectrum of the two exterior problems $(-\Delta+iV_1)^{\sharp}$ in $\Omega_1=\mathbb{R}^d\backslash K_1$ (with $\#\in\{D,N\}$) and $(-\Delta+iV_2)^{\flat}$ in $\Omega_2=\mathbb{R}^d\backslash K_2$ (with $\flat\in\{D,N\}$) under the condition that $V_1=V_2$ outside a large open ball containing K_1 and K_2 .

Proof of Theorem 2.2. Since the proof relies on semi-classical analysis, we reintroduce the parameter h (we no longer assume h=1). Under Assumption 2.1 there exists R>0 such that $K\subset B(0,R)$ and a potential V_0 satisfying Assumptions (2.1) and (2.2) in \mathbb{R}^d and such that $V\equiv V_0$ in $\mathbb{R}^d\setminus B(0,R)$. By Remark 3.6 we need only consider the case when $K=\emptyset$, with V satisfying (2.1) and (2.2) in \mathbb{R}^d .

We use the same framework as in [14, 2]. We cover \mathbb{R}^d by balls $B(a_j, h^{\rho})$ of size h^{ρ} $(\frac{1}{3} < \rho < \frac{2}{3})$ and consider an associated partition of unity $\chi_{j,h}$ such that

- $\bullet \sum_{j \in \mathcal{J}_i(h)} \chi_{j,h}(x)^2 = 1,$
- supp $\chi_{j,h} \subset B(a_j(h), h^{\rho})$,
- For $|\alpha| \le 2$, $\sum_{j} |\partial^{\alpha} \chi_{j,h}(x)|^2 \le C_{\alpha} h^{-2|\alpha|\varrho}$.

 Λ being given, we construct the approximate resolvent $(A_h - z)$ (with Re $z \leq \Lambda h^{\frac{2}{3}}$) by

$$\mathcal{R}_h := \sum_{j \in \mathcal{J}} \chi_{j,h} (\mathcal{A}_{j,h} - z)^{-1} \chi_{j,h}.$$

We then use the uniform estimate [14]:

$$\sup_{\text{Re } z \le \omega h^{\frac{2}{3}}} \| (\mathcal{A}_{j,h} - z)^{-1} \| \le C_{\omega} [\mathbf{j}h]^{-\frac{2}{3}},$$
 (3.5)

where $\mathbf{j} = |\nabla V(a_j)|, C_{\omega}$ is independent of $j, h \in (0, h_0]$ and

$$A_{j,h} := -h^2 \Delta + i V_0(a_j) + i \nabla V_0(a_j) \cdot (x - a_j)$$
(3.6)

is the linear approximation of A_h at the point a_j . As in [14, 2], we then get

$$\mathcal{R}_h \circ (\mathcal{A}_h - z) = I + \mathcal{E}(h) \,, \tag{3.7}$$

where

$$\mathcal{E}(h) = \sum_{j \in \mathcal{J}} \chi_{j,h} i \left(V_0 - V_0(a_j) - \nabla V_0(a_j) \cdot (x - a_j) \right) (\mathcal{A}_{j,h} - z)^{-1} \chi_{j,h} - h^2 [\Delta, \chi_{j,h}] (\mathcal{A}_{j,h} - z)^{-1} \chi_{j,h}.$$

The estimation of the second term in the sum can be done in precisely the same manner as in [14]. For the first term we have by (2.1)

$$\|\chi_{j,h}(V_0 - V_0(a_j) - \nabla V_0(a_j) \cdot (x - a_j))(A_{j,h} - z)^{-1}\chi_{j,h}\| \le C_{\omega}h^{2\rho - 2/3}$$
.

By the above and [14]

$$\|\mathcal{E}(h)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} = \mathcal{O}(h^{2-2\rho-\frac{2}{3}}) + \mathcal{O}(h^{2\rho-\frac{2}{3}}). \tag{3.8}$$

To obtain (3.8), use has been made of (2.1), (2.2) (of Assumption 2.7) which permit the use of (3.5). The bound on $|D^2V_0|/|\nabla V_0|^{2/3}$ is necessary in order to estimate the error in the linear approximation of V in the ball $B(a_j, h^{\rho})$. Note that the cardinality of $\mathcal{J}_i(h)$ is now infinite, but it has been established in [2] that the cardinality of the balls $B(a_k, 2h^{\rho})$ intersecting a given $B(a_j, h^{\rho})$ is uniformly bounded in j, h. By (3.8) $I + \mathcal{E}(h)$ is invertible for sufficiently small h. Hence, by (3.7) we have that

$$\sup_{\operatorname{Re} z \le \Lambda h^{\frac{2}{3}}} \| (\mathcal{A}_h - z)^{-1} \| \le C \sup_{\operatorname{Re} z \le \Lambda h^{\frac{2}{3}}} \| \mathcal{R}_h \| \le \frac{C_{\Lambda}}{h^{2/3}},$$

where c_0 is the lower bound on $|\nabla V_0|$ given in (2.2). We may now conclude that for any Λ , the spectrum (including the essential spectrum) of $\mathcal{A}_h = -h^2\Delta + iV$ in \mathbb{R}^d is contained in $\{z \in \mathbb{C} \mid \operatorname{Re} z \geq \Lambda[c_0 h]^{\frac{2}{3}}\}$ for h small enough.

4 The left margin of the spectrum

This section is devoted to the proof of Theorem 2.9. As the proof is very similar to the proof in a bounded domain [2], and therefore we bring only its main ingredients.

4.1 Lower bound

By lower bound, we mean

$$\underline{\lim_{h \to 0}} \frac{1}{h^{2/3}} \inf \left\{ \operatorname{Re} \, \sigma(\mathcal{A}_h^D) \right\} \ge \Lambda_m^{\#}, \tag{4.1}$$

where Λ_m^D is given in (2.14) and Λ_m^N in (2.16). .

We keep the notation of [2, Section 6]. For some $1/3 < \varrho < 2/3$ and for every $h \in (0, h_0]$, we choose two sets of indices $\mathcal{J}_i(h)$, $\mathcal{J}_{\partial}(h)$, and a set of points

$$\{a_j(h) \in \Omega : j \in \mathcal{J}_i(h)\} \cup \{b_k(h) \in \partial\Omega : k \in \mathcal{J}_\partial(h)\},$$
 (4.2a)

such that $B(a_i(h), h^{\varrho}) \subset \Omega$,

$$\bar{\Omega} \subset \bigcup_{j \in \mathcal{J}_i(h)} B(a_j(h), h^{\varrho}) \cup \bigcup_{k \in \mathcal{J}_{\partial}(h)} B(b_k(h), h^{\varrho}), \qquad (4.2b)$$

and such that the closed balls $\bar{B}(a_j(h), h^{\varrho}/2)$, $\bar{B}(b_k(h), h^{\varrho}/2)$ are all disjoint.

Now we construct in \mathbb{R}^d two families of functions

$$(\chi_{j,h})_{j\in\mathcal{J}_i(h)}$$
 and $(\zeta_{j,h})_{j\in\mathcal{J}_\partial(h)}$, (4.2c)

and a function $\chi_{R,h}$ such that, for every $x \in \bar{\Omega}$,

$$\sum_{j \in \mathcal{J}_i(h)} \chi_{j,h}(x)^2 + \sum_{k \in \mathcal{J}_\partial(h)} \zeta_{k,h}(x)^2 = 1, \qquad (4.2d)$$

and such that

- Supp $\chi_{j,h} \subset B(a_j(h), h^{\varrho})$ for $j \in \mathcal{J}_i(h)$,
- Supp $\zeta_{i,h} \subset B(b_i(h), h^{\varrho})$ for $j \in \mathcal{J}_{\partial}$,
- $\chi_{j,h} \equiv 1$ (respectively $\zeta_{j,h} \equiv 1$) on $\bar{B}(a_j(h), h^{\varrho}/2)$ (respectively $\bar{B}(b_j(h), h^{\varrho}/2)$).

To verify that the approximate resolvent constructed in the sequel satisfies the boundary conditions on $\partial\Omega$, we require in addition that

$$\left. \frac{\partial \zeta_{k,h}}{\partial \nu} \right|_{\partial \Omega} = 0 \tag{4.3}$$

for # = N.

Note that, for all $\alpha \in \mathbb{N}^n$, we can assume that there exist positive h_0 and C_{α} , such that, $\forall h \in (0, h_0], \forall x \in \overline{\Omega}$,

$$|\partial^{\alpha} \chi_{R,h}|^2 + \sum_{j} |\partial^{\alpha} \chi_{j,h}(x)|^2 \le C_{\alpha} h^{-2|\alpha|\varrho} \quad \text{and} \quad \sum_{j} |\partial^{\alpha} \zeta_{j,h}(x)|^2 \le C_{\alpha} h^{-2|\alpha|\varrho}. \tag{4.4}$$

We now define the approximate resolvent as in [2]

$$\mathcal{R}_h = \sum_{j \in \mathcal{J}_i(h)} \chi_{j,h} (\mathcal{A}_{j,h} - \lambda)^{-1} \chi_{j,h} + \sum_{j \in \mathcal{J}_{\partial}(h)} \eta_{j,h} R_{j,h} \eta_{j,h}, \qquad (4.5)$$

where $R_{j,h}$ is given by [2, Eq. (6.14)], and $\eta_{j,h} = \mathbf{1}_{\Omega}\zeta_{j,h}$. As in (3.7) we write

$$\mathcal{R}_h \circ (\mathcal{A}_h - z) = I + \mathcal{E}(h), \qquad (4.6)$$

where

$$\mathcal{E}(h) = \sum_{j \in \mathcal{J}} \chi_{j,h} (\mathcal{A}_h - \mathcal{A}_{j,h}) (\mathcal{A}_{j,h} - z)^{-1} \chi_{j,h}
-h^2 [\Delta, \chi_{j,h}] (\mathcal{A}_{j,h} - z)^{-1} \chi_{j,h}
+ \sum_{j \in \mathcal{J}_{\partial}(h)} (\mathcal{A}_h - z) \eta_{j,h} R_{j,h} \eta_{j,h} .$$
(4.7)

The estimate of the first sum can be now made in the same manner as in the proof of Theorem 2.2, whereas control of the second sum can be achieved as in [2]. We may thus conclude that for any $\epsilon > 0$ there exists $C_{\epsilon} > 0$ such that for sufficiently small h

$$\sup_{\text{Re } z \le h^{2/3}(\Lambda_m^{\#} - \epsilon)} \|\mathcal{E}(h)\| \le C \left(h^{2 - 2\rho - \frac{2}{3}} + h^{2\rho - \frac{2}{3}} \right).$$

Since for sufficiently small h $I + \mathcal{E}$ becomes invertible, we can now use (4.6) to conclude that for any $\epsilon > 0$ there exists $C_{\epsilon} > 0$ such that for sufficiently small h

$$\sup_{\operatorname{Re} z \le h^{2/3}(\Lambda_m^{\#} - \epsilon)} \| (\mathcal{A}_h - \lambda)^{-1} \| \le \frac{C_{\epsilon}}{h^{2/3}}.$$

This completes the proof of (4.1).

4.2 The proof of upper bounds

To prove that

$$\overline{\lim_{h\to 0}} \frac{1}{h^{2/3}} \inf \left\{ \operatorname{Re} \, \sigma(\mathcal{A}_h^{\#}) \right\} \leq \Lambda_m^{\#},$$

we use the same procedure presented in [2, Section 7]. The only thing we care to mention is that to estimate the contribution of the interior of Ω (i.e. the first sum in (4.5) and (4.7)) we use the same approach as in the proof of Theorem 2.2. The rest of the proof, being precisely the same as in [2, Section 7] is skipped.

5 Numerical illustration

In this section, we provide a numerical evidence for the existence of a discrete spectrum of the Bloch-Torrey operator $\mathcal{A}_h^N = -h^2\Delta + ix_1$ in the case of the exterior of the unit disk: $\Omega_{\infty} = \{x \in \mathbb{R}^2 : |x| > 1\}$. In contrast to the remaining part of this note, this section relies on numerics and does not pretend for a mathematical rigor: it only serves for illustration purposes.

Since a numerical construction of the operator \mathcal{A}_h^N is not easily accessible for an unbounded domain, we consider the operator $\mathcal{A}_{h,R}^N = -h^2\Delta + ix_1$ in a circular annulus $\Omega_R = \{x \in \mathbb{R}^2 : 1 < |x| < R\}$ with two radii 1 and R. As $R \to +\infty$, the bounded domain Ω_R approaches to the exterior of the disk Ω_∞ . We set Neumann boundary condition at the inner circle and the Dirichlet boundary condition at the outer circle. Given that Ω_R is a bounded domain, the operator $\mathcal{A}_{h,R}^N$ has a discrete spectrum (as ix_1 is a bounded perturbation of the Laplace operator). The operator $\mathcal{A}_{h,R}$ can be represented via projections onto the Laplacian eigenbasis by an infinite-dimensional matrix $-h^2\Lambda + i\mathcal{B}$, where the diagonal matrix Λ is formed by Laplacian eigenvalues and the elements of the matrix \mathcal{B} are the projections of x_1 onto two Laplacian eigenfunctions (see [6, 7, 8, 11] for details). In practice, the

matrix $-h^2\Lambda + i\mathcal{B}$ is truncated and then numerically diagonalized, yielding a well-controlled approximation of eigenvalues of the operator $\mathcal{A}_{h,R}^N$, for fixed h and R. For convenience, the eigenvalues are ordered according their increasing real part.

As shown in [11], for small enough h, the quasimodes of the operator $\mathcal{A}_{h,R}^N$ are localized near the boundary of the annulus, i.e., near two circles. The quasimodes that are localized near the inner circle are almost independent of the location of the outer circle. Since the spectrum of the operator \mathcal{A}_h^N in the limiting (unbounded) domain Ω_{∞} is discrete, some eigenvalues of $\mathcal{A}_{h,R}^N$ are expected to converge to that of \mathcal{A}_h^N as R increases.

Table 1 shows several eigenvalues of the operator $\mathcal{A}_{h,R}^N$ as the outer radius R grows. The symmetry of the domain implies that if λ is an eigenvalue, then the complex conjugate $\bar{\lambda}$ is also an eigenvalue. For this reason, we only present the eigenvalues with odd indices with positive imaginary part. One can see that the eigenvalues λ_1 , λ_3 and λ_7 are almost independent of R. These eigenvalues correspond to the eigenmodes localized near the inner circle. We interpret this behavior as the convergence of the eigenvalues to that of the operator \mathcal{A}_h^N for the limiting (unbounded) domain Ω_{∞} . In contrast, the imaginary part of the eigenvalues λ_5 and λ_9 grows almost linearly with R, as expected from the asymptotic behavior reported in [11]. These eigenvalues correspond to the eigenmodes localized near the outer circle and thus diverge as the outer circle tends to infinity $(R \to +\infty)$. These numerical results illustrate the expected behavior of the spectrum. To illustrate the quality of the numerical computation, we also present in Table 1 the approximate eigenvalues based on their asymptotics derived in [11]:

$$\lambda_{\text{app}}^{N(n,k)} = i + h^{2/3} |a'_n| e^{\pi i/3} + h(2k-1) \frac{e^{-\pi i/4}}{\sqrt{2}} + h^{4/3} \frac{e^{\pi i/6}}{2|a'_n|} + O(h^{5/3}),$$

$$\lambda_{\text{app}}^{D(n,k)} = iR + h^{2/3} |a_n| e^{-\pi i/3} + h(2k-1) \frac{e^{-\pi i/4}}{\sqrt{2R}} + O(h^{5/3}),$$
(5.1)

where a_n and a'_n are the zeros of the Airy function and its derivative, respectively. Note that $\lambda_{\text{app}}^{N(n,k)}$ corresponds to the inner circle of radius 1 where Neumann boundary condition is prescribed, whereas $\lambda_{\text{app}}^{D(n,k)}$ corresponds to the outer circle of radius R where we impose a Dirichlet boundary condition. These approximate eigenvalues (truncated at $O(h^{5/3})$) show an excellent agreement with the numerically computed eigenvalues of the operator $\mathcal{A}_{h,R}^N$. This agreement confirms the accuracy of both the numerical procedure and the asymptotic formulas (5.1).

6 Conclusion

While we have confined the discussion in this work to Dirichlet and Neumann boundary conditions for simplicity, we could have also treated the Robin case or the transmission case (see [2]) with $\Omega^+ = \mathbb{R}^d \setminus \overline{\Omega}^-$. Note that we do not assume that K is connected. In the case of the Dirichlet problem, the main theorem was obtained in [4, Theorem 1.1] under the stronger assumption that, at each point x of \mathcal{S}^D , the Hessian of $V_{\partial} := V_{/\partial\Omega}$ is positive definite if $\partial_{\nu}V(x) < 0$ or negative definite if

$\lambda_n \setminus R$	1.5	2	3
λ_1	0.0250 + 1.0318i	0.0250 + 1.0317i	0.0251 + 1.0315i
$\lambda_{ m app}^{N(1,1)}$	0.0251 + 1.0317i	0.0251 + 1.0317i	0.0251 + 1.0317i
λ_3	0.0409 + 1.0160i	0.0409 + 1.0160i	0.0410 + 1.0158i
$\lambda_{ m app}^{N(1,3)}$	0.0411 + 1.0157i	0.0411 + 1.0157i	0.0411 + 1.0157i
λ_5	0.0501 + 1.4157i	0.0497 + 1.9162i	0.0498 + 2.9161i
$\lambda_{ m app}^{D(1,1)}$	0.0500 + 1.4157i	0.0496 + 1.9162i	0.0491 + 2.9167i
λ_7	0.0567 + 1.0003i	0.0567 + 1.0003i	0.0560 + 1.0000i
$\lambda_{ m app}^{N(1,5)}$	0.0571 + 0.9997i	0.0571 + 0.9997i	0.0571 + 0.9997i
λ_9	0.0635 + 1.4026i	0.0612 + 1.9048i	0.0593 + 2.9065i
$\lambda_{ m app}^{D(1,3)}$	0.0631 + 1.4027i	0.0609 + 1.9049i	0.0583 + 2.9075i

Table 1: Several eigenvalues of the operator $\mathcal{A}_{h,R}^N$ in the circular annulus $\Omega_R = \{x \in \mathbb{R}^2 : 1 < |x| < R\}$ computed numerically by diagonalizing the truncated matrix representation $-h^2\Lambda + i\mathcal{B}$, for h = 0.008 and R = 1.5, 2, 3. For comparison, gray shadowed lines show the approximate eigenvalues from Eqs. (5.1).

 $\partial_{\nu}V(x) > 0$, with $\partial_{\nu}V := \nu \cdot \nabla V$. This additional assumption reflects some technical difficulties in the proof, that was overcome in [2] by using tensor products of semigroups, a point of view that was missing in [4].

This generalization allows us to obtain the asymptotics of the left margin of $\sigma(\mathcal{A}_h^{\#})$, for instance, when $V(x_1, x_2) = x_1$ and Ω is the exterior of a disk, where the above assumption is not satisfied.

For this particular potential, an extension to the case when Ω is unbounded is of significant interest in the physics literature [10].

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