KREIN'S IDENTITY AND TRACE FORMULAS FOR HALF-LINE SCHRÖDINGER OPERATORS

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ABSTRACT

We consider self-adjoint extensions of the minimal operator generated by the differential expression $\mathcal{L} = -d^2/dx^2 + V$ on the half-line $[0, \infty)$, where V is a real-valued function integrable with respect to the weight $1 + x$. The self-adjoint extensions are of Schrödinger-type and form a one-parameter family formally given by $H_\alpha = -d^2/dx^2 + V$, $\alpha \in [0, \pi)$, with the boundary condition $\sin(\alpha) f'(0) = \cos(\alpha) f(0)$ at $x = 0$. We derive a formula that relates the resolvent operator of H_α to the resolvent operator of H_0 in terms of the Jost solution corresponding to the underlying differential equation $\mathcal{L}u = zu$. Combining this resolvent formula and properties of the Jost solution, we compute the trace of the difference of the resolvents of H_α and the free operator $H_\alpha^{(0)}$ with $V \equiv 0$ in terms of the parameter α and the Jost function for $\mathcal{L}u = zu$.

DEDICATION

This thesis is dedicated to my mother, Mary Sofo, who has been a countless source of love and support.

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CHAPTER 1

INTRODUCTION

1.1. Overview

The central topic of this thesis is the family of self-adjoint operators generated by the formal differential operator

$$\mathcal{L} = -\frac{d^2}{dx^2} + V \tag{1.1}$$

acting on suitable functions on the interval $[0, \infty)$, where $V : [0, \infty) \to \mathbb{R}$, in $L^2(0, \infty)$ and it is assumed that

$$\int_0^\infty (1 + x)|V(x)|\, dx < \infty. \tag{1.2}$$

Here, $L^2(0, \infty)$ is the set of (equivalence classes of) complex-valued functions on $(0, \infty)$ which are square integrable with respect to Lebesgue measure.

These self-adjoint operators are usually called *Schrödinger operators* and play an important role in quantum mechanics where they arise in the study of Schrödinger's equation

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V\psi, \tag{1.3}$$

for the wave function $\psi = \psi(x, t)$. To obtain a self-adjoint operator H from $\mathcal{L}$, we must impose a boundary condition at $x = 0$ on functions in the domain of H. For example, by imposing the boundary condition

$$f(0) = 0, \tag{1.4}$$

we obtain a self-adjoint realization of $\mathcal{L}$ which physically corresponds to an impenetrable barrier at $x = 0$, [**10**, p. 166]. The boundary condition in (1.4) is usually called a *Dirichlet* boundary condition, and we denote the corresponding self-adjoint operator by H_0.

The function V is called the *electrostatic potential* because in physical applications, V is a smooth function and $-V'(x)$ is the force on a charged particle at x. In the special case when $V(x) = 0$ for all $x \in [0, \infty)$, there is no force on the charged particle, and the particle is called a *free* particle. In this case we use the symbol $H_0^{(0)}$ to denote the corresponding self-adjoint operator generated by $\mathcal{L}$ with the Dirichlet boundary condition (1.4).

Since H_0 and $H_0^{(0)}$ are both self-adjoint operators, any point $z \in \mathbb{C}\backslash\mathbb{R}$ belongs to their resolvent sets. That is, the operators $H_0 - zI_{L^2(0,\infty)}$ and $H_0^{(0)} - zI_{L^2(0,\infty)}$ are bijections in $L^2(0, \infty)$, so their inverses $(H_0 - zI_{L^2(0,\infty)})^{-1}$ and $(H_0^{(0)} - zI_{L^2(0,\infty)})^{-1}$ exist and are bounded operators defined on all of $L^2(0, \infty)$. Moreover, the difference of these two resolvent operators belongs to the trace class $\mathcal{B}_1(L^2(0, \infty))$, [**10**, Lemma 4.5.1 and Proposition 4.5.3]:

$$(H_0^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1} \in \mathcal{B}_1(L^2(0, \infty)), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.5}$$

and therefore has a trace equal to the sum of its eigenvalues,

$$\operatorname{tr}_{L^2(0,\infty)} \big((H_0^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1}\big) = \sum_{n=1}^{N_0} \lambda_0(z, n), \tag{1.6}$$

where $N_0 \in \mathbb{N} \cup \{\infty\}$ denotes the number of eigenvalues and $\{\lambda_0(z, n)\}_{n=1}^{N_0}$ is an enumeration of the eigenvalues of $(H_0^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1}$.

In practice, it is not possible to obtain expressions for the eigenvalues $\{\lambda_0(z, n)\}_{n=1}^{N_0}$ for general V, so other representations for the trace in (1.6) are of interest. For example, the trace in (1.6) can be computed in terms of the *Jost function* associated to $\mathcal{L}u = zu$. The assumption in (1.2) guarantees that for each $z \in \mathbb{C}\backslash[0, \infty)$, there exists a unique solution

$\theta(\zeta, \cdot\,) : [0, \infty) \to \mathbb{C}$ to $\mathcal{L}u = zu$ that satisfies

$$\theta(\zeta, x) = e^{i\zeta x}[1 + o(1)] \tag{1.7}$$

as $x \to \infty$. Here, $o(1)$ denotes a term that converges to zero as $x \to \infty$ the precise form of which is immaterial, and ζ is the unique square root of z fixed according to $\operatorname{Im}(\zeta) \geq 0$. For $z \in \mathbb{C}\backslash\mathbb{R}$, the condition in (1.7) implies $\theta(\zeta, \cdot\,) \in L^2(0, \infty)$ and the function $\theta(\zeta, \cdot\,)$ is called the *Jost solution* to $\mathcal{L}u = zu$. In turn, the function w defined in the upper half of the complex plane by

$$w(\zeta) = \theta(\zeta, 0) \tag{1.8}$$

is called the *Jost function*. The Jost function is analytic in the open upper half of $\mathbb{C}$ and it is an important function for two reasons. First, the squares of its zeros are the eigenvalues of the Schrödinger operator H_0 with Dirichlet boundary conditions (see Remark 1.46 below). Second, the trace in (1.6) can be computed in terms of the Jost function, a fact that is summarized in the following theorem.

Theorem 1.1 (Proposition 4.5.3 in [**10**]). *If V satisfies* (1.2)*, then*

$$\operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_0^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_0 - zI_{L^2(0,\infty)}\big)^{-1}\Big) = \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.9}$$

where $\dot{w}(\zeta)$ denotes the complex derivative of $w(\zeta)$ with respect to ζ.

The formula in (1.9) is called a trace formula as it provides a formula to compute the trace of the difference of resolvents in terms of other, related functions.

The Dirichlet boundary condition (1.4) is not the only boundary condition at $x = 0$ that yields a self-adjoint realization of $\mathcal{L}$. In fact, there are uncountably many boundary conditions at $x = 0$ that give rise to a self-adjoint realization of $\mathcal{L}$. These boundary conditions can be characterized in terms of a single real-valued parameter: every boundary condition of the form

$$\sin(\alpha)f'(0) = \cos(\alpha)f(0), \tag{1.10}$$

where $\alpha \in [0, \pi)$ is fixed, gives rise to a self-adjoint realization of $\mathcal{L}$, which we denote by H_α. In the case of a free particle, $V \equiv 0$, we denote the self-adjoint realization by $H_\alpha^{(0)}$. The Dirichlet boundary condition (1.4) is now a special case which comes from choosing $\alpha = 0$.

Like the Dirichlet case, for each $z \in \mathbb{C}\backslash\mathbb{R}$, the difference of the resolvent operators of $H_\alpha^{(0)}$ and H_α also belongs to the trace class $\mathcal{B}_1(L^2(0, \infty))$:

$$(H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_\alpha - zI_{L^2(0,\infty)})^{-1} \in \mathcal{B}_1(L^2(0, \infty)), \tag{1.11}$$

and then

$$\operatorname{tr}_{L^2(0,\infty)} \left((H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_\alpha - zI_{L^2(0,\infty)})^{-1}\right) = \sum_{n=1}^{N_\alpha} \lambda_\alpha(z, n), \tag{1.12}$$

where $N_\alpha \in \mathbb{N} \cup \{\infty\}$ denotes the number of eigenvalues and $\{\lambda_\alpha(z, n)\}_{n=1}^{N_\alpha}$ is an enumeration of the eigenvalues of $(H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_\alpha - zI_{L^2(0,\infty)})^{-1}$.

The individual eigenvalues $\lambda_\alpha(z, n)$ are no simpler to compute than those in the Dirichlet case, so it is of interest to have an alternative expression for the trace in (1.12). In particular, it is natural to ask if (1.9) may be generalized from the case $\alpha = 0$ to arbitrary $\alpha \in [0, \pi)$.

The Dirichlet trace formula (1.9) was generalized to arbitrary $\alpha \in [0, \pi)$ in 2011 by Demirel and Usman, [**2**]. To be precise, Demirel and Usman work with a boundary condition at $x = 0$ in the form

$$f'(0) = \gamma f(0), \tag{1.13}$$

where $\gamma \in \mathbb{R}$ is a fixed parameter. Writing $\gamma = \cot(\alpha)$, the formulation of the boundary condition in (1.13) is equivalent to the formulation of the boundary condition in (1.10) when $\alpha \neq 0$.

The arguments in [**2**] rely on the fact that $(H_{\cot^{-1}(\gamma)} - zI_{L^2(0,\infty)})^{-1}$ is an integral operator with an integral kernel that can be computed in terms of $\theta(\zeta, \cdot\,)$ and the solution $\phi(\zeta, \cdot\,) : [0, \infty) \to \mathbb{C}$ to $\mathcal{L}u = zu$ determined by the initial conditions

$$\phi(\zeta, 0) = 1 \quad \text{and} \quad \phi'(\zeta, 0) = \gamma. \tag{1.14}$$

The difference of resolvent operators $(H^{(0)}_{\cot^{-1}(\gamma)} - zI_{L^2(0,\infty)})^{-1} - (H_{\cot^{-1}(\gamma)} - zI_{L^2(0,\infty)})^{-1}$ is then also an integral operator with an integral kernel. Demirel and Usman derive properties of $\phi(\zeta, \cdot\,)$ and use them to compute the trace by integrating this integral kernel along the diagonal. This approach is a generalization of the approach used to prove Theorem 1.1 in [**10**]. The result of Demirel and Usman is summarized in the following theorem.

Theorem 1.2 (Theorem 1.1 in [**2**]). *If $\gamma \in \mathbb{R}$, then*

$$\begin{aligned} &\operatorname{tr}_{L^2(0,\infty)}\Big((H^{(0)}_{\cot^{-1}(\gamma)} - zI_{L^2(0,\infty)})^{-1} - (H_{\cot^{-1}(\gamma)} - zI_{L^2(0,\infty)})^{-1}\Big) \\ &\quad = \frac{1}{2\zeta}\left(\frac{\dot{\omega}(\zeta)}{\omega(\zeta)} + \frac{i}{\gamma - i\zeta}\right), \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{1.15}$$

where

$$\omega(\zeta) = \gamma\theta(\zeta, 0) - \theta'(\zeta, 0), \quad z = \zeta^2,\ \operatorname{Im}(\zeta) > 0,\ z \in \mathbb{C}\backslash\mathbb{R}. \tag{1.16}$$

Written explicitly in terms of $\alpha = \cot^{-1}(\gamma)$, (1.15) takes the form

$$\operatorname{tr}_{L^2(0,\infty)}\Big((H^{(0)}_{\alpha} - zI_{L^2(0,\infty)})^{-1} - (H_{\alpha} - zI_{L^2(0,\infty)})^{-1}\Big)$$

$$= \frac{\cos(\alpha)\dot{w}(\zeta) - \sin(\alpha)\dot{\theta}'(\zeta,0)}{2\zeta[\cos(\alpha)w(\zeta) - \sin(\alpha)\theta'(\zeta,0)]} + \frac{i\sin(\alpha)}{2\zeta[\cos(\alpha) - i\zeta\sin(\alpha)]}. \tag{1.17}$$

In this thesis, we derive (1.17) directly using an approach that is different from that in [**2**]. Both (1.9) and (1.17) are trace formulas for self-adjoint realizations of the same underlying differential expression. Thus, we view the trace formula problem as a problem in the theory of self-adjoint extensions. Taking the result in (1.9) for granted, our approach is to first derive a formula that relates the operator $(H_\alpha - zI_{L^2(0,\infty)})^{-1}$ to $(H_0 - zI_{L^2(0,\infty)})^{-1}$ and the operator $(H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1}$ to $(H_0^{(0)} - zI_{L^2(0,\infty)})^{-1}$. With these relations, we have

$$\begin{aligned}
&(H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_\alpha - zI_{L^2(0,\infty)})^{-1} \\
&\quad = (H_0^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1} + T_{1,\alpha}(z) + T_{2,\alpha}(z), \quad z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned} \tag{1.18}$$

where $T_{1,\alpha}(z)$ and $T_{2,\alpha}(z)$ are operators of rank one. These formulas are special cases of Krein's resolvent formula, and their application allows us to relate the trace in (1.12) to the trace for the Dirichlet boundary condition in (1.9) by

$$\begin{aligned}
&\operatorname{tr}_{L^2(0,\infty)}\big((H_\alpha^{(0)} - zI_{L^2(0,\infty)})^{-1} - (H_\alpha - zI_{L^2(0,\infty)})^{-1}\big) \\
&\quad = \operatorname{tr}_{L^2(0,\infty)}\big((H_0 - zI_{L^2(0,\infty)})^{-1} - (H_0^{(0)} - zI_{L^2(0,\infty)})^{-1}\big) \\
&\qquad + \operatorname{tr}_{L^2(0,\infty)}\big(T_{1,\alpha}(z)\big) + \operatorname{tr}_{L^2(0,\infty)}\big(T_{2,\alpha}(z)\big), \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{1.19}$$

We explicitly compute the operators $T_{1,\alpha}(z)$ and $T_{2,\alpha}(z)$ in (1.18), and we compute their traces using properties of $\theta(\zeta,\,\cdot\,)$ derived in [**10**].

In the remainder of this chapter, we recall the basic background on Sturm–Liouville operators needed to rigorously define the Schrödinger operators H_α and the Jost solution and Jost function. In Chapter 2, we recall the abstract formulation of Krein's resolvent identity which relates the resolvent operators of two self-adjoint extensions of a symmetric operator. In Section 2.2., we derive the explicit form of Krein's resolvent identity which relates $(H_\alpha - zI_{L^2(0,\infty)})^{-1}$ to $(H_0 - zI_{L^2(0,\infty)})^{-1}$ and a rank one operator in Theorem 2.13. Chapter 3 contains our main result. We recall several important properties of solutions to $\mathcal{L}u = zu$ and investigate some of their consequences in, for example, Corollary 3.4. These results are then combined with Theorem 1.1 and Theorem 2.13 to prove our main result, Theorem 3.6, which is an alternative proof of (1.17).

1.2. Background on Sturm–Liouville Operators

In this section, we recall some of the basic elements of the theory of Sturm–Liouville operators of Schrödinger-type on intervals $(a, b) \subseteq \mathbb{R}$ to be used later. By now, Sturm–Liouville theory is a well-developed subject, and this material may be found in a number of standard sources (e.g., [**6**, Chapter 15], [**7**, Chapter 9], [**8**, §8.4], and [**9**]). We closely follow the presentation of the subject given in [**6**, Chapter 15].

To define the operators we will work with, we will first recall the following definitions of sets of measure zero and the spaces $L^1_{loc}(\alpha, \beta)$, $AC[\alpha, \beta]$ and $AC_{loc}(\alpha, \beta)$. Intervals $I \subset \mathbb{R}$ of the form (α, β), $[\alpha, \beta)$, $(\alpha, \beta]$, and $[\alpha, \beta]$, with $-\infty < \alpha < \beta < \infty$ will be called *finite intervals*. If I is a finite interval, its length is denoted by $|I| = \beta - \alpha$. If $-\infty \leq a < b \leq \infty$, then a and b are called the *endpoints* of the interval (a, b).

Definition 1.3 ([**5**], p. 5–6). *A subset $N \subset \mathbb{R}$ is called a set of (Lebesgue) measure zero if for every $\varepsilon > 0$, there exists a countable collection of finite intervals $\{I_k(\varepsilon)\}_{k \in \mathcal{I}(\varepsilon)}$, with $\mathcal{I}(\varepsilon) \subseteq \mathbb{N}$ an appropriate indexing set, such that*

$$N \subseteq \bigcup_{k \in \mathcal{I}(\varepsilon)} I_k(\varepsilon) \quad \textit{and} \quad \sum_{j \in \mathcal{I}(\varepsilon)} |I_k(\varepsilon)| < \varepsilon. \tag{1.20}$$

A statement $P(x)$ about points $x \in S \subseteq \mathbb{R}$ is said to hold almost everywhere (abbreviated a.e.) in S if $P(x)$ is true for all $x \in S \backslash N$, for some set $N \subset S$ of measure zero. The fact that $P(x)$ holds almost everywhere in S, is abbreviated by writing

$$P(x) \text{ for a.e. } x \in S. \tag{1.21}$$

Definition 1.4. *Let $-\infty \leq \alpha < \beta \leq \infty$. $L^1_{loc}(\alpha, \beta)$ is the set of all (equivalence classes of) Lebesgue measurable functions $f : (\alpha, \beta) \to \mathbb{C}$ such that*

$$\int_c^d |f(x)|\, dx < \infty \text{ for all intervals } [c, d] \subset (\alpha, \beta). \tag{1.22}$$

Note that the condition $[c, d] \subset (\alpha, \beta)$ in (1.22) implies that $[c, d]$ is *compactly contained* in (α, β). If $f \in L^1(\alpha, \beta)$, then $f \in L^1_{\mathrm{loc}}(\alpha, \beta)$; the converse statement is false.

Example 1.5. *If $(\alpha, \beta) = (0, \infty)$ and*

$$f(x) = x, \quad x \in (0, \infty), \tag{1.23}$$

then $f \in L^1_{loc}(0, \infty)$ since $|f|$ is continuous, hence bounded, on any interval $[c, d] \subset (0, \infty)$. However, $f \notin L^1(0, \infty)$.

Definition 1.6 (§2.7 in [**7**], Appendix E in [**6**]). *Let $-\infty < \alpha < \beta < \infty$. A function $f : [\alpha, \beta] \to \mathbb{C}$ is absolutely continuous on $[\alpha, \beta]$ if and only if there exists a function $h \in L^1(\alpha, \beta)$ such*

$$f(x) = f(\alpha) + \int_\alpha^x h(t)\, dt, \quad x \in [\alpha, \beta]. \tag{1.24}$$

The set of all absolutely continuous functions on $[\alpha, \beta]$ is denoted by $AC[\alpha, \beta]$.

Every absolutely continuous function is continuous, so

$$AC[\alpha, \beta] \subset C[\alpha, \beta]. \tag{1.25}$$

If $f \in AC[\alpha, \beta]$, then f is differentiable almost everywhere on (α, β) by [**6**, Theorem E.1], and its derivative f' is an integrable function,

$$f' \in L^1(\alpha, \beta). \tag{1.26}$$

In fact, if f is given by (1.24), then $f' = h$ almost everywhere on (α, β). Therefore, the Fundamental Theorem of Calculus holds for absolutely continuous functions.

There is also a local notion of absolute continuity for functions on intervals of infinite length.

Definition 1.7. *Let $-\infty \leq \alpha < \beta \leq \infty$. A function $f : (\alpha, \beta) \to \mathbb{C}$ is locally absolutely continuous on (α, β) if and only if $f \in AC[c, d]$ for all $[c, d] \subset (\alpha, \beta)$ for all $[c, d] \subset (\alpha, \beta)$. The set of all locally absolutely continuous functions on (α, β) is denoted by $AC_{loc}(\alpha, \beta)$.*

If $f \in AC_{loc}(\alpha, \beta)$, then $f \in C(\alpha, \beta)$. Moreover, f is differentiable almost everywhere on (α, β), and its derivative f' is a locally integrable function,

$$f' \in L^1_{loc}(\alpha, \beta). \tag{1.27}$$

Definition 1.8 (Wronskian). *If $I \subseteq \mathbb{R}$ is an interval and $f, g : I \to \mathbb{C}$ are continuously differentiable, then the Wronskian of f with g at the point $x \in I$ is denoted by $W(f, g)(x)$ and defined to be*

$$W(f, g)(x) = f(x)g'(x) - f'(x)g(x), \quad x \in I. \tag{1.28}$$

With these preliminary definitions, we return to our discussion of some elements of Sturm–Liouville theory of Schrödinger-type operators on intervals $(a, b) \subseteq \mathbb{R}$. Throughout this section, we will assume the following hypothesis.

Hypothesis 1.9. *Suppose that $-\infty \le a < b \le \infty$. Let*

$$V \in L^1_{loc}(a,b) \text{ be real-valued a.e.} \tag{1.29}$$

and define the formal differential expression $\mathcal{L}$ on (a,b) by

$$\mathcal{L} = -\frac{d^2}{dx^2} + V(x). \tag{1.30}$$

Assuming Hypothesis 1.9, the action of the differential expression $\mathcal{L}$ on a twice differentiable function $f : (a,b) \to \mathbb{C}$ is

$$(\mathcal{L}f)(x) = -f''(x) + V(x)f(x), \tag{1.31}$$

for all $x \in (a,b)$ for which the right-hand side is well-defined.

We should note that in [**6**, Chapter 15], the function $V(x)$ is assumed to be continuous. However, this assumption is not necessary, [**9**, p. 27].

In order to use the action of $\mathcal{L}$ to define an operator in the Hilbert space $L^2(a,b)$, a domain of definition for the operator must be specified. We begin by defining the class $\mathfrak{D}(a,b)$ by

$$\mathfrak{D}(a,b) = \{f \in C_0(a,b) \,|\, f, f' \in AC_{loc}(a,b),\, \mathcal{L}f \in L^2(a,b)\}, \tag{1.32}$$

where

$$C_0(a,b) = \{f \in C(a,b) \,|\, f(x) = 0,\, x \in (a,b)\backslash[c,d], \text{ for some } [c,d] \subset (a,b)\}. \tag{1.33}$$

The operator $\mathring{H}$ is defined by

$$(\mathring{H}f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (a,b),\ f \in \operatorname{dom}(\mathring{H}) = \mathfrak{D}(a,b). \tag{1.34}$$

The operator $\mathring{H}$ is densely defined [**4**, §17.4], though this fact is not obvious, and it is a *symmetric* operator.

Definition 1.10 (Symmetric operator). *If $\mathcal{H}$ is a Hilbert space with inner product $\langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{H}}$, then a densely defined linear operator $A : \operatorname{dom}(A) \subseteq \mathcal{H} \to \mathcal{H}$ is symmetric if*

$$\langle u, Av\rangle_{\mathcal{H}} = \langle Au, v\rangle_{\mathcal{H}}, \quad u, v \in \operatorname{dom}(A). \tag{1.35}$$

To show that $\mathring{H}$ is symmetric; we integrate by parts twice:

$$\begin{aligned}
\langle f, \mathring{H} g\rangle_{L^2(a,b)} &= \int_a^b \overline{f(x)}[-f''(x) + V(x)g(x)]\,dx \\
&= -\int_a^b \overline{f(x)}g''(x)\,dx + \int_a^b \overline{f(x)}V(x)g(x)\,dx \\
&= -\overline{f(x)}g'(x)|_a^b + \int_a^b \overline{f'(x)}g'(x)\,dx + \int_a^b \overline{V(x)f(x)}g(x)\,dx \\
&= \overline{f'(x)}g(x)|_a^b - \int_a^b \overline{f''(x)}g(x)\,dx + \int_a^b \overline{V(x)f(x)}g(x)\,dx \\
&= \int_a^b \overline{-f''(x) + V(x)f(x)}g(x)\,dx \\
&= \langle \mathring{H} f, g\rangle_{L^2(a,b)}, \quad f, g \in \operatorname{dom}(\mathring{H}).
\end{aligned} \tag{1.36}$$

Note that we have used the fact that V is real-valued in (1.36).

Since $\mathring{H}$ is densely defined and symmetric, it is closable by [**7**, Lemma 2.4 (ii)]. The closure of $\mathring{H}$ is called the *minimal operator associated to $\mathcal{L}$*, and it is denoted by H_{min}:

$$H_{min} = \overline{\mathring{H}} = (\mathring{H})^{**}. \tag{1.37}$$

The operator closure in (1.37) may be computed as the double adjoint by [**7**, Lemma 2.4 (ii)]. The minimal operator is symmetric (by the remarks following [**7**, Corollary 2.2]) since it is the closure of a symmetric operator. The *maximal operator associated to $\mathcal{L}$* is denoted by H_{max} and defined explicitly by

$$(H_{max} f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (a, b), \tag{1.38}$$

$$f \in \operatorname{dom}(H_{max}) = \big\{g \in L^2(a, b) \,\big|\, g, g' \in AC_{loc}(a, b),\ \mathcal{L}g \in L^2(a, b)\big\}.$$

The maximal and minimal operators associated to $\mathcal{L}$ are adjoint to one another ([**4**, Theorem 2 in §17.4] or [**9**, Theorem 3.9]):

$$(H_{min})^* = H_{max}, \quad (H_{max})^* = H_{min}. \tag{1.39}$$

Definition 1.11. *If $A : \mathrm{dom}(A) \subseteq \mathcal{H} \to \mathcal{H}$ and $B : \mathrm{dom}(B) \subseteq \mathcal{H} \to \mathcal{H}$ are two linear operators, then B is called an extension of A if* $\mathrm{dom}(A) \subseteq \mathrm{dom}(B)$ *and*

$$Av = Bv, \quad v \in \mathrm{dom}(A). \tag{1.40}$$

In this case, A is also called a restriction of B.

We will be concerned with extensions of H_{min} that are self-adjoint, provided they exist. The next proposition shows that the action of a self-adjoint extension of H_{min} coincides with the action of H_{max}.

Proposition 1.12. *Assume Hypothesis* 1.9. *If H is a self-adjoint extension of H_{min}, then H is a restriction of H_{max}.*

Proof. Let H denote a self-adjoint extension of H_{min}, so that

$$H_{min} \subseteq H. \tag{1.41}$$

Taking the adjoint on both sides and applying [**7**, (2.28)] (which states that $B^* \subseteq A^*$ if $A \subseteq B$ for densely defined operators A and B), we obtain

$$H = H^* \subseteq H_{min}^* = H_{max}, \tag{1.42}$$

using that H is self-adjoint and the first equality in (1.39). Thus, H is a restriction of H_{max}. □

Remark 1.13. The importance of Proposition 1.12 is that it shows the action of any self-adjoint extension of H_{min} coincides with the action of H_{max}. That is, if H is a self-adjoint extension of H_{min}, then

$$(Hf)(x) = (H_{max}f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (a,b), \quad f \in \operatorname{dom}(H). \tag{1.43}$$

Therefore, a self-adjoint extension is defined by specifying its domain; the action of the self-adjoint extension on vectors in its domain is already determined by H_{max}.

Assuming H_{min} has a self-adjoint extension H, Proposition 1.12 shows that H must be a self-adjoint restriction of H_{max}. However, Proposition 1.12 does not guarantee the existence of a self-adjoint extension of H_{min}. It is natural to ask, "When does H_{min} have a self-adjoint extension?" To determine whether the symmetric operator H_{min} has self-adjoint extensions (equivalently, whether H_{max} has self-adjoint restrictions), or not, we must study properties of $\mathcal{L}$ near the endpoints of the interval (a,b).

Definition 1.14 (Regular endpoint). *The differential expression $\mathcal{L}$ is called regular at a if $a \in \mathbb{R}$ and $V \in L^1(a,c)$ for some $c \in (a,b)$. If $\mathcal{L}$ is not regular at a, $\mathcal{L}$ is called singular at a. The differential expression $\mathcal{L}$ is called regular at b if $b \in \mathbb{R}$ and $V \in L^1(c,b)$ for some $c \in (a,b)$. If $\mathcal{L}$ is not regular at b, $\mathcal{L}$ is called singular at b.*

When $\mathcal{L}$ is regular at an endpoint, more can be said about the behavior of functions in $\operatorname{dom}(H_{min})$ and $\operatorname{dom}(H_{max})$ near the regular endpoint.

Proposition 1.15 (Proposition 15.5 in [**6**]). *Assume Hypothesis 1.9, and suppose that $\mathcal{L}$ is regular at a. Then the following items hold:*

(i) If $f \in \operatorname{dom}(H_{max})$, then f and f' can be extended to continuous functions on $[a,b)$.

(ii) The set $\{(f(a), f'(a)) \in \mathbb{C}^2 \,|\, f \in \operatorname{dom}(H_{max})\}$ *is equal to* $\mathbb{C}^2$*.*

(iii) If $f \in \operatorname{dom}(H_{min})$*, then* $f(a) = f'(a) = 0$*.*

(iv) If, in addition, $\mathcal{L}$ *is regular at* b *then* $f(a) = f'(a) = f(b) = f'(b) = 0$ *for all* $f \in \operatorname{dom}(H_{min})$*.*

If a is a regular endpoint of $\mathcal{L}$, then the minimal operator may be computed directly using boundary conditions and the Wronskian by [**9**, Theorem 3.12]:

$$\begin{aligned}
&(H_{min} f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (a,b), \qquad (1.44)\\
&f \in \operatorname{dom}(H_{min}) = \Big\{ g \in \operatorname{dom}(H_{max}) \,\Big|\, g(a) = g'(a) = 0 \text{ and } \lim_{x \to b^-} W(g,h)(x) = 0 \\
&\qquad\qquad \text{for all } h \in \operatorname{dom}(H_{max}) \Big\}.
\end{aligned}$$

Definition 1.16 (Solution). *If* $z \in \mathbb{C}$ *and* $g \in L^1_{loc}(a,b)$*, then* f *is called a solution to*

$$\mathcal{L}f - zf = g \tag{1.45}$$

on (a,b) *if and only if* $f, f' \in AC_{loc}((a,b))$ *and*

$$(\mathcal{L}f)(x) - zf(x) = g(x) \text{ for a.e. } x \in (a,b). \tag{1.46}$$

We will adhere to the convention of writing $z \in \mathbb{C}$ as $z = \zeta^2$ where $\zeta \in \mathbb{C}$ is chosen to satisfy $\operatorname{Im}(\zeta) \geq 0$ throughout this thesis.

Notation 1.17. $\zeta \in \mathbb{C}$ *always denotes a complex number which satisfies* $\operatorname{Im}(\zeta) \geq 0$*.*

The next result shows that a solution to (1.45) has additional properties near a regular endpoint.

Proposition 1.18 (Theorem 9.1 in [**7**]). *Assume Hypothesis* 1.9. *Suppose* $z \in \mathbb{C}$ *and* $g \in L^1_{loc}(a,b)$. *The following items hold:*

(*i*) *If* $\mathcal{L}$ *is regular at* a *and* f *is a solution to* (1.45), *then the finite limits*

$$f(a) := \lim_{x \to a^+} f(x) \quad \textit{and} \quad f'(a) := \lim_{x \to a^+} f'(x) \tag{1.47}$$

exist. That is, f *and* f' *extend to continuous functions on* $[a,b)$. *An analogous statement holds if* $\mathcal{L}$ *is regular at* b.

(*ii*) *Let* x_0 *be a point in* (a,b) *or a regular endpoint. For each* $z = \zeta^2 \in \mathbb{C}$, *and pair of constants* $c_1, c_2 \in \mathbb{C}$, *there exists a unique solution* $f(\zeta, x)$ *to the initial-value problem*

$$\begin{cases} \mathcal{L}f - zf = g, \\ f(\zeta, x_0) = c_1, \quad f'(\zeta, x_0) = c_2, \end{cases} \tag{1.48}$$

where the prime denotes differentiation with respect to the second variable, $x \in (a,b)$. *Moreover, for any fixed* $x \in (a,b)$, $f(\zeta, x)$ *is an entire function of the variable* $z = \zeta^2$.

Remark 1.19. By item (*ii*) in Proposition 1.18, the solution space to the homogeneous differential equation

$$\mathcal{L}f = zf, \tag{1.49}$$

with $z \in \mathbb{C}$ fixed, is a two-dimensional vector space (over $\mathbb{C}$).

A pair $\{u, v\}$ of linearly independent solutions u and v to $\mathcal{L}f = zf$ is called a *fundamental system of solutions*. We can employ the Wronskian to determine if functions are linearly independent. If $W(f,g)(x_0) \neq 0$ for some $x_0 \in (a,b)$, then f and g are linearly independent. If f and g are solutions to (1.49), then their Wronskian is actually constant, and the solutions f and g are linearly independent if and only if their Wronskian is nonzero.

From the point of view of the possible existence of self-adjoint extensions of H_{min}, the importance of the differential equation (1.49) is the fact that the solutions to (1.49) which lie in $L^2(a,b)$ form the null space of $H_{max} - zI_{L^2(a,b)}$. The dimensions of the two spaces $\ker(H_{max} \pm iI_{L^2(a,b)})$ determine whether H_{min} has self-adjoint extensions, or not.

DEFINITION 1.20 (Deficiency indices). *If A is a densely defined, closed, symmetric operator in the Hilbert space $\mathcal{H}$, then the deficiency indices of A are denoted $(d_-(A), d_+(A))$, where $d_\pm(A) \in \mathbb{N}_0 \cup \{\infty\}$ and are defined by*

$$d_\pm(A) = \dim(\ker(A^* \mp iI_{\mathcal{H}})). \tag{1.50}$$

By Remark 1.19, $d_\pm(H_{min})$ are each at most two. The next result shows that $d_+(H_{min}) = d_-(H_{min})$.

PROPOSITION 1.21 (Proposition 15.4 in [**6**]). *Assume Hypothesis* 1.9. *The minimal operator H_{min} has deficiency indices $(0,0)$, $(1,1)$, or $(2,2)$.*

By von Neumann's theory of self-adjoint extensions, a symmetric operator has self-adjoint extensions if and only if its deficiency indices coincide.

THEOREM 1.22 (von Neumann, Theorem 8.6 in [**8**]). *A densely defined, closed, symmetric operator A in $\mathcal{H}$ has a self-adjoint extension if and only if its deficiency indices are equal,*

$$d_+(A) = d_-(A), \tag{1.51}$$

and A is self-adjoint if and only if $d_+(A) = d_-(A) = 0$.

Therefore, by Proposition 1.21, the minimal operator H_{min} always possesses self-adjoint extensions. If H_{min} has deficiency indices $(0,0)$, then H_{min} is self-adjoint and, therefore, has no nontrivial self-adjoint extension by [**7**, Corollary 2.2].

By Proposition 1.21, there are exactly three possibilities for the deficiency indices of H_{min}:

$$(d_-(H_{min}), d_+(H_{min})) \in \{(0,0), (1,1), (2,2)\}. \tag{1.52}$$

Next, we would like to characterize exactly when each of the three possible cases arises. The following definition, which deals with certain integrability properties of functions near an endpoint of (a,b), is a first step in this direction.

Definition 1.23. *Let $f : (a,b) \to \mathbb{C}$ be a measurable function. Then f is said to lie in L^2 near a if and only if there exists a point $c \in (a,b)$ such that*

$$\int_a^c |f(x)|^2 \, dx < \infty. \tag{1.53}$$

Analogously, f is said to lie in L^2 near b if there exists a point $d \in (a,b)$ such that

$$\int_d^b |f(x)|^2 \, dx < \infty. \tag{1.54}$$

If $z \in \mathbb{C}\backslash\mathbb{R}$ and c is an endpoint of (a,b), then the equation $\mathcal{L}f = zf$ has a nontrivial solution that lies in L^2 near c.

Proposition 1.24 (Proposition 15.6 in [**6**]). *If $z \in \mathbb{C}\backslash\mathbb{R}$, then there exist nontrivial solutions u_z and v_z to $\mathcal{L}f = zf$ such that u_z lies in L^2 near a, and v_z lies in L^2 near b.*

In the case of at least one regular endpoint, Proposition 1.24 rules out the possibility that H_{min} has deficiency indices $(0,0)$. For example, if a is a regular endpoint, then the nontrivial solution v_z from Proposition 1.24, which lies in L^2 near b, must also lie in L^2 near a by Proposition 1.18 (i). Thus, $v_z \in L^2(a,b)$. Since $\mathcal{L}v_z = zv_z$ implies $(H_{max} - zI_{L^2(a,b)})v_z = 0$, we see that $v_z \in \ker(H_{max} - zI_{L^2(a,b)})$. Since v_z is nontrivial, choosing $z = \pm i$ shows that $d_\pm(H_{min}) \geq 1$. This result, together with the case of two regular endpoints, is summarized in the following corollary.

Corollary 1.25 (Corollary 15.7 in [**6**]). *If $\mathcal{L}$ is regular at a or b, then the deficiency indices of H_{min} are $(1,1)$ or $(2,2)$. If $\mathcal{L}$ is regular at a and b, then the deficiency indices of H_{min} are $(2,2)$.*

The following alternative is due to H. Weyl and is the key ingredient in characterizing when the deficiency indices of H_{min} are $(1,1)$ or $(2,2)$.

Theorem 1.26 (Weyl's Alternative, Theorem 15.8 in [**6**]). *Assume Hypothesis 1.9. If c denotes an endpoint of (a,b), then the following alternative holds. Either,*

(i) For each $z \in \mathbb{C}$, every solution to (1.49) lies in L^2 near c, or

(ii) For each $z \in \mathbb{C}$, there exists one solution of (1.49) which does not lie in L^2 near c.

The important feature of Theorem 1.26 is that the alternative is uniform in $z \in \mathbb{C}$. Therefore, the alternative that arises in practice (either (i) or (ii)) is completely determined by $\mathcal{L}$, and therefore by V.

Definition 1.27 (Limit point/limit circle classification). *Let c denote an endpoint of (a,b). If alternative (i) of Theorem 1.26 holds, then one says that $\mathcal{L}$ is in the limit circle case at c. If alternative (ii) of Theorem 1.26 holds, then one says that $\mathcal{L}$ is in the limit point case at c.*

Corollary 1.28. *Assume Hypothesis* 1.9. *Let c denote an endpoint of (a, b). If c is a regular endpoint, then $\mathcal{L}$ is in the limit circle case at c.*

Proof. If c is a regular endpoint, then $c \in \mathbb{R}$ and all solutions to (1.49) have finite limits at c by Proposition 1.18. Hence, every solution to (1.49) is bounded in a neighborhood of c and must therefore lie in L^2 near c. $\square$

Proposition 1.29 (Lemma 15.9 in [**6**]). *Assume Hypothesis* 1.9. *If $\mathcal{L}$ is in the limit point case at b, then*

$$\lim_{x \to b^-} W(f, g)(x) = 0, \quad f, g \in \operatorname{dom}(H_{max}). \tag{1.55}$$

A similar result holds if $\mathcal{L}$ is in the limit point case at a.

By Proposition 1.21, the deficiency indices of H_{min} are $(0, 0)$, $(1, 1)$, or $(2, 2)$. Weyl's limit point/limit circle classification completely characterizes when each case arises.

Theorem 1.30 (Theorem 15.10 in [**6**]). *Assume Hypothesis* 1.9. *The minimal operator H_{min} has deficiency indices:*

(i) $(2, 2)$ *if $\mathcal{L}$ is in the limit circle case at a and b,*

(ii) $(1, 1)$ *if $\mathcal{L}$ is in the limit point case at one endpoint and in the limit circle case at the other endpoint; and*

(iii) $(0, 0)$ *if $\mathcal{L}$ is in the limit point case at both endpoints.*

1.3. Schrödinger Operators on the Half-Line, $(0, \infty)$

In this section, we apply the results of Section 1.2 to define Schrödinger operators on the half-line, $(a, b) = (0, \infty)$. However, we strengthen the hypothesis on the potential coefficient V and assume the following hypothesis.

Hypothesis 1.31. *Suppose that*

$$V \in L^1(0,\infty) \ \textit{is real-valued a.e.,} \tag{1.56}$$

with

$$\int_0^\infty (1+x)|V(x)|\, dx < \infty, \tag{1.57}$$

and define the differential expression $\mathcal{L}$ *on* $(0,\infty)$ *by*

$$\mathcal{L} = -\frac{d^2}{dx^2} + V(x). \tag{1.58}$$

By assuming Hypothesis 1.31, we see that Hypothesis 1.9 is satisfied with $(a,b) = (0,\infty)$. Moreover, due to the assumption in (1.57), which implies $\int_0^\infty |V(x)|\, dx < \infty$, we see that 0 is a regular endpoint for $\mathcal{L}$.

Assuming Hypothesis 1.31, we recall H_{max}, the *maximal operator associated with* $\mathcal{L}$ in $L^2(0,\infty)$ which is defined by

$$\begin{aligned} &(H_{max} f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (0,\infty), \\ &f \in \operatorname{dom}(H_{max}) = \big\{ g \in L^2(0,\infty) \,\big|\, g, g' \in AC[0,R],\ R > 0,\ \mathcal{L}g \in L^2(0,\infty) \big\}, \end{aligned} \tag{1.59}$$

and the operator $\mathring{H}$:

$$\begin{aligned} &\mathring{H} f = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (0,\infty), \\ &f \in \operatorname{dom}(\mathring{H}) = \big\{ g \in \operatorname{dom}(H_{max}) \,\big|\, f(x) = 0,\ x \in (0,\infty)\backslash[c,d], \text{ for some } [c,d] \subset (0,\infty) \big\}. \end{aligned} \tag{1.60}$$

As noted in Section 1.2, the operator $\mathring{H}$ is densely defined and symmetric in the Hilbert space $L^2(0,\infty)$. It is closable, and its closure, H_{min}, is the *minimal operator associated to* $\mathcal{L}$ in $L^2(0,\infty)$. The minimal and maximal operators are adjoint to one another (cf. (1.39)):

$$(H_{min})^* = H_{max} \quad \text{and} \quad (H_{max})^* = H_{min}. \tag{1.61}$$

Next, we introduce the *regular* and *Jost solutions* to the eigenvalue differential equation

$$(\mathcal{L}u)(x) = -u''(x) + V(x)u(x) = zu(x), \quad x \in [0,\infty),\, z = \zeta^2 \in \mathbb{C}. \tag{1.62}$$

DEFINITION 1.32 (Regular Solution). *For each* $z = \zeta^2 \in \mathbb{C}$*, the regular solution* $\phi(\zeta, x)$ *of* $\mathcal{L}u = zu$ *is defined to be the unique solution to the initial-value problem*

$$\begin{cases} -\phi''(\zeta,x) + V(x)\phi(\zeta,x) = z\phi(\zeta,x), \quad x \in [0,\infty), \\ \phi(\zeta,0) = 0, \quad \phi'(\zeta,0) = 1. \end{cases} \tag{1.63}$$

The regular solution is well-defined by Proposition 1.34(ii).

In order to define the Jost solution for (1.62), we recall the following result which shows that the condition (1.57) allows us to compare the solutions of the equation $\mathcal{L}f = zf$ with the solutions $e^{\pm i\zeta x}$ of the equation $-f'' = zf$.

PROPOSITION 1.33 (Lemma 4.1.4 in [**10**]). *Assume Hypothesis* 1.31. *For all* $\zeta \neq 0$ *from the closed upper half-plane of* $\mathbb{C}$*, equation* (1.62) *has solutions* $\theta(\zeta,x)$ *and* $\tilde{\theta}(\zeta,x)$ *satisfying as* $x \to \infty$ *the conditions*

$$\theta(\zeta,x) = e^{i\zeta x}[1 + o(1)], \quad \theta'(\zeta,x) = i\zeta e^{i\zeta x}[1+o(1)], \tag{1.64}$$

$$\tilde{\theta}(\zeta,x) = e^{-i\zeta x}[1 + o(1)], \quad \tilde{\theta}'(\zeta,x) = -i\zeta e^{-i\zeta x}[1+o(1)], \tag{1.65}$$

where in each case $o(1)$ *represents a* ζ*-dependent term that converges to zero as* $x \to \infty$*. For any fixed* $x \geq 0$*, the functions* $\theta(\zeta,x)$ *and* $\tilde{\theta}(\zeta,x)$ *are analytic in* ζ *in the open upper half-plane of* $\mathbb{C}$ *and continuous in* ζ *up to the real axis, with the possible exception of the point* $\zeta = 0$.

Proposition 1.34. *Assume Hypothesis* 1.31. *The differential expression* $\mathcal{L}$ *is in the limit circle case at* 0 *and in the limit point case at* ∞. *In particular,* H_{min} *has deficiency indices* $(1,1)$.

Proof. The endpoint 0 is a regular endpoint. Therefore, $\mathcal{L}$ is in the limit circle case by Corollary 1.28. By Weyl's alternative, Theorem 1.26, to show the limit point claim, it is enough to find a $z \in \mathbb{C}$ for which $\mathcal{L}f = zf$ has a solution which does not lie in L^2 near ∞. If we take $z = -1$, then $\zeta = i$, and by (1.65),

$$\tilde{\theta}(i,x) = e^{x}[1+o(1)] \text{ as } x \to \infty, \tag{1.66}$$

so clearly $\tilde{\theta}(i,\,\cdot\,) \notin L^2(c,\infty)$ for all $c \in (0,\infty)$. That is, $\tilde{\theta}(i,\,\cdot\,)$ does not lie in L^2 near ∞. Therefore, alternative (ii) must hold in Theorem 1.26, and $\mathcal{L}$ is in the limit point case at ∞.

Since $\mathcal{L}$ is in the limit point case at ∞ and in the limit circle case at 0, Theorem 1.30(ii) implies the deficiency indices of H_{min} are $(1,1)$. $\square$

Assuming Hypothesis 1.31, 0 is a regular endpoint for $\mathcal{L}$. Therefore, the characterization of H_{min} in (1.44) applies. Furthermore, since $\mathcal{L}$ is in the limit point case at ∞ by Proposition 1.34, Proposition 1.29 implies that the Wronskian condition in (1.44):

$$\lim_{x\to\infty} W(g,h)(x) = 0, \quad h \in \operatorname{dom}(H_{max}), \tag{1.67}$$

is, in fact, redundant. Hence, the minimal operator H_{min} is given explicitly as

$$\begin{aligned}&(H_{min}f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (0,\infty), \\ &f \in \operatorname{dom}(H_{min}) = \big\{g \in \operatorname{dom}(H_{max}) \,\big|\, g(0) = g'(0) = 0\big\}.\end{aligned} \tag{1.68}$$

Definition 1.35 (Jost solution). *For each* $\zeta \neq 0$ *from the closed upper half-plane of* $\mathbb{C}$, *the function* $\theta(\zeta,\,\cdot\,)$ *in Proposition* 1.33 *is the Jost solution to* (1.62).

REMARK 1.36. If $z = \zeta^2 \in \mathbb{C}\backslash[0, \infty)$, then actually $\text{Im}(\zeta) > 0$, and the condition $\theta(\zeta, x) = e^{i\zeta x}[1 + o(1)]$ as $x \to \infty$ immediately implies $\theta(\zeta, \cdot\,) \in L^2(0, \infty)$. Here we have also used the fact that $\theta(\zeta, x)$ has a finite limit at $x \to 0^+$, since 0 is a regular endpoint (see Definition 1.14 and Proposition 1.18). We also conclude that $\mathcal{L}\theta(\zeta, \cdot\,) = \zeta^2\theta(\zeta, \cdot\,) \in L^2(0, \infty)$. Thus,

$$\theta(\zeta, \cdot\,) \in \ker(H_{max} - zI_{L^2(0,\infty)}), \quad z \in \mathbb{C}\backslash[0, \infty),\ z = \zeta^2. \tag{1.69}$$

Since $\mathcal{L}$ is in the limit point case at ∞, there does not exist another square integrable solution to $\mathcal{L}f = zf$ that is linearly independent to the Jost solution. Otherwise, every solution to $\mathcal{L}f = zf$ would be square integrable, and $\mathcal{L}$ would be in the limit circle case at ∞. Therefore, any other solution to $\mathcal{L}f = zf$ which is square integrable on $(0, \infty)$ is a constant multiple of the Jost solution.

As an immediate consequence of Remark 1.36, we obtain a spanning vector for $\ker(H_{max} - zI_{L^2(0,\infty)})$ for each $z \in \mathbb{C}\backslash\mathbb{R}$.

COROLLARY 1.37. *Assume Hypothesis* 1.31. *Then the Jost solution* $\theta(\zeta, \cdot\,)$ *spans* $\ker(H_{max} - zI_{L^2(0,\infty)})$.

Since H_{min} has equal and finite deficiency indices, Theorem 1.22 implies that H_{min} has self-adjoint extensions. In fact, since the deficiency indices of H_{min} are $(1, 1)$, von Neumann's theory of self-adjoint extensions implies that H_{min} has a one-parameter family of self-adjoint extensions H_α, $\alpha \in [0, \pi)$, parametrized by a separated self-adjoint boundary condition at $x = 0$:

$$(H_\alpha f)(x) = -f''(x) + V(x)f(x) \text{ for a.e. } x \in (0, \infty), \tag{1.70}$$

$$f \in \operatorname{dom}(H_\alpha) = \{g \in \operatorname{dom}(H_{max}) \mid \cos(\alpha)g(0) = \sin(\alpha)g'(0)\}, \quad \alpha \in [0,\pi).$$

The preceding claim is made precise in the following proposition.

Proposition 1.38 (Example 15.5 in [**6**]). *For each $\alpha \in [0,\pi)$, H_α defined in* (1.70) *is a self-adjoint extension of H_{min}. Conversely, if H is a self-adjoint extension of H_{min}, then $H = H_\alpha$ for some $\alpha \in [0,\pi)$.*

The regular and Jost solutions of $\mathcal{L}f = zf$ permit one to define the *Jost function.*

Definition 1.39 (Jost function). *The Wronskian of the Jost and regular solutions is denoted by w and is called the Jost function:*

$$\begin{aligned} w(\zeta) &:= W(\theta(\zeta,\,\cdot\,), \phi(\zeta,\,\cdot\,)) \\ &= \theta(\zeta,0)\underbrace{\phi'(\zeta,0)}_{=1} - \theta'(\zeta,0)\underbrace{\phi(\zeta,0)}_{=0} \\ &= \theta(\zeta,0), \quad \zeta \neq 0. \end{aligned} \tag{1.71}$$

Proposition 1.40 (p. 165 in [**10**]). *Assume Hypothesis* 1.31*. The Jost function $w(\zeta)$ is analytic in* $\operatorname{Im}(\zeta) > 0$ *and continuous in* $\operatorname{Im}(\zeta) \geq 0$ *with the possible exception of the point* $\zeta = 0$*. Moreover,*

$$w(\zeta) = 1 + O(|\zeta|^{-1}) \ \text{ as } |\zeta| \to \infty. \tag{1.72}$$

In particular,

$$\lim_{|\zeta|\to\infty} w(\zeta) = 1. \tag{1.73}$$

Remark 1.41. If $z = \zeta^2 \in \mathbb{C}$ with $\zeta = a + ib$, $a \in \mathbb{R}$, $b \in [0,\infty)$, then $\overline{z} = (\overline{\zeta})^2$. However, $\overline{\zeta} = a - ib$ has a nonpositive imaginary part. It is $-\overline{\zeta} = -a + ib$ that is the square root of $\overline{z}$ with a nonnegative imaginary part. As a consequence, we have [**10**, equation (1.28), p. 165]

$$\theta(\zeta, x) = \overline{\theta(-\overline{\zeta}, x)} \quad \text{and} \quad w(\zeta) = \overline{w(-\overline{\zeta})}. \tag{1.74}$$

In particular, when $z \in \mathbb{C}\backslash\mathbb{R}$, $\theta(-\overline{\zeta}, \,\cdot\,)$ is a spanning vector for $\ker(H_{max} - \overline{z}I_{L^2(0,\infty)})$.

For $\zeta = k > 0$, the functions $\theta(k, \,\cdot\,)$ and $\theta(-k, \,\cdot\,)$ satisfy the same differential equation

$$-u''(x) + V(x)u(x) = k^2 u(x), \quad x \in [0, \infty), \tag{1.75}$$

and since their Wronskian is equal to a constant, we may apply the asymptotics in (1.64) to compute

$$\begin{aligned} W(\theta(k, \,\cdot\,), \theta(-k, \,\cdot\,)) &= \lim_{x\to\infty} W(\theta(k, \,\cdot\,), \theta(-k, \,\cdot\,))(x) \\ &= \lim_{x\to\infty} [\theta(k, x)\theta'(-k, x) - \theta'(k, x)\theta(-k, x)] \\ &= \lim_{x\to\infty} \Big\{ e^{ikx}[1 + o(1)](-ik)e^{-ikx}[1 + o(1)] \\ &\qquad\qquad - ike^{ikx}[1 + o(1)]e^{-ikx}[1 + o(1)] \Big\} \\ &= -2ik, \end{aligned} \tag{1.76}$$

which shows that $\theta(k, \,\cdot\,)$ and $\theta(-k, \,\cdot\,)$ are actually linearly independent for $k > 0$. Hence, $\{\theta(k, \,\cdot\,), \theta(-k, \,\cdot\,)\}$ forms a fundamental system for (1.75). Thus, the regular solution $\phi(k, \,\cdot\,)$ to (1.75) may be expressed as a linear combination

$$\phi(k, x) = c(k)\theta(k, x) + d(k)\theta(-k, x), \quad x \in [0, \infty). \tag{1.77}$$

Taking the Wronskian throughout (1.77) with $\theta(-k, \,\cdot\,)$, we have

$$W(\theta(-k, \,\cdot\,), \phi(k, \,\cdot\,))(x) = c(k)W(\theta(-k, \,\cdot\,), \theta(k, \,\cdot\,))(x), \quad x \in [0, \infty). \tag{1.78}$$

By uniqueness of solutions to (1.63), $\phi(k,\,\cdot\,) = \phi(-k,\,\cdot\,)$, so applying (1.76) in (1.78), we obtain

$$W(\theta(-k,\,\cdot\,), \phi(-k,\,\cdot\,))(x) = 2ikc(k), \tag{1.79}$$

or that

$$c(k) = (2ik)^{-1} w(-k), \quad k > 0. \tag{1.80}$$

In a similar way, we determine

$$d(k) = -(2ik)^{-1} w(k), \quad k > 0. \tag{1.81}$$

Therefore, (1.77) becomes

$$\phi(k,x) = (2ik)^{-1}[w(-k)\theta(k,x) - w(k)\theta(-k,x)], \quad x \in [0,\infty),\, k > 0. \tag{1.82}$$

By combining the representation for the regular solution for $k > 0$ in (1.82) with (1.74), we can show the Jost function does not vanish for $k > 0$.

PROPOSITION 1.42. *Assume Hypothesis* 1.31. *If $k > 0$, then $w(k) \neq 0$.*

PROOF. Let $k > 0$. If $w(k) = 0$, then $w(-k) = \overline{w(k)} = 0$, by the second equality in (1.74). However, (1.82) immediately implies $\phi(k,x) \equiv 0$, which is a contradiction. $\square$

We define

$$A(k) = |w(k)|, \quad \eta(k) = \arg(w(k)), \quad k \in \mathbb{R}\backslash\{0\}, \tag{1.83}$$

which allows us to write

$$w(k) = A(k)e^{i\eta(k)}, \quad k \in \mathbb{R}\backslash\{0\}. \tag{1.84}$$

Initially, the function $\eta(k)$ is only determined up to additive multiples of 2π, but one can impose the condition $\eta(k) \to 0$ as $k \to \infty$ (see [**10**, p. 166]) which determines $\eta(k)$ uniquely.

Definition 1.43 (Scattering amplitude and scattering phase). *For each $k \in \mathbb{R}\backslash\{0\}$, the coefficients $A(k)$ and $\eta(k)$ in* (1.83) *are called the scattering amplitude and the scattering phase, respectively.*

The functions $A(k)$ and $\eta(k)$ are important because they give the asymptotics of the regular solution $\phi(k, x)$ as $x \to \infty$.

Theorem 1.44 (Equations (1.21) and (1.22) in [**3**]). *Assume Hypothesis* 1.31. *If $k \in \mathbb{R}\backslash\{0\}$, then the regular solution $\phi(k, \cdot)$ satisfies*

$$\begin{aligned} \phi(k,x) &= \frac{A(k)}{k}\sin(kx - \eta(k)) + o(1), \\ \phi'(k,x) &= A(k)\cos(kx - \eta(k)) + o(1), \end{aligned} \tag{1.85}$$

as $x \to \infty$, where in each case $o(1)$ represents a k-dependent term that converges to zero as $x \to \infty$.

Theorem 1.44 justifies the terminology for $A(k)$ and $\eta(k)$ introduced in Definition 1.43. We also introduce the scattering matrix.

Definition 1.45 (Scattering matrix). *For each $k > 0$, the function $S(k)$ defined by*

$$\frac{w(-k)}{w(k)} = e^{-2i\eta(k)} \tag{1.86}$$

is called the scattering matrix.

Although the quantity defined by (1.86) is scalar-valued, it is customary to refer to it as the scattering *matrix*.

The scattering matrix gets its name from the fact that for $k > 0$, the solution

$$\psi(k,x) = \frac{k}{w(k)}\phi(k,x), \quad x \in [0,\infty), \tag{1.87}$$

satisfies [**10**, p. 166]

$$\psi(k,x) = \frac{i}{2}\big[e^{-ikx} - S(k)e^{ikx}\big] + o(1) \tag{1.88}$$

as $x \to \infty$. In quantum mechanics, e^{-ikx} represents a wave of particles incoming from $+\infty$ toward an impenetrable infinite barrier located at $x = 0$. These waves interact with the potential $V(x)$, reflect from the barrier, and part of the wave scatters back to $+\infty$. Similarly e^{ikx} represents a wave of particles moving to $+\infty$. Thus, the scattering matrix $S(k)$ measures the proportion of particles that scatter to ∞ after interaction with $V(x)$ and reflection from the barrier.

Remark 1.46. The significance of the Jost function, w, is that it contains information about the eigenvalues of the self-adjoint extension H_0. In fact, if $w(\zeta) = 0$ for some $\zeta \in \mathbb{C}$, then the regular and Jost solutions must be linearly dependent. Consequently, if $\mathrm{Im}(\zeta) > 0$, then $\theta(\zeta, \cdot\,) \in L^2(0,\infty)$ is an eigenfunction of H_0 with the corresponding eigenvalue $z = \zeta^2$. Since H_0 can only have negative eigenvalues (if any), it follows that the Jost function can only vanish on the imaginary axis.

In the special case when $V(x) = 0$ for a.e. $x \in (0,\infty)$, we append the superscript (0) to the operators $\mathring{H}$, H_{min}, H_{max}, and H_α, and the functions $\phi(\zeta,x)$, $\theta(\zeta,x)$, and $w(\zeta)$ and write $\mathring{H}^{(0)}$, $H^{(0)}_{min}$, $H^{(0)}_{max}$, $H^{(0)}_\alpha$, $\phi^{(0)}(\zeta,x)$, $\theta^{(0)}(\zeta,x)$, and $w^{(0)}(\zeta)$, respectively. In fact, in this case, we explicitly compute:

$$
\begin{aligned}
\phi^{(0)}(\zeta, x) &= \zeta^{-1} \sin(\zeta x), \quad x \in [0, \infty),\ \zeta \neq 0, \\
\theta^{(0)}(\zeta, x) &= e^{i\zeta x}, \quad x \in [0, \infty),\ \zeta \neq 0, \\
w^{(0)}(\zeta) &= 1, \quad \zeta \neq 0.
\end{aligned} \tag{1.89}
$$

In particular, since $w^{(0)}(\zeta)$ does not vanish for $\mathrm{Im}(\zeta) > 0$, the operator $H_0^{(0)}$ has no negative eigenvalues by Remark 1.46.

CHAPTER 2

KREIN'S RESOLVENT IDENTITY FOR HALF-LINE SCHRÖDINGER OPERATORS

2.1. Abstract Formulation of Krein's Resolvent Identity

HYPOTHESIS 2.1. *Let A_0 be a densely defined, closed, symmetric operator in the Hilbert space $\mathcal{H}$ with equal and finite deficiency indices,*

$$m = d_-(A_0) = d_+(A_0) \in \mathbb{N}_0, \tag{2.1}$$

and suppose that A_1 and A_2 are two self-adjoint extensions of A_0:

$$A_0 \subseteq A_j, \quad A_j^* = A_j, \quad j \in \{1, 2\}. \tag{2.2}$$

DEFINITION 2.2 (Common part). *A linear operator $C : \mathrm{dom}(C) \subseteq \mathcal{H} \to \mathcal{H}$ which satisfies*

$$C \subseteq A_j, \quad j \in \{1, 2\}, \tag{2.3}$$

is called a common part of A_1 and A_2.

REMARK 2.3. The operator A_0 is a common part of A_1 and A_2.

LEMMA 2.4. *Assume Hypothesis 2.1. If the operator C_{max} is defined by*

$$\mathrm{dom}(C_{max}) = \{u \in \mathrm{dom}(A_1) \cap \mathrm{dom}(A_2) \,|\, A_1 u = A_2 u\}, \tag{2.4}$$

$$C_{max} u = A_1 u = A_2 u, \quad u \in \mathrm{dom}(C_{max}), \tag{2.5}$$

then C_{max} is a common part of A_1 and A_2, and if C is any other common part of A_1 and A_2, then C is a restriction of C_{max}, that is

$$C \subseteq C_{max}. \tag{2.6}$$

Proof. To show C_{max} is a common part, we must show $C_{max} \subseteq A_j$, $j \in \{1, 2\}$. Clearly, $dom(C_{max}) \subseteq dom(A_j)$. By definition,

$$A_j u = C_{max} u, \quad u \in dom(C_{max}). \tag{2.7}$$

Hence, $C_{max} \subseteq A_j$, $j \in \{1, 2\}$. Let C denote a common part of A_1 and A_2, so that

$$C \subseteq A_j, \quad j \in \{1, 2\}. \tag{2.8}$$

If $u \in dom(C)$, then $u \in dom(A_j)$, $j \in \{1, 2\}$, and

$$Cu = A_1 u = A_2 u. \tag{2.9}$$

Thus, $u \in dom(C_{max})$ and

$$C_{max} u = A_1 u = A_2 u = Cu. \tag{2.10}$$

Evidently, this proves $C \subseteq C_{max}$. □

Remark 2.5. The operator C_{max} is symmetric:

$$\langle u, C_{max} v \rangle_{\mathcal{H}} = \langle u, A_1 v \rangle_{\mathcal{H}} = \langle A_1 u, v \rangle_{\mathcal{H}} = \langle C_{max} u, v \rangle_{\mathcal{H}}, \quad u, v \in \mathrm{dom}(C_{max}), \tag{2.11}$$

and $A_0 \subset C_{max}$.

Definition 2.6 (Maximal common part). *C_{max} is the maximal common part of A_1 and A_2.*

Definition 2.7 (Relatively prime). *A_1 and A_2 are relatively prime with respect to A_0 if and only if $C_{max} = A_0$*

Remark 2.8. A_1 and A_2 are relatively prime if and only if the condition $u \in \mathrm{dom}(A_1) \cap \mathrm{dom}(A_2)$ implies $u \in \mathrm{dom}(A_0)$.

Lemma 2.9. *Assume Hypothesis* 2.1. *Then A_1 and A_2 are self-adjoint extensions of C_{max}. Thus, C_{max} has equal deficiency indices. In fact,*

$$d_+(C_{max}) = d_-(C_{max}) =: r \leq m. \tag{2.12}$$

Proof. By Lemma 2.4, in particular (2.6), C_{max} is an extension of A_0 since A_0 is a common part of A_1 and A_2. It follows that $\mathrm{dom}(A_0) \subset \mathrm{dom}(C_{max})$, so that C_{max} is densely defined. In addition, C_{max} is a restriction of A_j for $j \in \{1, 2\}$. To see this, note that if $u \in \mathrm{dom}(C_{max})$, then $u \in \mathrm{dom}(A_j)$ for $j \in \{1, 2\}$ by the very definition of $\mathrm{dom}(C_{max})$, and then by the definition of C_{max}, we have $C_{max}u = A_1u = A_2u$. Since A_1 and A_2 are self-adjoint, it follows that both A_1 and A_2 are self-adjoint extensions of C_{max}. Since C_{max} has self-adjoint extensions, the deficiency indices of C_{max} must be equal by Theorem 1.22, so we set

$$r := d_+(C_{max}) = d_-(C_{max}). \tag{2.13}$$

To complete the proof, we must show that $r \leq m$. To show this inequality, it suffices to prove that

$$\ker(C_{max}^* \mp iI_{\mathcal{H}}) \subseteq \ker(A_0^* \mp iI_{\mathcal{H}}). \tag{2.14}$$

Let $u_\pm \in \ker(C_{max}^* \mp iI_{\mathcal{H}})$ so that $C_{max}^* u_\pm = \pm i u_\pm$. Since $A_0 \subseteq C_{max}$ implies $C_{max}^* \subseteq A_0^*$, we have $A_0^* u_\pm = \pm i u_\pm$. We conclude that $u_\pm \in \ker(A_0^* \mp iI_{\mathcal{H}})$. $\square$

In order to abbreviate notation, we introduce the following notation for the resolvent operators of A_j, $j \in \{1, 2\}$:

$$R_j(z) = (A_j - zI_{\mathcal{H}})^{-1}, \quad z \in \rho(A_j),\, j \in \{1, 2\}. \tag{2.15}$$

THEOREM 2.10 (Abstract Krein's Resolvent Identity, Section VII.84 in [**1**]). *Assume Hypothesis 2.1. Fix $z \in \rho(A_1) \cap \rho(A_2)$, and let $\{g_k(z)\}_{k=1}^r$ and $\{g_k(\overline{z})\}_{k=1}^r$ be bases for $\ker(C_{max}^* - zI_{\mathcal{H}})$ and $\ker(C_{max}^* - \overline{z}I_{\mathcal{H}})$, respectively. Then there exist (complex) scalars $\{\beta_{j,k}(z)\}_{j,k=1}^r$ such that*

$$R_2(z) - R_1(z) = \sum_{j,k=1}^{r} \beta_{j,k}(z) \langle g_j(\overline{z}), \cdot \rangle_{\mathcal{H}} g_k(z). \tag{2.16}$$

In particular,

$$\begin{aligned} \operatorname{tr}_{\mathcal{H}}(R_2(z) - R_1(z)) &= \operatorname{tr}_{\mathcal{H}} \left[\sum_{j,k=1}^{r} \beta_{j,k}(z) \langle g_j(\overline{z}), \cdot \rangle_{\mathcal{H}} g_k(z) \right] \\ &= \sum_{j,k=1}^{r} \beta_{j,k}(z) \operatorname{tr}_{\mathcal{H}} \left[\langle g_j(\overline{z}), \cdot \rangle_{\mathcal{H}} g_k(z) \right] \\ &= \sum_{j,k=1}^{r} \beta_{j,k}(z) \langle g_j(\overline{z}), g_k(z) \rangle_{\mathcal{H}}. \end{aligned} \tag{2.17}$$

The identity in (2.16) is called Krein's resolvent identity.

2.2. Krein's Resolvent Identity for H_0 and H_α

We recall that the operator H_{min} defined by (1.68) is closed, densely defined and symmetric with deficiency indices $(1, 1)$. Let $\alpha \in (0, \pi)$. The operators H_α and H_0 defined by (1.70) are both self-adjoint extensions of H_{min}. Therefore, Hypothesis 2.1 is satisfied with $A_0 = H_{min}$, $A_1 = H_0$, $A_2 = H_\alpha$, and $\mathcal{H} = L^2(0, \infty)$. Next, we determine the maximal common of the operators H_0 and H_α.

LEMMA 2.11. *The minimal operator H_{min} is the maximal common part of H_0 and H_α. Therefore, H_0 and H_α are relatively prime with respect to H_{min}.*

PROOF. Let C_{max} denote the maximal common part of H_0 and H_α. To prove the claim, it suffices to show $\operatorname{dom}(C_{max}) = \operatorname{dom}(H_{min})$. Since, H_{min} is a common part of H_0 and H_α, it follows from Lemma 2.4 that $H_{min} \subseteq C_{max}$; in particular, $\operatorname{dom}(H_{min}) \subseteq \operatorname{dom}(C_{max})$. Conversely, if $f \in \operatorname{dom}(C_{max})$, then $f \in \operatorname{dom}(H_0) \cap \operatorname{dom}(H_\alpha)$. As a result, $f \in \operatorname{dom}(H_{max})$ with

$$f(0) = 0 \quad \text{and} \quad \sin(\alpha) f'(0) = \cos(\alpha) f(0). \tag{2.18}$$

Combining the two equations, and noting $\sin(\alpha) \neq 0$ if $\alpha \in (0, \pi)$, we obtain $f'(0) = 0$. Having shown $f \in \operatorname{dom}(H_{max})$ with $f(0) = f'(0) = 0$, we conclude that $f \in \operatorname{dom}(H_{min})$. This shows that $\operatorname{dom}(C_{max}) \subset \operatorname{dom}(H_{min})$, and we finally conclude that $C_{max} = H_{min}$. By Definition 2.7, H_0 and H_α are relatively prime. $\square$

Hypothesis 2.1 is satisfied with $A_0 = H_{min}$, $A_1 = H_0$, $A_2 = H_\alpha$, and $\mathcal{H} = L^2(0, \infty)$, and we know that $C_{max} = H_{min}$ by Lemma 2.11. Since the deficiency indices of H_{min} are $r = 1$, Theorem 2.10 implies that the difference of the resolvents of H_0 and H_α is a rank one operator with a range contained in $\ker(H_{min}^* - zI_{L^2(0,\infty)})$:

$$(H_\alpha - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1} = -p_\alpha(z) \langle g_1(\overline{z}), \cdot \rangle_{L^2(0,\infty)} g_1(z), \tag{2.19}$$
$$z \in \rho(H_0) \cap \rho(H_\alpha),$$

where $g_1(z)$ is a basis vector for $\ker(H_{min}^* - zI_{L^2(0,\infty)})$ and $p_\alpha(z)$ is an appropriate complex scalar. The main result of this chapter is the derivation of the precise form of Krein's resolvent identity for the operators H_0 and H_α when $g_1(z) = \theta(\zeta, \cdot)$ is chosen as a basis vector for $\ker(H_{min}^* - zI_{L^2(0,\infty)})$. The derivation entails the computation of the corresponding coefficient $p_\alpha(z)$. The proof of the identity relies on the fact that $(H_0 - zI_{L^2(0,\infty)})^{-1}$, $z \in \rho(H_0)$, is an integral operator.

PROPOSITION 2.12 (Proposition 4.2.1 in [**10**]). *For each* $z \in \rho(H_0)$, *the resolvent* $(H_0 - zI_{L^2(0,\infty)})^{-1}$ *is an integral operator with integral kernel given by*

$$G_0(z;x,x') = \frac{1}{w(\zeta)} \begin{cases} \phi(\zeta,x)\theta(\zeta,x'), & 0 \le x \le x' < \infty, \\ \phi(\zeta,x')\theta(\zeta,x), & 0 \le x' \le x < \infty. \end{cases} \tag{2.20}$$

We now state and prove the main result of this chapter.

THEOREM 2.13 (Krein's Resolvent Identity for H_0 and H_α). *Assume Hypothesis* 1.31. *If* $\alpha \in (0,\pi)$, *then the resolvent operators of* H_0 *and* H_α *satisfy*

$$(H_\alpha - zI_{L^2(0,\infty)})^{-1} - (H_0 - zI_{L^2(0,\infty)})^{-1} = -p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),\,\cdot\,\rangle_{L^2(0,\infty)}\theta(\zeta,\,\cdot\,), \tag{2.21}$$

$$z = \zeta^2 \in \rho(H_0) \cap \rho(H_\alpha),$$

where

$$p_\alpha(z) = \frac{\sin(\alpha)}{\theta(\zeta,0)[\sin(\alpha)\theta'(\zeta,0) - \cos(\alpha)\theta(\zeta,0)]}, \quad z = \zeta^2 \in \rho(H_0) \cap \rho(H_\alpha). \tag{2.22}$$

PROOF. Let $z \in \rho(H_0) \cap \rho(H_\alpha)$ be fixed, and define the bounded operator $T_\alpha(z)$ by

$$T_\alpha(z) = (H_0 - zI_{L^2(0,\infty)})^{-1} - p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),\,\cdot\,\rangle_{L^2(0,\infty)}\theta(\zeta,\,\cdot\,), \tag{2.23}$$

$$\mathrm{dom}(T_\alpha(z)) = L^2(0,\infty).$$

To prove the theorem, it suffices to show

$$(H_\alpha - zI_{L^2(0,\infty)})T_\alpha(z) = I_{L^2(0,\infty)}, \tag{2.24}$$

where

$$\mathrm{dom}((H_\alpha - zI_{L^2(0,\infty)})T_\alpha(z)) = \{f \in \mathrm{dom}(T_\alpha(z)) \,|\, T_\alpha(z)f \in \mathrm{dom}(H_\alpha)\}, \tag{2.25}$$

and that

$$T_\alpha(z)(H_\alpha - zI_{L^2(0,\infty)}) = I_{L^2(0,\infty)}\big|_{\mathrm{dom}(H_\alpha)}, \tag{2.26}$$

where $S|_{\mathcal{K}}$ denotes the restriction of an operator S to the subspace $\mathcal{K}$. Indeed, the identities in (2.24) and (2.26) imply that $T_\alpha(z)$ is the inverse of $H_\alpha - zI_{L^2(0,\infty)}$. Since the inverse of an invertible operator is unique, and $(H_\alpha - zI_{L^2(0,\infty)})^{-1}$ is the inverse of $H_\alpha - zI_{L^2(0,\infty)}$, we conclude that

$$T_\alpha(z) = (H_\alpha - zI_{L^2(0,\infty)})^{-1}. \tag{2.27}$$

It remains to justify the identities in (2.24) and (2.26). To this end, let $f \in L^2(0,\infty)$. We claim that

$$T_\alpha(z)f \in \operatorname{dom}(H_\alpha). \tag{2.28}$$

By the very definition of $T_\alpha(z)$,

$$T_\alpha(z)f = (H_0 - zI_{L^2(0,\infty)})^{-1}f - p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta,\,\cdot\,). \tag{2.29}$$

The fact that $\operatorname{dom}(H_{max})$ is a subspace, along with (2.29) and the containments

$$\big[(H_0 - zI_{L^2(0,\infty)})^{-1}f\big] \in \operatorname{dom}(H_0) \subset \operatorname{dom}(H_{max}) \quad \text{and} \quad \theta(\zeta,\,\cdot\,) \in \operatorname{dom}(H_{max}) \tag{2.30}$$

imply $T_\alpha(z)f \in \operatorname{dom}(H_{max})$. The first containment in (2.30) is clear; see Remark 1.36 for an explanation of the second containment. Thus, the proof of the containment in (2.28) reduces to showing that $T_\alpha(z)f$ satisfies the boundary condition for elements of $\operatorname{dom}(H_\alpha)$, that is that

$$\cos(\alpha)[T_\alpha(z)f](0) = \sin(\alpha)[T_\alpha(z)f]'(0). \tag{2.31}$$

To verify that $T_\alpha(z)f$ satisfies the boundary condition, we begin by computing the left-hand side in (2.31):

$$\begin{aligned}\cos(\alpha)[T_\alpha(z)f](0) &= \cos(\alpha)\big[(H_0 - zI_{L^2(0,\infty)})^{-1}f - p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta,\,\cdot\,)\big](0)\\ &= \cos(\alpha)\big[(H_0 - zI_{L^2(0,\infty)})^{-1}f\big](0)\end{aligned}$$

$$-\cos(\alpha)p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),f\rangle_{L^2(0,\infty)}\underbrace{\theta(\zeta,0)}_{=w(\zeta)}$$
$$=-\cos(\alpha)p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),f\rangle_{L^2(0,\infty)}w(\zeta),$$

where we use the fact that $\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big]\in\mathrm{dom}(H_0)$ and, therefore, satisfies the Dirichlet boundary condition at $x=0$:

$$\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big](0)=0. \tag{2.32}$$

To compute the right-hand side of (2.31), we begin with $[T_\alpha(z)f]'(0)$. By (2.29), we have

$$[T_\alpha(z)f]'(0)=\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big]'(0)-p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),f\rangle_{L^2(0,\infty)}\theta'(\zeta,0). \tag{2.33}$$

We use the integral kernel in (2.20) to compute $\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big]'(0)$. Equation (2.20) implies

$$\begin{aligned}\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big](x)&=\int_0^\infty G_0(z;x,x')f(x')\,dx' \qquad (2.34)\\&=\int_0^x G_0(z;x,x')f(x')\,dx'+\int_x^\infty G_0(z;x,x')f(x')\,dx'\\&=\frac{1}{w(\zeta)}\int_0^x\phi(\zeta,x')\theta(\zeta,x)f(x')\,dx\\&\quad+\frac{1}{w(\zeta)}\int_x^\infty\phi(\zeta,x)\theta(\zeta,x')f(x')\,dx,\quad x\in[0,\infty).\end{aligned}$$

Now, by differentiating, we have

$$\begin{aligned}\big[(H_0-zI_{L^2(0,\infty)})^{-1}f\big]'(x)=\frac{1}{w(\zeta)}\bigg[&\underbrace{\frac{d}{dx}\int_0^x\phi(\zeta,x')\theta(\zeta,x)f(x')\,dx'}_{=I_1(x)}\\&+\underbrace{\frac{d}{dx}\int_x^\infty\phi(\zeta,x)\theta(\zeta,x')f(x')\,dx'}_{=I_2(x)}\bigg],\quad x\in[0,\infty).\end{aligned} \tag{2.35}$$

Computing $I_1(x)$ and $I_2(x)$, we have

$$\begin{aligned} I_1(x) &= \frac{d}{dx}\left[\theta(\zeta,x)\int_0^x \phi(\zeta,x')f(x')\,dx'\right] \qquad (2.36)\\ &= \theta'(\zeta,x)\int_0^x \phi(\zeta,x')f(x')\,dx' + \theta(\zeta,x)\phi(\zeta,x)f(x) \ \text{ for a.e. } x\in[0,\infty), \end{aligned}$$

and upon reversing the order of integration in $I_2(x)$,

$$\begin{aligned} I_2(x) &= -\frac{d}{dx}\left[\phi(\zeta,x)\int_\infty^x \theta(\zeta,x')f(x')\,dx'\right] \qquad (2.37)\\ &= -\phi'(\zeta,x)\int_\infty^x \theta(\zeta,x')f(x')\,dx' - \phi(\zeta,x)\theta(\zeta,x)f(x) \ \text{ for a.e. } x\in[0,\infty). \end{aligned}$$

Then

$$\begin{aligned} &\frac{1}{w(\zeta)}\left[I_1(x)+I_2(x)\right] \qquad (2.38)\\ &= \frac{1}{w(\zeta)}\left[\theta'(\zeta,x)\int_0^x \phi(\zeta,x')f(x')\,dx' + \phi'(\zeta,x)\int_x^\infty \theta(\zeta,x')f(x')\,dx'\right], \quad x\in[0,\infty). \end{aligned}$$

Taking $x=0$ in (2.35) and applying (2.38), we have

$$\begin{aligned} \left[(H_0 - zI_{L^2(0,\infty)})^{-1}f\right]'(0) &= \frac{1}{w(\zeta)}\Bigg[\theta'(\zeta,0)\underbrace{\int_0^0 \phi(\zeta,x')f(x')\,dx'}_{=0}\\ &\qquad + \underbrace{\phi'(\zeta,0)}_{=1}\int_0^\infty \theta(\zeta,x')f(x')\,dx'\Bigg]\\ &= \frac{1}{w(\zeta)}\int_0^\infty \theta(\zeta,x')f(x')\,dx'\\ &= \frac{1}{w(\zeta)}\int_0^\infty \overline{\theta(-\overline{\zeta},x')}f(x')\,dx' \qquad (2.39)\\ &= \frac{1}{w(\zeta)}\langle\theta(-\overline{\zeta},\,\cdot\,),f\rangle_{L^2(0,\infty)}, \end{aligned}$$

where we have applied (1.74) in (2.39). Now, to show (2.31), we compute the difference between $\cos(\alpha)[T_\alpha(z)f](0)$ and $\sin(\alpha)[T_\alpha(z)f]'(0)$:

$$\begin{aligned} &\cos(\alpha)[T_\alpha(z)f](0) - \sin(\alpha)[T_\alpha(z)f]'(0)\\ &= \cos(\alpha)\{\underbrace{[(H_0 - zI_{L^2(0,\infty)})^{-1}f](0)}_{=0} - p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,),f\rangle_{L^2(0,\infty)}\theta(\zeta,0)\} \end{aligned}$$

$$
\begin{aligned}
&\quad - \sin(\alpha)\{[(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0) - p_\alpha(z)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)} \theta'(\zeta, 0)\} \\
&= -p_\alpha(z)\langle \theta(-\overline{\zeta}, \cdot), f\rangle_{L^2(0,\infty)}[\cos(\alpha)\theta(\zeta,0) - \sin(\alpha)\theta'(\zeta,0)] \\
&\quad - \sin(\alpha)[(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0) \\
&= p_\alpha(z)\langle \theta(-\overline{\zeta}, \cdot), f\rangle_{L^2(0,\infty)}[\sin(\alpha)\theta'(\zeta,0) - \cos(\alpha)\theta(\zeta,0)] \\
&\quad - \sin(\alpha)[(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0) \\
&= \frac{\sin(\alpha)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}}{\theta(\zeta,0)[\sin(\alpha)\theta'(\zeta,0) - \cos(\alpha)\theta(\zeta,0)]}[\sin(\alpha)\theta'(\zeta,0) - \cos(\alpha)\theta(\zeta,0)] \\
&\quad - \sin(\alpha)[(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0) \\
&= \frac{\sin(\alpha)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}}{\theta(\zeta,0)} - \sin(\alpha)[(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0) \\
&= \sin(\alpha)\left[\frac{\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}}{\theta(\zeta,0)} - [(H_0 - zI_{L^2(0,\infty)})^{-1} f]'(0)\right] \\
&= \sin(\alpha)\Bigg[\underbrace{\frac{\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}}{\theta(\zeta,0)} - \frac{\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}}{\theta(\zeta,0)}}_{=0}\Bigg] \\
&= 0. \qquad (2.40)
\end{aligned}
$$

This completes the proof of (2.28).

Having shown (2.28), we proceed to verify the identity in (2.24) by computing $(H_\alpha - zI_{L^2(0,\infty)})T_\alpha(z)f$ as follows:

$$
\begin{aligned}
&(H_\alpha - zI_{L^2(0,\infty)})T_\alpha(z)f \\
&\quad = (H_\alpha - zI_{L^2(0,\infty)})\big[(H_0 - zI_{L^2(0,\infty)})^{-1} f - p_\alpha(z)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta, \,\cdot\,)\big] \\
&\quad = (H_{max} - zI_{L^2(0,\infty)})\big[(H_0 - zI_{L^2(0,\infty)})^{-1} f - p_\alpha(z)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta, \,\cdot\,)\big] \\
&\quad = (H_{max} - zI_{L^2(0,\infty)})\big[(H_0 - zI_{L^2(0,\infty)})^{-1} f\big] \\
&\qquad - (H_{max} - zI_{L^2(0,\infty)})\big[p_\alpha(z)\langle \theta(-\overline{\zeta}, \,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta, \,\cdot\,)\big] \\
&\quad = (H_0 - zI_{L^2(0,\infty)})\big[(H_0 - zI_{L^2(0,\infty)})^{-1} f\big] \qquad (2.41)
\end{aligned}
$$

$$
\begin{aligned}
&\quad - (H_{max} - zI_{L^2(0,\infty)})\big[p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,), f\rangle_{L^2(0,\infty)}\theta(\zeta,\,\cdot\,)\big] \\
&= f - p_\alpha(z)\langle\theta(-\overline{\zeta},\,\cdot\,), f\rangle_{L^2(0,\infty)}\underbrace{(H_{max} - zI_{L^2(0,\infty)})\theta(\zeta,\,\cdot\,)}_{=0} \\
&= f \qquad (2.42) \\
&= I_{L^2(0,\infty)}f,
\end{aligned}
$$

where we used $H_0 \subset H_{max}$ to obtain (2.41). In (2.42), we have used the fact that $(H_{max} - zI_{L^2(0,\infty)})\theta(\zeta,\,\cdot\,) \equiv 0$ since $\theta(\zeta,\,\cdot\,)$ satisfies (1.62). This proves (2.24). It remains to prove (2.26).

To prove (2.26), we use (2.24) and properties of the operator adjoint. By (2.24) with z replaced by $\overline{z}$, we have

$$
(H_\alpha - \overline{z}I_{L^2(0,\infty)})T_\alpha(\overline{z}) = I_{L^2(0,\infty)}. \qquad (2.43)
$$

Taking adjoints on both sides of (2.43), and using the relation $(AB)^* \supseteq B^*A^*$, we have

$$
\begin{aligned}
I_{L^2(0,\infty)} = I^*_{L^2(0,\infty)} &= [(H_\alpha - \overline{z}I_{L^2(0,\infty)})T_\alpha(\overline{z})]^* \\
&\supseteq T_\alpha(\overline{z})^*(H_\alpha - \overline{z}I_{L^2(0,\infty)})^* \\
&= T_\alpha(\overline{z})^*(H_\alpha^* - (\overline{z}I_{L^2(0,\infty)})^*) \\
&= T_\alpha(\overline{z})^*(H_\alpha - zI_{L^2(0,\infty)}) \qquad (2.44) \\
&= T_\alpha(z)(H_\alpha - zI_{L^2(0,\infty)}). \qquad (2.45)
\end{aligned}
$$

To get (2.44), we used the fact that $(A - wI)^* = A^* - \overline{w}I$ for any densely defined operator A and any $w \in \mathbb{C}$ together with the self-adjointness property of H_α, $H_\alpha^* = H_\alpha$. In (2.45), we used $T_\alpha(w) = T_\alpha(\overline{w})^*$ for any $w \in \rho(H_0) \cap \rho(H_\alpha)$, which follows from (2.23), (1.74), and the procedure for taking the adjoint of a rank one operator: if $\mathcal{H}$ is a separable Hilbert space and $f, g \in \mathcal{H}$, then the operator A defined by

$$Ah = \langle f, h \rangle_{\mathcal{H}} g, \quad h \in \operatorname{dom}(A) = \mathcal{H}, \tag{2.46}$$

is a bounded linear operator on $\mathcal{H}$, and its adjoint is given by

$$A^* = \langle g, h \rangle_{\mathcal{H}} f, \quad h \in \mathcal{H}. \tag{2.47}$$

With (2.45) we have now shown that $T_\alpha(z)(H_\alpha - zI_{L^2(0,\infty)})$ is a restriction of the identity operator $I_{L^2(0,\infty)}$. Since $T_\alpha(z) \in \mathcal{B}(L^2(0,\infty))$ (in particular $\operatorname{dom}(T_\alpha(z)) = L^2(0,\infty)$), we have

$$\operatorname{dom}(T_\alpha(z)(H_\alpha - zI_{L^2(0,\infty)})) = \operatorname{dom}(H_\alpha), \tag{2.48}$$

and we conclude that $T_\alpha(z)(H_\alpha - zI_{L^2(0,\infty)})$ is the restriction of the identity operator to $\operatorname{dom}(H_\alpha)$, which is precisely the statement in (2.26). $\square$

CHAPTER 3

A TRACE FORMULA FOR HALF-LINE SCHRÖDINGER OPERATORS

If $\mathcal{H}$ is a separable Hilbert space and $f, g \in \mathcal{H}$, then the operator A defined by

$$Ah = \langle f, h \rangle_{\mathcal{H}} g, \quad h \in \operatorname{dom}(A) = \mathcal{H}, \tag{3.1}$$

is a bounded linear operator on $\mathcal{H}$. It is customary to write

$$A = \langle f, \cdot \rangle_{\mathcal{H}} g. \tag{3.2}$$

Clearly, A is a finite rank operator since the range of A is contained in the one-dimensional subspace spanned by the vector g. In fact, A has rank equal to zero if at least one one of f or g is the zero vector; otherwise, A has rank equal to one.

Proposition 3.1. *If $\mathcal{H}$ is a separable Hilbert space and $f, g \in \mathcal{H}$, then the operator $A = \langle f, \cdot \rangle_{\mathcal{H}} g$ belongs to the trace class $\mathcal{B}_1(\mathcal{H})$ with*

$$\operatorname{tr}_{\mathcal{H}}(A) = \langle f, g \rangle_{\mathcal{H}}. \tag{3.3}$$

Proof. If at least one of f or g is the zero vector, then A is the zero operator and all of the claims are trivial. Therefore, we may assume without loss that $f, g \in \mathcal{H} \backslash \{0\}$. Since A is finite rank, and every finite rank operator belongs to the trace class, it follows that $A \in \mathcal{B}_1(\mathcal{H})$.

To compute $\operatorname{tr}_{\mathcal{H}}(A)$, let $\{h_j\}_{j=1}^{\nu}$, where $\nu = \dim(\mathcal{H}) \in \mathbb{N} \cup \{\infty\}$ is the dimension of the separable Hilbert space $\mathcal{H}$, denote an orthonormal basis of $\mathcal{H}$, chosen so that $h_1 = \|g\|_{\mathcal{H}}^{-1} g$.

This choice implies

$$\langle h_j, g\rangle_{\mathcal{H}} = \delta_{1,j}\|g\|_{\mathcal{H}}, \quad 1 \le j \le \nu,\, j \in \mathbb{N}, \tag{3.4}$$

and then by the definition of the trace functional,

$$\begin{aligned}
\operatorname{tr}_{\mathcal{H}}(A) &= \sum_{j=1}^{\nu} \langle h_j, A h_j\rangle_{\mathcal{H}} \\
&= \sum_{j=1}^{\nu} \big\langle h_j, \langle f, h_j\rangle_{\mathcal{H}} g\big\rangle_{\mathcal{H}} \\
&= \sum_{j=1}^{\nu} \langle f, h_j\rangle_{\mathcal{H}} \langle h_j, g\rangle_{\mathcal{H}} \\
&= \langle f, \|g\|_{\mathcal{H}}^{-1} g\rangle_{\mathcal{H}} \|g\|_{\mathcal{H}} \\
&= \langle f, g\rangle_{\mathcal{H}}.
\end{aligned} \tag{3.5}$$

$\square$

To prove the main theorem of this chapter, we need several properties of solutions to $\mathcal{L}f = zf$. The first result shows that the product of two solutions is a derivative.

Proposition 3.2 (Lemma 4.5.2 in [**10**]). *Assume Hypothesis* 1.9. *For any two solutions $u(\zeta, x)$ and $v(\zeta, x)$ of $\mathcal{L}f = \zeta^2 f$, one has*

$$2\zeta u(\zeta, x) v(\zeta, x) = \big(u'(\zeta, x)\dot{v}(\zeta, x) - u(\zeta, x)\dot{v}'(\zeta, x)\big)'. \tag{3.6}$$

Proof. Take $v(\zeta, x)$ as a solution to $\mathcal{L}f = \zeta^2 f$, then

$$-v''(\zeta, x) + V(x) v(\zeta, x) = \zeta^2 v(\zeta, x). \tag{3.7}$$

Differentiate throughout with respect to ζ to obtain

$$-\dot{v}''(\zeta, x) + V(x)\dot{v}(\zeta, x) = \zeta^2 \dot{v}(\zeta, x) + 2\zeta v(\zeta, x). \tag{3.8}$$

If we multiply by $u(\zeta, x)$, we have

$$-u(\zeta,x)\dot{v}''(\zeta,x)+V(x)u(\zeta,x)\dot{v}(\zeta,x)=\zeta^2 u(\zeta,x)\dot{v}(\zeta,x)+2\zeta u(\zeta,x)v(\zeta,x). \tag{3.9}$$

Now take $u(\zeta, x)$ as a solution to $\mathcal{L}f = \zeta^2 f$ and multiply by $\dot{v}(\zeta, x)$:

$$-u''(\zeta,x)\dot{v}(\zeta,x)+V(x)u(\zeta,x)\dot{v}(\zeta,x)=\zeta^2 u(\zeta,x)\dot{v}(\zeta,x). \tag{3.10}$$

Taking the difference of the above two equations, we then have

$$u''(\zeta,x)\dot{v}(\zeta,x)-u(\zeta,x)\dot{v}''(\zeta,x)=2\zeta u(\zeta,x)v(\zeta,x). \tag{3.11}$$

Note that

$$\begin{aligned} &u''(\zeta,x)\dot{v}(\zeta,x)-u(\zeta,x)\dot{v}''(\zeta,x) \\ &\quad = u''(\zeta,x)\dot{v}(\zeta,x)+u'(\zeta,x)\dot{v}'(\zeta,x)-u'(\zeta,x)\dot{v}'(\zeta,x)-u(\zeta,x)\dot{v}''(\zeta,x) \\ &\quad = [u'(\zeta,x)\dot{v}(\zeta,x)]'-[u(\zeta,x)\dot{v}'(\zeta,x)]' \\ &\quad = [u'(\zeta,x)\dot{v}(\zeta,x)-u(\zeta,x)\dot{v}'(\zeta,x)]'. \end{aligned} \tag{3.12}$$

Then $2\zeta u(\zeta,x)v(\zeta,x) = [u'(\zeta,x)\dot{v}(\zeta,x)-u(\zeta,x)\dot{v}'(\zeta,x)]'$, as desired. □

The next result gives the limiting behavior of the ζ-derivative of $e^{-i\zeta x}\theta(\zeta, x)$ and its x-derivative as $x \to \infty$.

Proposition 3.3 (Lemma 4.1.7 in [**10**]). *Assume Hypothesis* 1.31 *and define the function $b(\zeta, x)$ by*

$$b(\zeta,x)=e^{-i\zeta x}\theta(\zeta,x), \quad x\in[0,\infty). \tag{3.13}$$

For each fixed $x \geq 0$, $\dot{b}(\zeta, x)$ is a continuous function of ζ in the closed upper half plane, with the possible exception of $\zeta = 0$, and

$$\lim_{x\to\infty}\dot{b}(\zeta,x)=0, \tag{3.14}$$

$$\lim_{x\to\infty} \dot{b}'(\zeta, x) = 0. \tag{3.15}$$

As a consequence of this proposition, we obtain similar results for $\theta(\zeta, \cdot)$.

COROLLARY 3.4. *If Hypothesis* 1.31 *holds and* $\zeta^2 = z \in \mathbb{C}\backslash\mathbb{R}$, *then*

$$\lim_{x\to\infty} \dot{\theta}(\zeta, x) = 0,$$

$$\lim_{x\to\infty} \dot{\theta}'(\zeta, x) = 0.$$

PROOF. Let $b(\zeta, x)$ be defined as in (3.13). Taking the derivative of $b(\zeta, x)$ with respect to ζ using the product rule, we have

$$\dot{b}(\zeta, x) = -ixe^{-i\zeta x}\theta(\zeta, x) + e^{-i\zeta x}\dot{\theta}(\zeta, x), \quad x \in [0, \infty), \tag{3.16}$$

and then

$$\dot{\theta}(\zeta, x) = e^{i\zeta x}\dot{b}(\zeta, x) + ix\theta(\zeta, x), \quad x \in [0, \infty). \tag{3.17}$$

As a result, by (1.64) and (3.14)

$$\begin{aligned}
\lim_{x\to\infty} \dot{\theta}(\zeta, x) &= \lim_{x\to\infty} e^{i\zeta x}\dot{b}(\zeta, x) + i \lim_{x\to\infty} x\theta(\zeta, x) \\
&= \lim_{x\to\infty} e^{i\zeta x}\dot{b}(\zeta, x) + i \lim_{x\to\infty} xe^{i\zeta x}[1 + o(1)] \\
&= 0, \qquad (3.18)
\end{aligned}$$

since $e^{i\zeta x} = e^{i\mathrm{Re}(\zeta)x}e^{-\mathrm{Im}(\zeta)x}$ goes to zero exponentially as $x \to \infty$ if $\zeta^2 = z \in \mathbb{C}\backslash\mathbb{R}$.

Now, differentiating (3.17) with respect to x,

$$\dot{\theta}'(\zeta, x) = i\zeta e^{i\zeta x}\dot{b}(\zeta, x) + e^{i\zeta x}\dot{b}'(\zeta, x) + i\theta(\zeta, x) + ix\theta'(\zeta, x), \quad x \in [0, \infty), \tag{3.19}$$

and then by (1.64), (3.14), and (3.15)

$$\lim_{x\to\infty} \dot{\theta}'(\zeta, x) = i\zeta \lim_{x\to\infty}[e^{i\zeta x}\dot{b}(\zeta, x)] + \lim_{x\to\infty}[e^{i\zeta x}\dot{b}'(\zeta, x)] + i \lim_{x\to\infty} \theta(\zeta, x) + i \lim_{x\to\infty}[x\theta'(\zeta, x)] = 0.$$

$\square$

As a final preparation, we recall the following result which computes the trace of the difference of the resolvents of $H_0^{(0)}$ and H_0.

Proposition 3.5 (Proposition 4.5.3 in [**10**]). *If Hypothesis* 1.31 *holds, then*

$$\operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_0^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_0 - zI_{L^2(0,\infty)}\big)^{-1}\Big) = \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.20}$$

With these preparations in place, we may now state and prove the main theorem of this thesis.

Theorem 3.6. *If Hypothesis* 1.31 *holds, then*

$$\begin{aligned}
&\operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_\alpha^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_\alpha - zI_{L^2(0,\infty)}\big)^{-1}\Big) \\
&\quad = \frac{\cos(\alpha)\dot{w}(\zeta) - \sin(\alpha)\dot{\theta}'(\zeta,0)}{2\zeta[\cos(\alpha)w(\zeta) - \sin(\alpha)\theta'(\zeta,0)]} + \frac{i\sin(\alpha)}{2\zeta[\cos(\alpha) - i\zeta\sin(\alpha)]}, \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{3.21}$$

Proof. Let $z \in \mathbb{C}\backslash\mathbb{R}$. It follows that $\operatorname{Im}(\zeta) > 0$. The main strategy for the proof is to apply Krein's resolvent identity, specifically Theorem 2.13, to relate the resolvent of $H_\alpha^{(0)}$ to the resolvent of $H_0^{(0)}$ and to relate the resolvent of H_α to the resolvent of H_0. By (2.21), and linearity of the trace functional,

$$\begin{aligned}
&\operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_\alpha^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_\alpha - zI_{L^2(0,\infty)}\big)^{-1}\Big) \\
&\quad = \operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_0^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_0 - zI_{L^2(0,\infty)}\big)^{-1} \\
&\qquad - p_\alpha^{(0)}(z)\langle\theta^{(0)}(-\overline{\zeta},\cdot),\cdot\rangle_{L^2(0,\infty)}\theta^{(0)}(\zeta,\cdot) + p_\alpha(z)\langle\theta(-\overline{\zeta},\cdot),\cdot\rangle_{L^2(0,\infty)}\theta(\zeta,\cdot)\Big) \\
&\quad = \operatorname{tr}_{L^2(0,\infty)}\Big(\big(H_0^{(0)} - zI_{L^2(0,\infty)}\big)^{-1} - \big(H_0 - zI_{L^2(0,\infty)}\big)^{-1}\Big) \\
&\qquad - p_\alpha^{(0)}(z)\operatorname{tr}_{L^2(0,\infty)}\Big(\langle\theta^{(0)}(-\overline{\zeta},\cdot),\cdot\rangle_{L^2(0,\infty)}\theta^{(0)}(\zeta,\cdot)\Big) \\
&\qquad + p_\alpha(z)\operatorname{tr}_{L^2(0,\infty)}\Big(\langle\theta(-\overline{\zeta},\cdot),\cdot\rangle_{L^2(0,\infty)}\theta(\zeta,\cdot)\Big) \\
&\quad = \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)} - p_\alpha^{(0)}(z)\langle\theta^{(0)}(-\overline{\zeta},\cdot),\theta^{(0)}(\zeta,\cdot)\rangle_{L^2(0,\infty)} + p_\alpha(z)\langle\theta(-\overline{\zeta},\cdot),\theta(\zeta,\cdot)\rangle_{L^2(0,\infty)},
\end{aligned} \tag{3.22}$$

where in the last line, we applied Proposition 3.5.

Using (1.89), the inner product $\langle\theta^{(0)}(-\overline{\zeta},\cdot),\theta^{(0)}(\zeta,\cdot)\rangle_{L^2(0,\infty)}$ may be explicitly computed as follows:

$$\begin{aligned}
\langle\theta^{(0)}(-\overline{\zeta},\cdot),\theta^{(0)}(\zeta,\cdot)\rangle &= \int_0^\infty \overline{e^{-i\overline{\zeta}x}}e^{i\zeta x}dx \\
&= \int_0^\infty \overline{e^{-ix[\overline{\mathrm{Re}(\zeta)+i\mathrm{Im}(\zeta)}]}}e^{i\zeta x}dx \\
&= \int_0^\infty \overline{e^{-ix[\mathrm{Re}(\zeta)-i\mathrm{Im}(\zeta)]}}e^{i\zeta x}dx \\
&= \int_0^\infty \overline{e^{-ix\mathrm{Re}(\zeta)-x\mathrm{Im}(\zeta)}}e^{ix[\mathrm{Re}(\zeta)+i\mathrm{Im}(\zeta)]}dx \\
&= \int_0^\infty e^{ixRe(\zeta)-x\mathrm{Im}(\zeta)}e^{ix\mathrm{Re}(\zeta)-x\mathrm{Im}(\zeta)}dx \\
&= \int_0^\infty e^{2ix\mathrm{Re}(\zeta)}e^{-2x\mathrm{Im}(\zeta)}dx \\
&= \int_0^\infty e^{2ix[\mathrm{Re}(\zeta)+i\mathrm{Im}(\zeta)]}dx \\
&= \int_0^\infty e^{2ix\zeta}dx \\
&= \lim_{t\to\infty}\frac{e^{2ix\zeta}}{2i\zeta}\bigg|_0^t \\
&= \left[\lim_{t\to\infty}\frac{e^{2i\mathrm{Re}(\zeta)t}e^{-2\mathrm{Im}(\zeta)t}}{2i\zeta}\right]-\frac{1}{2i\zeta} \\
&= -\frac{1}{2i\zeta} \\
&= \frac{i}{2\zeta},
\end{aligned} \tag{3.23}$$

where we used $\mathrm{Im}(\zeta)>0$ to conclude that $\lim_{t\to\infty}e^{-2\mathrm{Im}(\zeta)t}=0$.

The inner product $\langle\theta(-\overline{\zeta},\cdot),\theta(\zeta,\cdot)\rangle_{L^2(0,\infty)}$ may also be computed using Proposition 3.2 as follows:

$$
\begin{aligned}
&\langle \theta(-\overline{\zeta},\cdot),\theta(\zeta,\cdot)\rangle \\
&\quad= \int_0^\infty \overline{\theta(-\overline{\zeta},x)}\theta(\zeta,x)dx \\
&\quad= \int_0^\infty \theta(\zeta,x)\theta(\zeta,x)dx \\
&\quad= \int_0^\infty \frac{1}{2\zeta}\Big[\theta'(\zeta,x)\dot{\theta}(\zeta,x)-\theta(\zeta,x)\dot{\theta}'(\zeta,x)\Big]'dx \\
&\quad= \frac{1}{2\zeta}\Big[\theta'(\zeta,x)\dot{\theta}(\zeta,x)-\theta(\zeta,x)\dot{\theta}'(\zeta,x)\Big]\Big|_0^\infty \\
&\quad= \frac{1}{2\zeta}\lim_{x\to\infty}\Big[\underbrace{\theta'(\zeta,x)}_{\to 0}\underbrace{\dot{\theta}(\zeta,x)}_{\to 0}-\underbrace{\theta(\zeta,x)}_{\to 0}\underbrace{\dot{\theta}'(\zeta,x)}_{\to 0}-\Big[\theta'(\zeta,0)\dot{\theta}(\zeta,0)-\theta(\zeta,0)\dot{\theta}'(\zeta,0)\Big]\Big] \\
&\quad= -\frac{1}{2\zeta}\Big[\theta'(\zeta,0)\dot{\theta}(\zeta,0)-\theta(\zeta,0)\dot{\theta}'(\zeta,0)\Big], \qquad (3.24)
\end{aligned}
$$

where in the last equality we applied (1.64) and Corollary 3.4 to conclude that the first two terms converge to zero as $x \to \infty$ if $\mathrm{Im}(\zeta) > 0$.

Returning to (3.22), and applying (3.23), (3.24), and (1.89), we then have

$$
\begin{aligned}
&\mathrm{tr}_{L^2(0,\infty)}\Big(\big(H_\alpha^{(0)}-zI_{L^2(0,\infty)}\big)^{-1}-\big(H_\alpha-zI_{L^2(0,\infty)}\big)^{-1}\Big) \\
&\quad= \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)}-\frac{i}{2\zeta}p_\alpha^{(0)}(z)-\frac{1}{2\zeta}p_\alpha(z)[\theta'(\zeta,0)\dot{\theta}(\zeta,0)-\theta(\zeta,0)\dot{\theta}'(\zeta,0)] \\
&\quad= \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)}-\frac{i}{2\zeta}\frac{\sin(\alpha)}{\underbrace{\theta^{(0)}(\zeta,0)}_{=1}[\sin(\alpha)\underbrace{\theta^{(0)\prime}(\zeta,0)}_{=i\zeta}-\cos(\alpha)\underbrace{\theta^{(0)}(\zeta,0)}_{=1}]} \\
&\qquad -\frac{1}{2\zeta}\frac{\sin(\alpha)[\theta'(\zeta,0)\dot{\theta}(\zeta,0)-\theta(\zeta,0)\dot{\theta}'(\zeta,0)]}{\underbrace{\theta(\zeta,0)}_{=w(\zeta)}[\sin(\alpha)\theta'(\zeta,0)-\cos(\alpha)\underbrace{\theta(\zeta,0)}_{=w(\zeta)}]} \\
&\quad= \frac{\dot{w}(\zeta)}{2\zeta w(\zeta)}+\frac{i}{2\zeta}\frac{\sin(\alpha)}{\cos(\alpha)-i\zeta\sin(\alpha)}+\frac{1}{2\zeta}\frac{\sin(\alpha)[\theta'(\zeta,0)\dot{w}(\zeta)-w(\zeta)\dot{\theta}'(\zeta,0)]}{w(\zeta)[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]} \\
&\quad= \frac{\dot{w}(\zeta)[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}{2\zeta w(\zeta)[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}+\frac{i\sin(\alpha)}{2\zeta[\cos(\alpha)-i\zeta\sin(\alpha)]}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{\sin(\alpha)[\theta'(\zeta,0)\dot{w}(\zeta)-w(\zeta)\dot{\theta}'(\zeta,0)]}{2\zeta w(\zeta)[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}\\
&=\frac{\cos(\alpha)\dot{w}(\zeta)w(\zeta)-\sin(\alpha)w(\zeta)\dot{\theta}'(\zeta,0)}{2\zeta w(\zeta)[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}+\frac{i\sin(\alpha)}{2\zeta[\cos(\alpha)-i\zeta\sin(\alpha)]}\\
&=\frac{\cos(\alpha)\dot{w}(\zeta)-\sin(\alpha)\dot{\theta}'(\zeta,0)}{2\zeta[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}+\frac{i\sin(\alpha)}{2\zeta[\cos(\alpha)-i\zeta\sin(\alpha)]}\\
&=\frac{\cos(\alpha)\dot{\theta}(\zeta,0)-\sin(\alpha)\dot{\theta}'(\zeta,0)}{2\zeta[\cos(\alpha)\theta(\zeta,0)-\sin(\alpha)\theta'(\zeta,0)]}+\frac{i\sin(\alpha)}{2\zeta[\cos(\alpha)-i\zeta\sin(\alpha)]}\\
&=\frac{\cos(\alpha)\dot{w}(\zeta)-\sin(\alpha)\dot{\theta}'(\zeta,0)}{2\zeta[\cos(\alpha)w(\zeta)-\sin(\alpha)\theta'(\zeta,0)]}+\frac{i\sin(\alpha)}{2\zeta[\cos(\alpha)-i\zeta\sin(\alpha)]},
\end{aligned}
\tag{3.25}
$$

which concludes the proof. □

The main idea in the proof of Theorem 3.6 is the Krein resolvent identity which holds in an abstract setting. By abstracting the key elements from the proof, we obtain a general abstract result for pairs of self-adjoint operators. In order to introduce this abstract result, we introduce the following hypothesis.

HYPOTHESIS 3.7. *Let A_0 and B_0 denote densely defined closed symmetric operators in the Hilbert space $\mathcal{H}$, each with equal and finite deficiency indices:*

$$
d_\pm(A_0) := \dim(\ker(A_0^* \mp iI_{\mathcal{H}})) = m < \infty, \quad d_\pm(B_0) := \dim(\ker(B_0^* \mp iI_{\mathcal{H}})) = n < \infty,
\tag{3.26}
$$

for some $m, n \in \mathbb{N}_0$.

By von Neumann's theory of self-adjoint extensions, both A_0 and B_0 possess self-adjoint extensions.

HYPOTHESIS 3.8. *In addition to Hypothesis 3.7, suppose that:*

(i) A_1, A_2 are two self-adjoint extensions of A_0, and that B_1, B_2 are two self-adjoint extensions of B_0.

(ii) $r \in \mathbb{N}_0$ *denotes the common deficiency index of the maximal common part* A *of* A_1 *and* A_2 *so that*

$$d_{\pm}(A) = \dim(\ker(A^* \mp iI_{\mathcal{H}})) = r \le m, \tag{3.27}$$

(iii) $s \in \mathbb{N}_0$ *denotes the common deficiency index of the maximal common part* B *of* B_1 *and* B_2 *so that*

$$d_{\pm}(B) = \dim(\ker(B^* \mp iI_{\mathcal{H}})) = s \le n. \tag{3.28}$$

(iv) For each $z \in \rho(A_1) \cap \rho(A_2)$*, let* $\{f_k(z)\}_{k=1}^r$ *denote a basis for* $\ker(A^* - zI_{\mathcal{H}})$*, and for each* $\tilde{z} \in \rho(B_1) \cap \rho(B_2)$*, let* $\{g_k(\tilde{z})\}_{k=1}^s$ *denote a basis for* $\ker(B^* - \tilde{z}I_{\mathcal{H}})$*, so that*

$$(A_2 - zI_{\mathcal{H}})^{-1} = (A_1 - zI_{\mathcal{H}})^{-1} - \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}), \cdot\,)_{\mathcal{H}} f_j(z), \quad z \in \rho(A_1) \cap \rho(A_2), \tag{3.29}$$

$$(B_2 - \tilde{z}I_{\mathcal{H}})^{-1} = (B_1 - \tilde{z}I_{\mathcal{H}})^{-1} - \sum_{j,k=1}^{s} \beta_{j,k}(\tilde{z})(g_k(\overline{\tilde{z}}\,), \cdot\,)_{\mathcal{H}} g_j(\tilde{z}), \quad z \in \rho(B_1) \cap \rho(B_2). \tag{3.30}$$

for an appropriate choice of scalars

$$\{\alpha_{j,k}(z)\}_{1 \le j,k \le r} \subset \mathbb{C} \quad \textit{and} \quad \{\beta_{j,k}(\tilde{z})\}_{1 \le j,k \le s} \subset \mathbb{C} \tag{3.31}$$

by Krein's resolvent formula.

With these hypotheses in place, the trace of the resolvent difference of A_2 and B_2 may be computed in terms of the trace of the resolvent difference of A_1 and B_1.

Theorem 3.9. *If Hypothesis* 3.8 *holds and for some* $z_0 \in \mathbb{C}\backslash\mathbb{R}$,

$$\big[(A_1 - z_0 I_{\mathcal{H}})^{-1} - (B_1 - z_0 I_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}), \tag{3.32}$$

then

$$\big[(A_2 - zI_{\mathcal{H}})^{-1} - (B_2 - zI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.33}$$

and

$$
\begin{aligned}
&\operatorname{tr}_{\mathcal{H}}\big((A_2 - zI_{\mathcal{H}})^{-1} - (B_2 - zI_{\mathcal{H}})^{-1}\big)\\
&\quad = \operatorname{tr}_{\mathcal{H}}\big((A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\big)\\
&\qquad - \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}), f_j(z))_{\mathcal{H}} + \sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}), g_j(z))_{\mathcal{H}}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (3.34)
\end{aligned}
$$

Proof. We begin by noting that (3.32) implies

$$
\big[(A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \qquad (3.35)
$$

which follows from the following resolvent identity taken from [**8**, Exercise 7.8]:

$$
\begin{aligned}
(S_2 - z_0 I_{\mathcal{H}})^{-1} - (S_1 - z_0 I_{\mathcal{H}})^{-1} &= (S_2 - zI_{\mathcal{H}})(S_2 - z_0 I_{\mathcal{H}})^{-1}\\
\times \big[(S_2 - zI_{\mathcal{H}})^{-1} &- (S_1 - zI_{\mathcal{H}})^{-1}\big](S_1 - zI_{\mathcal{H}})(S_1 - z_0 I_{\mathcal{H}})^{-1}, \qquad (3.36)\\
&z, z_0 \in \rho(S_1) \cap \rho(S_2),
\end{aligned}
$$

for any pair of linear operators S_1 and S_2 in $\mathcal{H}$ with $\rho(S_1) \cap \rho(S_2) \neq \emptyset$.

Let $z \in \mathbb{C}\backslash\mathbb{R}$ be fixed. Subtracting (3.30) from (3.29), we have

$$
\begin{aligned}
&(A_2 - zI_{\mathcal{H}})^{-1} - (B_2 - zI_{\mathcal{H}})^{-1}\\
&\quad = (A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\\
&\qquad - \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}), \cdot\,)_{\mathcal{H}} f_j(z) + \sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}), \cdot\,)_{\mathcal{H}} g_j(z), \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (3.37)
\end{aligned}
$$

By the assumption in (3.35), the resolvent difference on the right-hand side of (3.37) belongs to the trace class $\mathcal{B}_1(\mathcal{H})$. In addition,

$$
\Bigg[- \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}), \cdot\,)_{\mathcal{H}} f_j(z) + \sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}), \cdot\,)_{\mathcal{H}} g_j(z)\Bigg] \in \mathcal{B}_1(\mathcal{H}), \qquad (3.38)
$$

since the operator under square brackets in (3.38) has finite rank at most equal to $r+s$, and every finite rank operator belongs to the trace class. Since the trace class is a vector space, the right-hand side of (3.37) belongs to the trace class $\mathcal{B}_1(\mathcal{H})$, and (3.33) follows.

To prove (3.34), we apply linearity of the trace functional $\operatorname{tr}_{\mathcal{H}}(\,\cdot\,)$ and Proposition 3.1:

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}}\big((A_2 - zI_{\mathcal{H}})^{-1} - (B_2 - zI_{\mathcal{H}})^{-1}\big)\\
&\quad = \operatorname{tr}_{\mathcal{H}}\Bigg((A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1} - \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} f_j(z)\\
&\qquad\qquad + \sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} g_j(z)\Bigg)\\
&\quad = \operatorname{tr}_{\mathcal{H}}\big((A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\big) - \operatorname{tr}_{\mathcal{H}}\Bigg(\sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} f_j(z)\Bigg)\\
&\qquad + \operatorname{tr}_{\mathcal{H}}\Bigg(\sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} g_j(z)\Bigg)\\
&\quad = \operatorname{tr}_{\mathcal{H}}\big((A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\big) - \sum_{j,k=1}^{r} \alpha_{j,k}(z)\operatorname{tr}_{\mathcal{H}}\big((f_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} f_j(z)\big)\\
&\qquad + \sum_{j,k=1}^{s} \beta_{j,k}(z)\operatorname{tr}_{\mathcal{H}}\big((g_k(\overline{z}),\,\cdot\,)_{\mathcal{H}} g_j(z)\big)\\
&\quad = \operatorname{tr}_{\mathcal{H}}\big((A_1 - zI_{\mathcal{H}})^{-1} - (B_1 - zI_{\mathcal{H}})^{-1}\big) - \sum_{j,k=1}^{r} \alpha_{j,k}(z)(f_k(\overline{z}), f_j(z))_{\mathcal{H}}\\
&\qquad + \sum_{j,k=1}^{s} \beta_{j,k}(z)(g_k(\overline{z}), g_j(z))_{\mathcal{H}}, \qquad (3.39)
\end{aligned}$$

which proves (3.37). $\square$

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VITA

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