TITCHMARSH–WEYL THEORY FOR SCHRÖDINGER OPERATORS ON UNBOUNDED DOMAINS

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Abstract. In this paper it is proved that the complete spectral data of self-adjoint Schrödinger operators on unbounded domains can be described with an associated Dirichlet-to-Neumann map. In particular, a characterization of the isolated and embedded eigenvalues, the corresponding eigenspaces, as well as the continuous and absolutely continuous spectrum in terms of the limiting behaviour of the Dirichlet-to-Neumann map is obtained. Furthermore, a sufficient criterion for the absence of singular continuous spectrum is provided. The results are natural multidimensional analogs of classical facts from singular Sturm–Liouville theory.

1. Introduction

The Titchmarsh–Weyl m-function associated with a Sturm–Liouville differential expression plays a fundamental role in the direct and inverse spectral theory of the corresponding ordinary differential operators. It was introduced by H. Weyl in his famous work [53] and was further studied by E. C. Titchmarsh in [51], who investigated the analytic nature of this function as well as its connection to the spectrum. For a one-dimensional Schrödinger differential expression $-\frac{d^2}{dx^2} + q$ on the half-line $(0, \infty)$ with a bounded, real-valued potential $q$ the Titchmarsh–Weyl m-function $m(\cdot)$ may be defined as

$$m(\lambda) f_\lambda(0) = f_\lambda'(0), \quad \lambda \in \mathbb{C} \setminus \mathbb{R},$$

where $f_\lambda$ is the unique solution in $L^2(0, \infty)$ of the equation $-f'' + qf = \lambda f$; equivalently $m(\lambda)$ combines two fundamental solutions to a solution in $L^2(0, \infty)$. The outstanding role of the function $\lambda \mapsto m(\lambda)$ in the direct and inverse spectral theory of the associated selfadjoint operators is due to the celebrated fact that the complete spectral data is encoded and can be recovered from the knowledge of $m(\cdot)$; cf. [18, 51]. Therefore the Titchmarsh–Weyl m-function became an indispensable tool in the spectral analysis of Sturm–Liouville differential operators, as well as more general Hamiltonian and canonical systems; for a small selection from the vast number of contributions see, e.g., [4, 6, 14, 19, 26, 30, 35, 36, 47, 48] for direct spectral problems and [11, 12, 17, 27, 28, 29, 38, 41, 49] for inverse problems.

The aim of the present paper is to develop Titchmarsh–Weyl theory in the multidimensional setting for partial differential operators. Our focus is on selfadjoint Schrödinger operators on unbounded domains. In our main results we prove that the $A$-dependent Dirichlet-to-Neumann map $M(\lambda)$ on the boundary of the domain, as the natural multidimensional analog of the Titchmarsh–Weyl m-function, determines the spectrum of the selfadjoint Schrödinger operator $A = -\Delta + q$ with a bounded, real valued potential $q$ and a Dirichlet boundary condition uniquely. We obtain an explicit characterization of the isolated and embedded eigenvalues, the corresponding eigenspaces, and the continuous and absolutely continuous spectrum in terms of the limiting behaviour of the Dirichlet-to-Neumann map $M(\lambda)$ when $\lambda$ approaches the real axis, and we provide a sufficient criterion for the absence of singular continuous spectrum. For instance, we show that $\lambda$ is an eigenvalue...
of $A$ if and only if the strong limit $s\lim_{\eta \searrow 0} \eta M(\lambda + i\eta)$ is non-trivial. Our main results Theorem 3.2, 3.4 and 3.5 extend to other selfadjoint realizations with Neumann and more general (nonlocal) Robin boundary conditions, and also remain valid for second order, formally symmetric, uniformly elliptic differential operators under appropriate assumptions on the coefficients. In order to avoid technical complications, in this paper we discuss only the case of an exterior domain with a $C^2$-boundary. The results can be extended to Lipschitz domains and to domains with non-compact boundaries; cf. Remark 3.7. We mention that for bounded domains matters simplify essentially: In that case the spectrum of $A$ is purely discrete and it is known that the poles of the function $M(\cdot)$ coincide with the eigenvalues of $A$, see, e.g., [43] and [10].

In the recent past there has been a strong interest in combining and applying modern techniques from operator theory to partial differential equations. In the context of Titchmarsh–Weyl theory for elliptic differential equations we point out the paper [3] by W.O. Amrein and D.B. Pearson, where a typical convergence result of Titchmarsh–Weyl theory for elliptic differential equations we point out [32, 39, 52] and to the more recent contributions [2, 7, 8, 15, 16, 24, 25, 33, 34, 42, 44, 46] for other aspects of Titchmarsh–Weyl theory and spectral theory of elliptic differential operators. However, to the best of our knowledge no attempts were made so far to extend the well-known results on the characterization of the spectrum of ordinary differential operators in terms of the Titchmarsh–Weyl $q$-functions in the one-dimensional situation was [26].

Let $\Omega$ be an open subset of $\mathbb{R}^n$, $n \geq 2$, such that $\mathbb{R}^n \setminus \overline{\Omega}$ is bounded, nonempty, and has a $C^2$-boundary $\partial \Omega$; for more general settings see Remark 3.7. With $H^s(\Omega)$ and $H^s(\partial \Omega)$ we denote the Sobolev spaces of the order $s > 0$ on $\Omega$ and $\partial \Omega$, respectively. Moreover, for $u \in H^2(\Omega)$ we denote by $u|_{\partial \Omega} \in H^{1/2}(\partial \Omega)$ the trace and by $\partial_n u|_{\partial \Omega} \in H^{1/2}(\partial \Omega)$ the trace of the derivative with respect to the outer unit normal.

Let $q : \Omega \to \mathbb{R}$ be a bounded, measurable function. As usual, we define the Dirichlet operator $A$ in $L^2(\Omega)$ corresponding to the Schrödinger differential expression $-\Delta + q$ by

$$Au = -\Delta u + qu, \quad \text{dom } A = \{ u \in H^2(\Omega) : u|_{\partial \Omega} = 0 \}. \quad (2.1)$$

It is well known that $A$ is a selfadjoint operator in $L^2(\Omega)$ and that the spectrum $\sigma(A)$ of $A$ is bounded from below and accumulates to $+\infty$; cf. [22, 23, 39].

Let $\lambda$ belong to the resolvent set $\rho(A)$ of $A$ and define

$$N_\lambda = \{ u \in H^2(\Omega) : -\Delta u + qu = \lambda u \}. \quad (2.2)$$

In order to define the Dirichlet-to-Neumann map associated with the differential expression $-\Delta + q$ recall that for each $\lambda \in \rho(A)$ and each $g \in H^{3/2}(\partial \Omega)$ the boundary value problem

$$-\Delta u + qu = \lambda u, \quad u|_{\partial \Omega} = g \quad (2.3)$$

has a unique solution $u_\lambda \in H^2(\Omega)$; this follows essentially from the surjectivity of the trace map $H^2(\Omega) \ni u \mapsto u|_{\partial \Omega} \in H^{3/2}(\partial \Omega)$. Thus for $\lambda \in \rho(A)$ the Poisson operator $\gamma(\lambda)$ from $L^2(\partial \Omega)$ to $L^2(\Omega)$ given by

$$\gamma(\lambda) g = u_\lambda, \quad \text{dom } \gamma(\lambda) = H^{3/2}(\partial \Omega), \quad (2.4)$$
is well-defined, where $u_\lambda$ is the unique solution of (2.3) in $H^2(\Omega)$. We remark that $\text{ran} \gamma(\lambda) = \mathcal{N}_\lambda$ holds.

**Definition 2.1.** For $\lambda \in \rho(A)$ the Dirichlet-to-Neumann map $M(\lambda)$ in $L^2(\partial \Omega)$ is defined by

$$M(\lambda)g = \partial_n u_\lambda|_{\partial \Omega}, \quad \text{dom} \ M(\lambda) = H^{3/2}(\partial \Omega),$$

where $u_\lambda$ is the unique solution of (2.3) in $H^2(\Omega)$.

The following proposition is crucial for the proofs of the main results in the next section.

**Proposition 2.2.** The linear space

$$\text{span} \{ \mathcal{N}_\lambda : \lambda \in \mathbb{C} \setminus \mathbb{R} \}$$

is dense in $L^2(\Omega)$.

**Proof.** Let us denote by $\tilde{q}$ the extension of the potential $q$ by zero to all of $\mathbb{R}^n$. Then

$$\tilde{A}u = -\Delta u + \tilde{q}u, \quad \text{dom} \ \tilde{A} = H^2(\mathbb{R}^n),$$

is a selfadjoint operator in $L^2(\mathbb{R}^n)$ which is semibounded from below by the essential infimum of $\tilde{q}$; it is no restriction to assume that $\tilde{A}$ has a positive lower bound $\mu$.

Choose a function $\tilde{v} \in L^2(\mathbb{R}^n)$ such that $\tilde{v}|_\Omega = 0$, and define $\tilde{u}_{\lambda,\tilde{v}} := (\tilde{A} - \lambda)^{-1}\tilde{v}$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. Then the restriction $u_{\lambda,\tilde{v}}$ of $\tilde{u}_{\lambda,\tilde{v}}$ to $\Omega$ satisfies $u_{\lambda,\tilde{v}} \in H^2(\Omega)$ and $-\Delta u_{\lambda,\tilde{v}} + qu_{\lambda,\tilde{v}} = \lambda u_{\lambda,\tilde{v}}$, thus $u_{\lambda,\tilde{v}} \in \mathcal{N}_\lambda$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Let $u \in L^2(\Omega)$ be orthogonal to $\mathcal{N}_\lambda$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and let $\tilde{u}$ denote the extension by zero of $u$ to $\mathbb{R}^n$. Then, in particular,

$$0 = (u_{\lambda,\tilde{v}}, \tilde{u}, (\tilde{A} - \lambda)^{-1}\tilde{v})_{L^2(\mathbb{R}^n)} = ((\tilde{A} - \lambda)^{-1}\tilde{u}, \tilde{v})_{L^2(\mathbb{R}^n)}$$

for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$, where $(\cdot, \cdot)$ and $(\cdot, \cdot)_{L^2(\mathbb{R}^n)}$ are the inner products in $L^2(\Omega)$ and $L^2(\mathbb{R}^n)$, respectively. Since this identity holds for an arbitrary $\tilde{v} \in L^2(\mathbb{R}^n)$ with $\tilde{v}|_\Omega = 0$, it follows

$$(\tilde{A} - \lambda)^{-1}\tilde{u} = 0 \quad \text{on} \quad \mathbb{R}^n \setminus \Omega$$

for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Following an idea of [5, Section 3] we consider the semigroup $T(t) = e^{-t\tilde{A}^{1/2}}$, $t \geq 0$, which is generated by the square root of the uniformly positive operator $\tilde{A}$. Then $t \mapsto T(t)\tilde{u}$ is twice differentiable and we have

$$\frac{d^2}{dt^2}T(t)\tilde{u} = \tilde{A}T(t)\tilde{u}$$

for $t > 0$, which implies

$$\left(-\frac{\partial^2}{\partial x^2} - \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2} + \tilde{q}(x)\right)T(t)\tilde{u}(x) = 0, \quad x \in \mathbb{R}^n, t > 0,$$

in the distributional sense. In particular, by elliptic regularity, $(x, t) \mapsto T(t)\tilde{u}(x)$ belongs locally to $H^2$ on $\mathbb{R}^n \times (0, \infty)$. Moreover, Stone’s formula for the spectral measure $E(\cdot)$ of $\tilde{A}$ and (2.7) yield that

$$E((a, b)\tilde{u}) = \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \int_a^b \left((\tilde{A} - (y - i\varepsilon))^{-1}\tilde{u} - (\tilde{A} - (y + i\varepsilon))^{-1}\tilde{u}\right) dy$$
vanishes on $\mathbb{R}^n \setminus \Omega$ for all $a < b$ such that $a, b$ are no eigenvalues of $\tilde{A}$. Consequently we have

$$T(t)\tilde{u} = \int_\mu e^{-t\lambda}dE(\lambda)\tilde{u} = 0 \quad \text{on} \quad \mathbb{R}^n \setminus \Omega$$

for each $t > 0$. Therefore the function $(x, t) \mapsto T(t)\tilde{u}(x)$ vanishes on $\mathbb{R}^n \setminus \Omega \times (0, \infty)$. From this and (2.3) it follows by a unique continuation argument that $T(t)\tilde{u}(x) = 0$ for all $(x, t) \in \mathbb{R}^n \times (0, \infty)$; see, e.g., [15] Theorem XIII.63. Thus $T(t)\tilde{u}$ vanishes identically on $\mathbb{R}^n$ for all $t > 0$ and, taking the limit $t \downarrow 0$, we obtain $\tilde{u} = 0$. This implies $u = 0$ and hence the linear space (2.6) is dense in $L^2(\Omega)$.

**Remark 2.3.** The proof of Proposition 2.2 shows that also span$\{N_\lambda : \lambda \in D\}$ is dense in $L^2(\Omega)$ with $D = \{x + iy : x \in \mathbb{R}, 0 < |y| < \varepsilon\}$ for an arbitrary $\varepsilon > 0$. In fact, with the help of Runge’s theorem it can be replaced by an arbitrary nonempty, open subset of $\rho(A)$.

**Remark 2.4.** The statement of Proposition 2.2 is equivalent to the fact that the symmetric restriction

$$Su = -\Delta u + qu, \quad \text{dom} \, S = \{u \in \text{dom} \, A : \partial_\nu u|_{\partial \Omega} = 0\},$$

of the Dirichlet operator in $L^2(\Omega)$ is simple or completely non-selfadjoint; cf. [11] Chapter VII-81] and [37]. The same property is known to hold for the minimal operator realizations of certain ordinary differential expressions which are in the limit point case at one endpoint, see [31].

3. Titchmarsh–Weyl theory for Schrödinger operators: A characterization of the Dirichlet spectrum

In this section we show how the isolated and embedded eigenvalues as well as the continuous spectrum of the Dirichlet operator $A$ in (2.1) can be recovered from the limiting behaviour of the Dirichlet-to-Neumann map $M(\lambda)$ in (2.5) when $\lambda$ approaches the real axis. Moreover, we characterize the absolutely continuous spectrum of $A$ and prove a criterion for the absence of singular continuous spectrum.

As a preparation we recall some statements on the Poisson operator $\gamma(\lambda)$ in (2.4), the Dirichlet-to-Neumann map $M(\lambda)$, and their relation to the resolvent of $A$. Their proofs are similar to the proof of [10, Lemma 2.4] and will be omitted. We also mention that in more abstract settings analog formulas are well known, see [7, 20].

**Lemma 3.1.** Let $\lambda, \zeta \in \rho(A)$, let $\gamma(\lambda), \gamma(\zeta)$ be the Poisson operators in (2.4), and let $M(\lambda), M(\zeta)$ be the Dirichlet-to-Neumann maps in (2.5). Then the following assertions hold.

(i) $\gamma(\lambda)$ is a bounded, densely defined operator from $L^2(\partial \Omega)$ to $L^2(\Omega)$. Its adjoint $\gamma(\lambda)^* : L^2(\partial \Omega) \to L^2(\Omega)$ is given by

$$\gamma(\lambda)^* u = -\partial_\nu ((A - \lambda)^{-1}u)|_{\partial \Omega}, \quad u \in L^2(\Omega).$$

(ii) The identity

$$\gamma(\lambda) = \left(1 + (\lambda - \zeta)(A - \lambda)^{-1}\right)\gamma(\zeta)$$

holds.

(iii) The relation

$$[\zeta - \lambda] \gamma(\zeta)^* \gamma(\lambda) g = M(\lambda)g - M(\zeta)^* g, \quad g \in H^{3/2}(\partial \Omega),$$

holds and $M(\overline{\lambda}) \subset M(\lambda)^*$.
(iv) $M(\lambda)$ is a densely defined, unbounded operator in $L^2(\partial \Omega)$ and satisfies

$$M(\lambda) = \text{Re } M(\zeta) - \gamma(\zeta)^* \left( (\lambda - \text{Re } \zeta) + (\lambda - \zeta)(A - \lambda)^{-1} \gamma(\zeta) \right).$$

(3.1)

In particular, the limit $\lim_{\eta \to 0} \eta M(\mu + i\eta)g$ exists in $L^2(\partial \Omega)$ for all $\mu \in \mathbb{R}$ and all $g \in H^{3/2}(\partial \Omega)$.

Observe that (3.1) also implies that the function $M(\cdot)$ is strongly analytic on $\rho(A)$. In the following we agree to say that the function $M(\cdot)$ can be continued analytically into $\lambda \in \mathbb{R}$ if and only if there exists an open neighborhood $\mathcal{O}$ of $\lambda$ in $\mathbb{C}$ such that the $L^2(\partial \Omega)$-valued function $M(\cdot)g$ can be continued analytically to $\mathcal{O}$ for all $g \in H^{3/2}(\partial \Omega)$. We say that $M(\cdot)$ has a pole at $\lambda$ if and only if there exists $g \in H^{3/2}(\partial \Omega)$ such that $M(\cdot)g$ has a pole at $\lambda$. The residual of $M(\cdot)$ at $\lambda$ is defined by

$$(\text{Res}_\lambda M)g := \text{Res}_\lambda(M(\cdot)g), \quad g \in H^{3/2}(\partial \Omega),$$

where $\text{Res}_\lambda(M(\cdot)g)$ is the usual residual of the $L^2(\partial \Omega)$-valued function $M(\cdot)g$ at $\lambda$.

In the next theorem we denote by $s\text{-}\lim$ the strong limit of an operator-valued function. Moreover, we denote by $\sigma_p(A)$ and $\sigma_c(A)$ the set of eigenvalues and the continuous spectrum of $A$, respectively. The following theorem is the multidimensional analog of the main theorem in [18] and of [35, Theorem 2], where several ODE situations were considered; see also [51]. The proof of item (i) is partly inspired by abstract considerations in [21]; the characterization of the isolated and embedded eigenvalues in the items (ii) and (iii) uses methods from the more abstract works [9] [40].

**Theorem 3.2.** Let $A$ be the selfadjoint Dirichlet operator in (2.1) and let $M(\lambda)$ be the Dirichlet-to-Neumann map in (2.5). For $\lambda \in \mathbb{R}$ the following assertions hold.

(i) $\lambda \in \rho(A)$ if and only if $M(\cdot)$ can be continued analytically into $\lambda$.

(ii) $\lambda \in \sigma_p(A)$ if and only if $s\text{-}\lim_{\eta \to 0} \eta M(\lambda + i\eta) \neq 0$. If $\lambda$ is an eigenvalue with finite multiplicity then the mapping

$$\tau : \ker(A - \lambda) \to \left\{ \lim_{\eta \to 0} \eta M(\lambda + i\eta)g : g \in H^{3/2}(\partial \Omega) \right\}, \quad u \mapsto \partial_\nu u|_{\partial \Omega},$$

(3.2)

is bijective; if $\lambda$ is an eigenvalue with infinite multiplicity then the mapping

$$\tau : \ker(A - \lambda) \to \text{cl}_\tau \left\{ \lim_{\eta \to 0} \eta M(\lambda + i\eta)g : g \in H^{3/2}(\partial \Omega) \right\}, \quad u \mapsto \partial_\nu u|_{\partial \Omega},$$

(3.3)

is bijective, where $\text{cl}_\tau$ denotes the closure in the normed space $\text{ran } \tau$.

(iii) $\lambda$ is an isolated eigenvalue of $A$ if and only if $\lambda$ is a pole of $M(\cdot)$. If $\lambda$ is an eigenvalue with finite multiplicity then the mapping

$$\tau : \ker(A - \lambda) \to \text{ran } \text{Res}_\lambda M, \quad u \mapsto \partial_\nu u|_{\partial \Omega},$$

(3.4)

is bijective; if $\lambda$ is an eigenvalue with infinite multiplicity then the mapping

$$\tau : \ker(A - \lambda) \to \text{cl}_\tau (\text{ran } \text{Res}_\lambda M), \quad u \mapsto \partial_\nu u|_{\partial \Omega},$$

(3.5)

is bijective with $\text{cl}_\tau$ as in (ii).

(iv) $\lambda \in \sigma_c(A)$ if and only if $s\text{-}\lim_{\eta \to 0} \eta M(\lambda + i\eta) = 0$ and $M(\cdot)$ cannot be continued analytically into $\lambda$.

**Proof.** (i) It follows from Lemma 3.1 (iv) that $M(\cdot)g$ is analytic on $\rho(A)$ for each $g \in H^{3/2}(\partial \Omega)$. In order to verify the other implication, note first that the identity

$$\gamma(\zeta)^*(A - z)^{-1} \gamma(\nu) = \frac{M(z)}{(z - \nu)(\zeta - z)} + \frac{M(\zeta)}{(z - \zeta)(\zeta - \nu)} - \frac{M(\nu)}{(z - \nu)(\zeta - \nu)}$$

(3.6)
holds for \( \zeta, \nu, z \in \rho(A) \) satisfying \( z \neq \nu, z \neq \overline{\zeta} \), and \( \nu \neq \overline{\zeta} \). Indeed, Lemma 3.1 (ii) together with the first statement in Lemma 3.1 (iii) implies
\[
\gamma(\zeta)^*(A - z)^{-1}\gamma(\nu) = \frac{1}{z - \nu} \left( M(z) - M(\overline{\zeta}) \right) - \frac{M(\nu) - M(\overline{\zeta})}{\zeta - \nu},
\]
and an easy computation yields \((3.6)\). Let us assume that \( M(\cdot) \) can be continued analytically to some \( \lambda \in \mathbb{R} \), that is, there exists an open neighborhood \( O \) of \( \lambda \) such that \( M(\cdot)g \) can be continued analytically to \( O \) for each \( g \in H^{3/2}(\partial \Omega) \). Choose \( a, b \in \sigma_p(A) \) with \( \lambda \in (a, b) \) and \([a, b] \subset O \). The spectral projection \( E((a, b)) \) of \( A \) corresponding to the interval \((a, b)\) is given by
\[
E((a, b)) = \lim_{\delta \to 0} \frac{1}{2\pi i} \int_a^b \left( (A - (t + i\delta))^{-1} - (A - (t - i\delta))^{-1} \right) dt,
\]
where the integral on the right-hand side converges in the strong sense. Let us fix \( \nu \in \mathbb{C} \setminus \mathbb{R} \). From \((3.6)\) and \((3.7)\) we obtain
\[
\gamma(\zeta)^* (A - z)^{-1} \gamma(\nu) = 0 \quad (3.8)
\]
for all \( g, h \in H^{3/2}(\partial \Omega) \) and all \( \zeta \in \mathbb{C} \setminus \mathbb{R}, \zeta \neq \overline{\tau} \), since \( (M(\cdot)g, h) \) admits an analytic continuation into \( O \) for all \( g, h \in H^{3/2}(\partial \Omega) \), where \( (\cdot, \cdot) \) is used for both the inner products in \( L^2(\Omega) \) and \( L^2(\partial \Omega) \). By Proposition 2.2 and Remark 2.3
\[
\text{span} \left\{ \gamma(\zeta)^* h : \zeta \in \mathbb{C} \setminus \mathbb{R}, \zeta \neq \overline{\tau}, h \in H^{3/2}(\partial \Omega) \right\}
\]
is dense in \( L^2(\Omega) \), thus \((3.8)\) implies \( E((a, b)) \gamma(\nu) = 0 \) for all \( g \in H^{3/2}(\partial \Omega) \). Since \( \nu \) was chosen arbitrarily in \( \mathbb{C} \setminus \mathbb{R} \) another application of Proposition 2.2 yields \( E((a, b)) = 0 \). This implies \( \lambda \in \rho(A) \).

(ii) We prove that the mapping \( \tau \) in \((3.3)\) is bijective for all \( \lambda \in \mathbb{R} \); from this it follows immediately that \( \lambda \) is an eigenvalue of \( A \) if and only if \( \text{s-lim}_{q \to 0} \eta M(\lambda + i\eta) \neq 0 \). Let us fix \( \lambda \in \mathbb{R} \). We prove first that the restriction \( \tau \) of the trace of the normal derivative to \( \ker(A - \lambda) \) is injective. Let \( u \in \ker(A - \lambda) \) with \( \partial_\nu u|_{\partial \Omega} = 0 \). Then, denoting the extensions by zero of \( u \) and \( q \) to all of \( \mathbb{R}^n \) by \( \tilde{u} \) and \( \tilde{q} \), respectively, we have \( \tilde{u} \in H^2(\mathbb{R}^n) \) and
\[
(-\Delta + \tilde{q} - \lambda) \tilde{u} = 0.
\]
By construction \( \tilde{u} \) vanishes on the open, nonempty set \( \mathbb{R}^n \setminus \overline{\Omega} \). Hence unique continuation implies \( \tilde{u} = 0 \); cf. [15], Theorem XIII.63]. Thus \( u = 0 \) and we have proved the injectivity of \( \tau \).

In order to prove the surjectivity of \( \tau \) note first that for each \( \zeta \in \mathbb{C} \setminus \mathbb{R} \) and each \( u \in \ker(A - \lambda) \) the identity
\[
\tau u = \partial_\nu u|_{\partial \Omega} = \partial_\nu \left( (A - \overline{\zeta})^{-1}(A - \overline{\zeta})u \right)|_{\partial \Omega} = (\overline{\zeta} - \lambda) \gamma(\zeta)^* u
\]
holds by Lemma 3.1 (i), where \( \gamma(\zeta) \) is the Poisson operator in \( (2.4) \); hence,
\[
\text{ran} \; \tau = \text{ran} \left( \gamma(\zeta)^* | \ker(A - \lambda) \right), \; \zeta \in \mathbb{C} \setminus \mathbb{R} \quad (3.9)
\]
In order to prove that \( \tau \) in \((3.3)\) is surjective, we set
\[
\mathcal{F}_\lambda := \left\{ \lim_{q \to 0} \eta M(\lambda + i\eta)g : g \in H^{3/2}(\partial \Omega) \right\}
\]
and show that
\[
\mathcal{F}_\lambda \subset \text{ran} \left( \gamma(\zeta)^* | \ker(A - \lambda) \right) \subset \mathcal{F}_\lambda, \; \zeta \in \mathbb{C} \setminus \mathbb{R} \quad (3.10)
\]
Let us fix some $\zeta \in \mathbb{C} \setminus \mathbb{R}$. If we denote by $P_{\lambda} = E(\{\lambda\})$ the orthogonal projection in $L^2(\Omega)$ onto $\ker(A - \lambda)$ then for $\nu \in \mathbb{C} \setminus \mathbb{R}$ and $g \in H^{3/2}(\partial \Omega)$ we have

$$\|\eta(A - (\lambda + i\eta))^{-1} - iP_{\lambda}\gamma(\nu)g\|^2 \geq \int_{\mathbb{R}} \left| \frac{\eta}{t - \lambda - i\eta} - i\mathbb{1}_{(\lambda)}(t) \right|^2 d(E(t)\gamma(\nu)g, \gamma(\nu)g)$$

and hence the dominated convergence theorem yields

$$\lim_{\eta \searrow 0} \eta(A - (\lambda + i\eta))^{-1}\gamma(\nu)g = iP_{\lambda}\gamma(\nu)g.$$ 

The formula (3.6) and the continuity of $\gamma(\zeta)^*$ imply

$$\lim_{\eta \searrow 0} \eta M(\lambda + i\eta)g = \lim_{\eta \searrow 0} \eta \gamma(\zeta)^*(A - (\lambda + i\eta))^{-1}\gamma(\nu)g = i\gamma(\zeta)^*P_{\lambda}\gamma(\nu)g$$

for all $\nu \neq \zeta$ and all $g \in H^{3/2}(\partial \Omega)$. Thus

$$\mathcal{F}_{\lambda} = \text{ran} \left( \gamma(\zeta)^* \upharpoonright \text{span}\{P_{\lambda}\gamma(\nu)g : \nu \in \mathbb{C} \setminus \mathbb{R}, \nu \neq \zeta, g \in H^{3/2}(\partial \Omega)\} \right).$$

(3.12)

It follows from Proposition 2.2 and Remark 2.3 that

$$\text{span}\{P_{\lambda}\gamma(\nu)g : \nu \in \mathbb{C} \setminus \mathbb{R}, \nu \neq \zeta, g \in H^{3/2}(\partial \Omega)\}$$

is dense in $\ker(A - \lambda)$, and, hence, from (3.12) and the continuity of $\gamma(\zeta)^*$ we obtain (3.10). Furthermore, with (3.9) we have $\mathcal{F}_{\lambda} \subset \text{ran} \tau \subset \overline{\mathcal{F}_{\lambda}}$. Since the closure $\text{cl}_r(\mathcal{F}_{\lambda})$ of $\mathcal{F}_{\lambda}$ in the normed space $\text{ran} \tau$ (equipped with the norm of $L^2(\partial \Omega)$) coincides with the intersection of the closure $\overline{\mathcal{F}_{\lambda}}$ (in $L^2(\partial \Omega)$) with $\text{ran} \tau$, that is, $\text{cl}_r(\mathcal{F}_{\lambda}) = \overline{\mathcal{F}_{\lambda}} \cap \text{ran} \tau$, we conclude $\text{ran} \tau = \text{cl}_r(\mathcal{F}_{\lambda})$. Therefore $\tau$ is surjective and, hence, bijective. Clearly, if dim $\ker(A - \lambda)$ is finite then equality holds in (3.11) which leads to the bijectivity of (3.2) and completes the proof of (ii).

(iii) Let $\lambda$ be an isolated point of $\sigma(A)$. Then there exists an open neighborhood $\mathcal{O}$ of $\lambda$ such that $z \mapsto (A - z)^{-1}$ is analytic on $\mathcal{O} \setminus \{\lambda\}$. Thus, by (i), $M(\cdot)$ is analytic on $\mathcal{O} \setminus \{\lambda\}$ in the strong sense. Moreover, $\lambda \in \sigma_p(A)$ and by (ii) there exists $g \in H^{3/2}(\partial \Omega)$ such that $\lim_{\eta \searrow 0} i\eta M(\lambda + i\eta)g \neq 0$. Hence $\lambda$ is a pole of $M(\cdot)$ and it follows from (3.11) and the corresponding property of the resolvent of $A$ that the order of the pole is one. Thus the limit

$$\lim_{z \to \lambda} (z - \lambda)M(z)g = \text{Res}_\lambda M(\cdot)g$$

exists for all $g \in H^{3/2}(\partial \Omega)$ and coincides with $\lim_{\eta \searrow 0} i\eta M(\lambda + i\eta)g$. Therefore (3.5) is a consequence of (3.3). Analogously, (3.3) follows from (3.2). If, conversely, $\lambda$ is a pole of $M(\cdot)$ then there exists an open neighborhood $\mathcal{O}$ of $\lambda$ such that $M(\cdot)$ is strongly analytic on $\mathcal{O} \setminus \{\lambda\}$ but not on $\mathcal{O}$. Hence, (i) implies $\lambda \in \sigma(A)$ and $\mathcal{O} \setminus \{\lambda\} \subset \rho(A)$; in particular, $\lambda$ is an eigenvalue of $A$.

(iv) Since $\sigma_c(A) = \mathbb{C} \setminus (\rho(A) \cup \sigma_p(A))$, the statement of (iv) follows immediately from (i) and (ii).}

The next theorem shows how the absolutely continuous spectrum of the Dirichlet operator $A$ in (2.4) can be expressed in terms of the limits of the function $M(\cdot)$ towards real points. The result is well known in the onedimensional setting for Sturm-Liouville differential operators. In a more abstract framework of extension theory of symmetric operators in Hilbert spaces and corresponding Weyl functions a similar result was proved in [13]. We present a somewhat more direct proof avoiding the integral representation of a Nevanlinna function. We will make use of the following lemma, which can partly be found in, e.g., the monograph [50]. Here,
if $\mu$ is a finite Borel measure on $\mathbb{R}$, we denote the set of all growth points of $\mu$ by $\text{supp} \mu$, that is,

$$\text{supp} \mu = \{ x \in \mathbb{R} : \mu((x - \varepsilon, x + \varepsilon)) > 0 \text{ for all } \varepsilon > 0 \}.$$ 

Moreover, for a Borel set $\chi \subset \mathbb{R}$ we define the absolutely continuous closure (also called essential closure) of $\chi$ by

$$\text{cl}_{ac}(\chi) := \{ x \in \mathbb{R} : |(x - \varepsilon, x + \varepsilon) \cap \chi| > 0 \text{ for all } \varepsilon > 0 \},$$

where $| \cdot |$ denotes the Lebesgue measure.

**Lemma 3.3.** Let $\mu$ be a finite Borel measure on $\mathbb{R}$ and denote by $F$ its Borel transform,

$$F(\lambda) = \int_{\mathbb{R}} \frac{1}{t - \lambda} d\mu(t), \quad \lambda \in \mathbb{C} \setminus \mathbb{R}.$$ 

Let $\mu_{ac}$ and $\mu_s$ be the absolutely continuous and singular part, respectively, of $\mu$ in the Lebesgue decomposition $\mu = \mu_{ac} + \mu_s$, and decompose $\mu_s$ into the singular continuous part $\mu_{sc}$ and the pure point part. Then the following assertions hold.

(i) $\text{supp} \mu_{ac} = \text{cl}_{ac}(\{ x \in \mathbb{R} : 0 < \text{Im} F(x + i0) < +\infty \}).$

(ii) The set $M_{ac} = \{ x \in \mathbb{R} : \text{Im} F(x + i0) = +\infty, \lim_{y \searrow 0} y F(x + iy) = 0 \}$ is a support for $\mu_{ac}$, that is, $\mu_{ac}(\mathbb{R} \setminus M_{ac}) = 0$.

**Proof.** Item (i) can be found in [50, Lemma 3.15]. In order to verify item (ii) let us set

$$(D\mu)(x) = \lim_{\varepsilon \searrow 0} \frac{\mu((x - \varepsilon, x + \varepsilon))}{2\varepsilon}$$

for all $x \in \mathbb{R}$ such that the limit exists (finite or infinite). By [50, Theorem A.38] the set $\{ x \in \mathbb{R} : (D\mu)(x) = +\infty \}$ is a support for $\mu_s$ and $(D\mu)(x) = +\infty$ implies $\text{Im} F(x + i0) = +\infty$, see [50, Theorem 3.23]. Consequently, also

$$\{ x \in \mathbb{R} : \text{Im} F(x + i0) = +\infty \}$$

is a support for $\mu_s$. Moreover, note that $i \mu(\{x\}) = \lim_{y \searrow 0} y F(x + iy)$ holds for all $x \in \mathbb{R}$; indeed,

$$\left| y F(x + iy) - i \mu(\{x\}) \right| \leq \int_{\mathbb{R}} \left| \frac{y}{t - (x + iy)} - i \mathbb{1}_{\{x\}}(t) \right| d\mu(t) \to 0, \quad y \searrow 0,$$

by the dominated convergence theorem. In particular, $\mu(\{x\}) = 0$ if and only if $\lim_{y \searrow 0} y F(x + iy) = 0$. Thus the claim of item (ii) follows. \hfill \Box

Now the absolutely continuous spectrum of $A$ can be characterized in the same form as for ordinary differential operators.

**Theorem 3.4.** Let $A$ be the selfadjoint Dirichlet operator in (2.1) and let $M(\lambda)$ be the Dirichlet-to-Neumann map in (2.5). Then the absolutely continuous spectrum of $A$ is given by

$$\sigma_{ac}(A) = \bigcup_{g \in H^{3/2}((\partial \Omega))} \text{cl}_{ac}(\{ x \in \mathbb{R} : 0 < -\text{Im} (M(x + i0)g, g) < +\infty \}).$$

(3.13)

In particular, if $a < b$ then $(a, b) \cap \sigma_{ac}(A) = \emptyset$ if and only if $\text{Im} (M(x + i0)g, g) = 0$ holds for all $g \in H^{3/2}((\partial \Omega))$ and for almost all $x \in (a, b)$.

**Proof.** Let us set

$$\mathcal{D} := \{ \gamma(\zeta)g : g \in H^{3/2}((\partial \Omega)), \zeta \in \mathbb{C} \setminus \mathbb{R} \} = \bigcup_{\zeta \in \mathbb{C} \setminus \mathbb{R}} \mathcal{N}_\zeta,$$

(3.14)
where $\mathcal{N}_C$ is defined in (2.2). By Proposition 2.2 span $\mathcal{D}$ is dense in $L^2(\Omega)$. Following standard arguments the absolutely continuous spectrum of $A$ is given by

$$
\sigma_{ac}(A) = \bigcup_{u \in L^2(\Omega)} \text{supp} \mu_{u,ac} = \bigcup_{\gamma(\zeta) \in \mathcal{D}} \text{supp} \mu_{\gamma(\zeta)g,ac}
$$

(3.15)

with $\mu_u := (E(\cdot)u, u)$ for $u \in L^2(\Omega)$, where $E(\cdot)$ denotes the spectral measure of $A$. With the help of the formula (3.1) we compute

$$
\text{Im}(M(x + iy)g, g) = -y\|\gamma(\zeta)g\|^2 - (|x - \zeta|^2 - y^2) \text{Im} \left( (A - (x + iy))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right) - 2(x - \text{Re} \gamma(\zeta)y \text{Re} \left( (A - (x + iy))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right),
$$

(3.16)

for all $x \in \mathbb{R}$, $y > 0$, $g \in H^{3/2}(\partial \Omega)$ and $\zeta \in \mathbb{C} \setminus \mathbb{R}$. Moreover,

$$
g \text{Re} \left( (A - (x + iy))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right) = \int_{\mathbb{R}} \frac{y(t-x)}{(t-x)^2 + y^2} \text{d}(E(t)\gamma(\zeta)g, \gamma(\zeta)g)
$$

converges to zero as $y \searrow 0$ by the dominated convergence theorem. Therefore (3.16) implies

$$
\text{Im}(M(x + i0)g, g) = -|x - \zeta|^2 \text{Im} \left( (A - (x + i0))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right),
$$

(3.17)

in particular,

$$
\{ x \in \mathbb{R} : 0 < -\text{Im}(M(x + i0)g, g) < +\infty \} = \{ x \in \mathbb{R} : 0 < \text{Im} \left( (A - (x + i0))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right) < +\infty \}
$$

(3.18)

holds for all $g \in H^{3/2}(\partial \Omega)$ and all $\zeta \in \mathbb{C} \setminus \mathbb{R}$. Note that the Borel transform of the measure $\mu_{\gamma(\zeta)g} = (E(\cdot)\gamma(\zeta)g, \gamma(\zeta)g)$ is given by

$$
F_{\gamma(\zeta)g}(x + iy) = \int_{\mathbb{R}} \frac{1}{t - (x + iy)} \text{d}(E(t)\gamma(\zeta)g, \gamma(\zeta)g) = \left((A - (x + iy))^{-1}\gamma(\zeta)g, \gamma(\zeta)g\right), \quad x \in \mathbb{R}, y > 0.
$$

(3.19)

Hence Lemma 3.3(i) implies

$$
\text{supp} \mu_{\gamma(\zeta)g,ac} = \text{cl}_{ac} \left( \{ x \in \mathbb{R} : 0 < -\text{Im}(M(x + i0)g, g) < +\infty \} \right) = \text{cl}_{ac} \left( \{ x \in \mathbb{R} : 0 < \text{Im} \left( (A - (x + i0))^{-1}\gamma(\zeta)g, \gamma(\zeta)g \right) < +\infty \} \right)
$$

and with the help of (3.18) we conclude

$$
\text{supp} \mu_{\gamma(\zeta)g,ac} = \text{cl}_{ac} \left( \{ x \in \mathbb{R} : 0 < -\text{Im}(M(x + i0)g, g) < +\infty \} \right).
$$

Now the assertion (3.13) follows from (3.15).

It remains to show that $(a, b) \cap \sigma_{ac}(A) = \emptyset$ if and only if $\text{Im}(M(x + i0)g, g) = 0$ for all $g \in H^{3/2}(\partial \Omega)$ and almost all $x \in (a, b)$. For abbreviation set

$$
M_{ac}(g) := \{ x \in \mathbb{R} : 0 < -\text{Im}(M(x + i0)g, g) < +\infty \}, \quad g \in H^{3/2}(\partial \Omega).
$$

If $(a, b) \cap \sigma_{ac}(A) = \emptyset$, then

$$
\emptyset = \text{cl}_{ac} (M_{ac}(g)) \cap (a, b) = \text{cl}_{ac} (M_{ac}(g) \cap (a, b))
$$

by (3.13) for each $g \in H^{3/2}(\partial \Omega)$. Therefore, for each $g$ and each $x \in (a, b)$ there exists $\varepsilon > 0$ such that

$$
|(x - \varepsilon, x + \varepsilon) \cap M_{ac}(g)| = 0.
$$

(3.20)

Note that for each $g \in H^{3/2}(\partial \Omega)$ and each $\zeta \in \mathbb{C} \setminus \mathbb{R}$ the set

$$
\{ x \in \mathbb{R} : \text{Im}(M(x + i0)g, g) = -\infty \} = \{ x \in \mathbb{R} : \text{Im} F_{\gamma(\zeta)g}(x + i0) = +\infty \}
$$

is a support for $\mu_{\gamma(\zeta)g,ac}$ and, thus, a set of Lebesgue measure zero; cf. the proof of Lemma 3.3. Hence (3.20) implies $\text{Im}(M(x + i0)g, g) = 0$ for all $g \in H^{3/2}(\partial \Omega)$ and
almost all $x \in (a,b)$. The converse implication follows immediately from \((3.13)\), since the absolutely continuous closure of a set of Lebesgue measure zero is empty. \hfill \Box

Next we formulate a sufficient criterion for the absence of singular continuous spectrum within some interval in terms of the limiting behaviour of the function $M(\cdot)$. Again the onedimensional counterpart for Sturm-Liouville operators is well known; an abstract operator theoretic version is contained in \([13]\).

\textbf{Theorem 3.5.} Let $A$ be the selfadjoint Dirichlet operator in \((2.1)\), let $M(\lambda)$ be the Dirichlet-to-Neumann map in \((2.5)\), and let $a < b$. If for each $g \in H^{3/2}(\partial \Omega)$ there exist at most countably many $x \in (a, b)$ such that

\[
\text{Im}(M(x + iy), g) \to -\infty \quad \text{and} \quad y(M(x + iy), g) \to 0 \quad \text{as} \quad y \searrow 0 \quad (3.21)
\]

then $(a, b) \cap \sigma_{ac}(A) = \emptyset$.

\textbf{Proof.} As in the proof of Theorem \(3.4\) we have

\[
\sigma_{ac}(A) = \bigcup_{\gamma(\zeta)g \in \mathcal{D}} \text{supp} \mu_{\gamma(\zeta)g, sc} \quad (3.22)
\]

with $\mathcal{D}$ defined in \((3.14)\) and $\mu_{\gamma(\zeta)g} = (E(\cdot)\gamma(\zeta)g, \gamma(\zeta)g)$. From \((3.21)\) it follows with the help of \((3.11)\) and \((3.17)\) that for each $g \in H^{3/2}(\partial \Omega)$ and each $\zeta \in \mathbb{C} \setminus \mathbb{R}$ there exist at most countably many $x \in (a, b)$ such that

\[
\text{Im} \left( (A - (x + iy))^{-1} \gamma(\zeta)g, \gamma(\zeta)g \right) \to +\infty \quad (3.23)
\]

and

\[
y \left( (A - (x + iy))^{-1} \gamma(\zeta)g, \gamma(\zeta)g \right) \to 0 \quad (3.24)
\]

as $y \searrow 0$. By Lemma \(3.9\)(ii) and \((3.19)\) the set of those $x$ satisfying \((3.23)\) and \((3.24)\) forms a support of $\mu_{\gamma(\zeta)g, sc}$. It follows that $\mu_{\gamma(\zeta)g, sc}$ has a countable support in $(a,b)$ for each $\gamma(\zeta)g \in \mathcal{D}$. Since the measures $\mu_{\gamma(\zeta)g, sc}$ do not have point masses, we have $(a,b) \cap \text{supp} \mu_{\gamma(\zeta)g, sc} = \emptyset$ for all $\gamma(\zeta)g \in \mathcal{D}$ and, hence, \((3.22)\) yields $\sigma_{ac}(A) \cap (a,b) = \emptyset$. \hfill \Box

As a corollary of the theorems of this section we provide sufficient criteria for the spectrum of the Dirichlet operator $A$ to be purely absolutely continuous or purely singularly continuous, respectively, in some interval.

\textbf{Corollary 3.6.} Let $A$ be the Dirichlet operator in \((2.1)\), let $M(\lambda)$ be the Dirichlet-to-Neumann map in \((2.5)\), and let $a < b$. Moreover, for all $x \in (a, b)$ let

\[
s_{-}\lim_{y \searrow 0} yM(x + iy) = 0.
\]

Then the following assertions hold.

(i) If for each $g \in H^{3/2}(\partial \Omega)$ there exist at most countably many $x \in (a,b)$ such that $\text{Im}(M(x + iy), g) \to -\infty$, then $\sigma(A) \cap (a,b) = \sigma_{ac}(A) \cap (a,b)$.

(ii) If $\text{Im}(M(x + iy), g) = 0$ holds for all $g \in H^{3/2}(\partial \Omega)$ and almost all $x \in (a,b)$, then $\sigma(A) \cap (a,b) = \sigma_{ac}(A) \cap (a,b)$.

\textbf{Remark 3.7.} The main results of the present paper, Theorem \(3.2\) as well as Theorem \(3.4\) and Theorem \(3.5\) remain true when the Dirichlet operator $A$ is replaced by the selfadjoint operator in $L^2(\Omega)$ subject to a Robin type boundary condition

\[
\Theta u|_{\partial \Omega} = \partial_{\nu} u|_{\partial \Omega},
\]

where $\Theta$ is a selfadjoint, bounded operator in $L^2(\partial \Omega)$, and $M(\lambda)$ is replaced by the corresponding Robin-to-Dirichlet map $M_{\Theta}(\lambda) = (\Theta - M(\lambda))^{-1}$. Moreover, the
results can be carried over to more general second order uniformly elliptic, formally symmetric differential expressions of the form

\[ \mathcal{L} = -\sum_{j,k=1}^{n} \partial_j a_{jk} \partial_k + \sum_{j=1}^{n} (a_j \partial_j - \partial_j a_j) + a \]

under suitable smoothness and boundedness conditions on the coefficients \(a_{jk}, a_j, a\), \(1 \leq j, k \leq n\), and to domains with less regular (e.g. Lipschitz) boundaries. Furthermore, it suffices to consider a local version of the Dirichlet-to-Neumann map on a part of \(\partial\Omega\); cf. [10] for more details in the case of a bounded domain \(\Omega\). Finally we remark that unbounded domains with non-compact boundaries can be treated in almost the same way.

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