ABSTRACT

On Functions Related to the Spectral Theory of Sturm–Liouville Operators

Jonathan Stanfill, Ph.D.

Mentor: Fritz Gesztesy, Ph.D.

Functions related to the spectral theory of differential operators have been extensively studied due to their many applications in mathematics and physics. In this dissertation, we will consider spectral ζ-functions, ζ-regularized functional determinants, and Donoghue m-functions associated with Sturm–Liouville operators. We apply our results to an array of examples, including regular Schrödinger operators as well as Jacobi and generalized Bessel operators in the singular context.

We begin by employing a recently developed unified approach to the computation of traces of resolvents and ζ-functions to efficiently compute values of spectral ζ-functions at positive integers associated with regular (three-coefficient) self-adjoint Sturm–Liouville differential expressions τ. Furthermore, we give the full analytic continuation of the ζ-function through a Liouville transformation and provide an explicit expression for the ζ-regularized functional determinant in terms of a particular set of a fundamental system of solutions of $\tau y = zy$.

Next we turn to Donoghue m-functions. Assuming the standard local integrability hypotheses on the coefficients of the singular Sturm–Liouville differential equation τ, we study all corresponding self-adjoint realizations in $L^2((a,b);rdx)$ and systematically construct the associated Donoghue m-functions in all cases where τ is in the limit circle case at least at one interval endpoint a or b.

Finally, we construct Donoghue m-functions for the Jacobi differential operator in $L^2\big((-1,1);(1-x)^\alpha(1+x)^\beta dx\big)$ associated with the differential expression $\tau_{\alpha,\beta} = -(1-x)^{-\alpha}(1+x)^{-\beta}(d/dx)\big((1-x)^{\alpha+1}(1+x)^{\beta+1}\big)(d/dx), \quad x \in (-1,1),\ \alpha,\beta \in \mathbb{R}$, whenever at least one endpoint, $x = \pm 1$, is in the limit circle case. In doing so, we provide a full treatment of the Jacobi operator's m-functions corresponding to coupled boundary conditions whenever both endpoints are in the limit circle case.

On Functions Related to the Spectral Theory of Sturm–Liouville Operators

by

Jonathan Stanfill, B.A., M.S.

A Dissertation

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Dorina Mitrea, Ph.D., Chairperson

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Approved by the Dissertation Committee

Fritz Gesztesy, Ph.D., Chairperson

Gerald B. Cleaver, Ph.D.

Lance L. Littlejohn, Ph.D.

Brian Simanek, Ph.D.

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J. Larry Lyon, Ph.D., Dean

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

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I begin by thanking the Department of Mathematics at Baylor University for accepting me into the doctoral program after years away from academia. This decision has changed the course of my life completely and I will be forever grateful.

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To Amanda for her love, constant support, and making this possible

CHAPTER ONE

Introduction

1.1 Background and Motivation

Our research is focused on functions related to the spectral theory of differential operators. The analysis of these objects is of widespread interest since in many areas of mathematics and physics one is often confronted with the problem of extracting relevant information from the spectrum of differential operators. In one dimension, these differential operators are often Sturm–Liouville operators associated with the second-order differential expression

$$\tau = \frac{1}{r(x)}\left[-\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] \text{ for a.e. } x \in (a,b) \subseteq \mathbb{R}. \tag{1.1.1}$$

The investigation of such problems naturally leads to the primary focus of this dissertation: the spectral ζ-function, ζ-regularized functional determinant, and Donoghue m-function. Though these objects will be our main focus, the heat kernel and Weyl–Titchmarsh–Kodaira m-function will play a role in the analysis and motivation of this research project. A description of each is given next.

The spectral ζ-function represents a generalization of the more familiar Riemann ζ-function in which the integers are replaced by the non-vanishing positive eigenvalues of a differential operator: Suppose S is a self-adjoint operator in a Hilbert space, $\mathcal{H}$, bounded from below, satisfying $(S - zI_{\mathcal{H}})^{-1} \in \mathcal{B}_1(\mathcal{H})$ (i.e., trace class) for some (and hence for all) $z \in \rho(S)$, the resolvent set of S. Then one denotes the spectrum of S by $\sigma(S) = \{\lambda_j\}_{j\in J}$ and defines the spectral ζ-function of the operator, S, as

$$\zeta(s;S) := \sum_{\substack{j\in J \\ \lambda_j \neq 0}} \lambda_j^{-s} \tag{1.1.2}$$

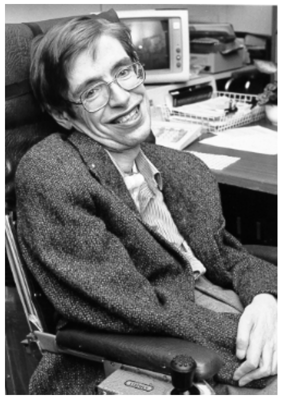

Figure 1.1. Stephen Hawking [102]

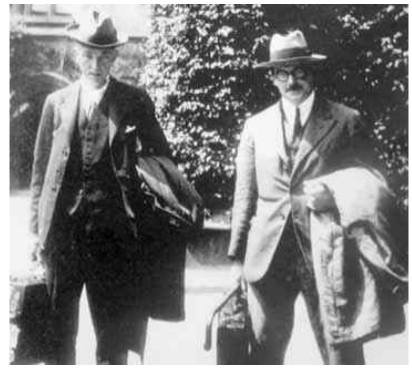

Figure 1.2: Left: G. H. Hardy, Right: John E. Littlewood [97]

with $J \subset \mathbb{Z}$ an appropriate index set where eigenvalues are counted according to their multiplicity and $\mathrm{Re}(s) > 0$ sufficiently large such that the sum converges absolutely.

The spectral ζ-function is of fundamental importance for the analysis of complex powers of elliptic operators and for the study of ζ-regularized functional determinants, formally defined as $\exp(-\zeta'(0; S))$. This topic includes Stephen Hawking (Figure 1.1) as one of its original investigators applying the functional determinant as a regulator in physical problems in [94], though many of the mathematical methods used can be traced back to G. H. Hardy and J. E. Littlewood (Figure 1.2) in [90] (see also [157]). The analytic continuation of the ζ-function is used in studying the small time asymptotic behavior of the trace of the heat kernel, which is the fundamental solution to the heat equation on a manifold endowed with appropriate boundary conditions. This small time asymptotic behavior is used in order to extract geometric information about the underlying manifold (see, e.g., [106, 115]) and in spectral analysis thanks to a relation that exists between the heat equation and the Atiyah-Singer index theorem (see [8, 9]).

The widespread use of both of these functions in physics can be found especially in the area of quantum field theory (see, e.g., [45, 46]). Many characteristics of quantum fields are encoded in the effective action (see, e.g., [45]) which is a functional that describes how the classical equations of motion are modified by quantum

Figure 1.3. Hermann Weyl [98]

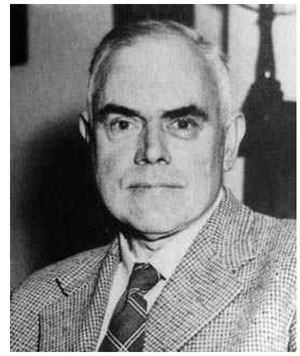

Figure 1.4. Edward Titchmarsh [99]

effects. The effective action can be expressed in terms of the ζ-regularized functional determinant of an elliptic operator and, therefore, spectral zeta function techniques are particularly suitable for its analysis. Zeta regularization methods continue to prove useful in cosmology to include investigating the Casimir effect related to the cosmological constant. Emilio Elizalde recently published a review [54] of spectral zeta functions and the cosmos as part of the special issue "The Casimir Effect: From a Laboratory Table to the Universe" discussing the entire history of this subject to date.

The Weyl and Donoghue m-functions are indispensable tools in the spectral analysis of self-adjoint extensions, T, of Sturm–Liouville differential operators (see, e.g., [15, Ch. 6], [78,182]). The Weyl m-function was first studied by Hermann Weyl (Figure 1.3) and its relation to spectral theory was later investigated by Edward Titchmarsh (Figure 1.4), who found a simple formula to determine the associated spectral measure. This formula was also discovered by Kunihiko Kodaira (Figure 1.5) around the same time (see [118, 119]); hence, the general terminology Weyl–Titchmarsh–Kodaira m-function (for more details and references, see [15, Introd.]). William F. Donoghue (Figure 1.6) introduced the analogue of the Donoghue m-function studied here in [49] and used it to settle certain inverse spectral problems. Interest in Weyl and Donoghue m-functions arises from the fact that they are gener-

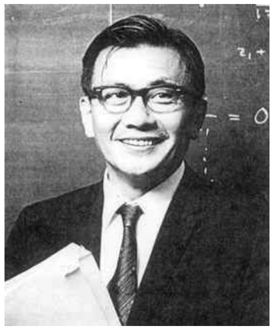

Figure 1.5. Kunihiko Kodaira [100]

Figure 1.6. William F. Donoghue [101]

alized Nevanlinna–Herglotz functions and an analog of the Stieltjes inversion formula applied to them yields that the spectrum (and its subdivisions) of T is related to the singularity structure of the m-functions on the real line.

1.2 Content of the Dissertation

We begin our analysis in Chapter Two by employing a recently developed unified approach to the computation of traces of resolvents and ζ-functions to efficiently compute values of spectral ζ-functions at positive integers associated with regular (three-coefficient) self-adjoint Sturm–Liouville differential expressions τ. Depending on the underlying boundary conditions, we express the ζ-function values in terms of a fundamental system of solutions of $\tau y = zy$ and their expansions about the spectral point $z = 0$. Furthermore, under strengthened hypotheses, we give the full analytic continuation of the ζ-function through a Liouville transformation and provide an explicit expression for the ζ-regularized functional determinant in terms of a particular set of this fundamental system of solutions. An array of examples illustrating the applicability of these methods is provided, including regular Schrödinger operators with zero, piecewise constant, and a linear potential on a compact interval.

We turn to the topic of Donoghue m-functions in Chapter Three. Let $\dot{A}$ be a densely defined, closed, symmetric operator in the complex, separable Hilbert space $\mathcal{H}$ with equal deficiency indices and denote by $\mathcal{N}_i = \ker\big((\dot{A})^* - iI_{\mathcal{H}}\big)$, $\dim(\mathcal{N}_i) =$

$k \in \mathbb{N} \cup \{\infty\}$, the associated deficiency subspace of $\dot{A}$. If A denotes a self-adjoint extension of $\dot{A}$ in $\mathcal{H}$, the Donoghue m-operator $M_{A,\mathcal{N}_i}^{Do}(\,\cdot\,)$ in $\mathcal{N}_i$ associated with the pair $(A, \mathcal{N}_i)$ is given by

$$M_{A,\mathcal{N}_i}^{Do}(z) = zI_{\mathcal{N}_i} + (z^2+1)P_{\mathcal{N}_i}(A - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.2.1}$$

with $I_{\mathcal{N}_i}$ the identity operator in $\mathcal{N}_i$, and $P_{\mathcal{N}_i}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}_i$. Assuming the standard local integrability hypotheses on the coefficients p, q, r, we study all self-adjoint realizations corresponding to the singular differential expression

$$\tau = \frac{1}{r(x)}\left[-\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] \text{ for a.e. } x \in (a,b) \subseteq \mathbb{R}, \tag{1.2.2}$$

in $L^2((a,b); rdx)$. As the principal aim of this chapter, we systematically construct the associated Donoghue m-functions (resp., 2×2 matrices) in all cases where τ is in the limit circle case at least at one interval endpoint a or b.

Finally, in Chapter Four we construct Donoghue m-functions for the Jacobi differential operator in $L^2\big((-1,1); (1-x)^{\alpha}(1+x)^{\beta}dx\big)$ associated with the differential expression

$$\begin{aligned}\tau_{\alpha,\beta} = -(1-x)^{-\alpha}(1+x)^{-\beta}(d/dx)\big((1-x)^{\alpha+1}(1+x)^{\beta+1}\big)(d/dx),& \\ x \in (-1,1),\ \alpha, \beta \in \mathbb{R},&\end{aligned} \tag{1.2.3}$$

whenever at least one endpoint, $x = \pm 1$, is in the limit circle case. In doing so, we provide a full treatment of the Jacobi operator's m-functions corresponding to coupled boundary conditions whenever both endpoints are in the limit circle case, a topic not covered in the literature.

1.3 Attributions

Each publication used throughout this dissertation employed multiple roles crucial to rigorous mathematical research, including: planning, organization, supervision, literary research, citation, notation, proofs, applications, LaTeX coding, styling and formatting, development, construction, proofreading, editing, submission, and revision.

Below we provide, in alphabetical order, the names of all authors listed within each publication used:

- Guglielmo Fucci
- Fritz Gesztesy
- Klaus Kirsten
- Lance Littlejohn
- Roger Nichols
- Mateusz Piorkowski
- Jonathan Stanfill

Furthermore, we confirm that each author contributed equally in all areas of research given above, and are listed alphabetically in each publication. Finally, we note that Chapters Two and Four were reproduced with permission from Springer Nature.

CHAPTER TWO

Spectral ζ-Functions and ζ-Regularized Functional Determinants for Regular Sturm–Liouville Operators

The content of this chapter relies on (but is not identical to) the paper published as: G. Fucci, F. Gesztesy, K. Kirsten, and J. Stanfill, *Spectral ζ-Functions and ζ-Regularized Functional Determinants for Regular Sturm–Liouville Operators*, Res. Math. Sci. **8**, No. 61; 44 pp. (2021).

2.1 Introduction

The principal motivation for this chapter is to illustrate how a recently developed unified approach to the computation of Fredholm determinants, traces of resolvents, and ζ-functions in [74] can be used to efficiently compute certain values of spectral ζ-functions associated with regular Sturm–Liouville operators as well as give the full analytic continuation of the ζ-function through a Liouville transformation and finally provide an explicit expression for the ζ-regularized functional determinant.

In Section 2.2 we begin by outlining the background for regular self-adjoint Sturm–Liouville operators on bounded intervals, that is, operators in $L^2((a,b);rdx)$ with separated and coupled boundary conditions and the associated spectral ζ-functions. Under appropriate hypotheses on the Sturm–Liouville operator associated with three-coefficient differential expressions of the type $\tau = r^{-1}[-(d/dx)p(d/dx) + q]$, certain values of the spectral ζ-function can be found via complex contour integration techniques to be equal to residues of explicit functions involving a canonical system of fundamental solutions $\phi(z,\,\cdot\,,a)$ and $\theta(z,\,\cdot\,,a)$ of $\tau y = zy$ for separated or coupled boundary conditions. Moreover, the zeros with respect to the parameter z of ϕ, θ, and some of their (boundary condition dependent) linear combinations are precisely the eigenvalues corresponding to the underlying operator, including multiplicity.

In Section 2.3 we provide a series expansion for $\phi(z,\,\cdot\,,a)$ and $\theta(z,\,\cdot\,,a)$ about $z=0$ using Volterra integral equations associated with the general three-coefficient regular self-adjoint Sturm–Liouville operator. This method leads to an expansion in powers of z of the fundamental solutions and their z-derivative involving their values at $z=0$ and the appropriate Volterra Green's function. We also investigate the $|z|\to\infty$ asymptotic expansion of the characteristic function appearing in the complex integral representation of the spectral ζ-function given in Section 2.2. This asymptotic expansion is then exploited in order to construct the analytic continuation of the spectral ζ-function and to obtain an explicit expression for the zeta regularized functional determinant.

Section 2.4 contains the main theorems that allow for the calculation of the values of spectral ζ-functions of general regular Sturm–Liouville operators on bounded intervals as ratios of series expansions of (boundary condition dependent) solutions of $\tau y = zy$ about $z=0$. In particular, we consider separated boundary conditions when zero is not an eigenvalue, or, when it is (necessarily) a simple eigenvalue, and coupled boundary conditions when either zero is not an eigenvalue, or, an eigenvalue of multiplicity (necessarily) at most two. (For more details in this context see [74] as well as [84, Ch. 3], [179, Sect. 8.4], [180, Sect. 13.2], and [182, Ch. 4].)

We continue by providing some examples in Section 2.5 illustrating the main theorems and corollaries of Section 2.4 and the zeta regularized functional determinant given in Section 2.3. In particular, we present the case of Schrödinger operators with zero potential imposing Dirichlet, Neumann, periodic, antiperiodic, and Krein–von Neumann boundary conditions. We then consider positive (piecewise) constant and negative constant potentials for Dirichlet boundary conditions, and finally the case of a linear potential.

Here we summarize some of the basic notation used in this chapter. If A is a linear operator mapping (a subspace of) a Hilbert space into another, then $\mathrm{dom}(A)$ and $\ker(A)$ denote the domain and the kernel (i.e., null space) of A. The spectrum, point spectrum, and resolvent set of a closed linear operator in a separable complex Hilbert space, $\mathcal{H}$, will be denoted by $\sigma(\,\cdot\,)$, $\sigma_p(\,\cdot\,)$, and $\rho(\,\cdot\,)$ respectively. If S is self-adjoint in $\mathcal{H}$, the multiplicity of an eigenvalue $z_0 \in \sigma_p(S)$ is denoted $m(z_0; S)$ (the geometric and algebraic multiplicities of S coincide in this case). The proper setting for our investigations is the Hilbert space $L^2((a,b); rdx)$, which we will occasionally abbreviate as $L^2_r((a,b))$. The spectral ζ-function of a self-adjoint linear operator S is denoted by $\zeta(s; S)$. In addition, $\mathrm{tr}_{\mathcal{H}}(T)$ denotes the trace of a trace class operator $T \in \mathcal{B}_1(\mathcal{H})$ and $\det_{\mathcal{H}}(I_{\mathcal{H}} - T)$ the Fredholm determinant of $I_{\mathcal{H}} - T$.

For consistency of notation, throughout this chapter we will follow the conventional notion that derivatives annotated with superscripts are understood as with respect to x and derivatives with respect to ξ will be abbreviated by $\cdot = d/d\xi$. We also employ the notation $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

2.2 Background on Self-Adjoint Regular Sturm–Liouville Operators

In the first part of this section we briefly recall basic facts on regular Sturm–Liouville operators and their self-adjoint boundary conditions. This material is standard and well-known, hence we just refer to some of the standard monographs on this subject, such as, [15, Sect. 6.3], [84, Ch. 3], [104, Sect. II.5], [149, Ch. V], [179, Sect. 8.4], [180, Sect. 13.2], [182, Ch. 4]. In the second part we discuss Fredholm determinants, traces of resolvents, and spectral ζ-functions associated with these regular Sturm–Liouville problems. For background as well as relevant material in this context we refer to [5], [12], [30], [31], [37], [48], [50], [61], [62], [63], [64], [65], [69], [74], [88], [95], [105], [128], [129], [130], [132], [141], [143], [144], [153], [161], [172], [174, Sects. 5.4, 5.5, 6.3], [178].

Throughout our discussion of regular Sturm–Liouville operators we make the following assumptions:

Hypothesis 2.2.1. *Let $(a,b) \subset \mathbb{R}$ be a finite interval and suppose that p, q, r are (Lebesgue) measurable functions on (a,b) such that the following items (i)–(iii) hold:*

(i) $r > 0$ a.e. on (a,b), $r \in L^1((a,b);dx)$.

(ii) $p > 0$ a.e. on (a,b), $1/p \in L^1((a,b);dx)$.

(iii) q is real-valued a.e. on (a,b), $q \in L^1((a,b);dx)$.

Given Hypothesis 2.2.1, we now study Sturm–Liouville operators associated with the general, three-coefficient differential expression τ of the type,

$$\tau = \frac{1}{r(x)}\left[-\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] \text{ for a.e. } x \in (a,b) \subseteq \mathbb{R}. \tag{2.2.1}$$

We start with the notion of minimal and maximal $L^2((a,b);rdx)$-realizations associated with the regular differential expression τ on the finite interval $(a,b) \subset \mathbb{R}$. Throughout this chapter the inner product in $L^2((a,b);rdx)$ is defined by

$$(f,g)_{L^2((a,b);rdx)} = \int_a^b r(x)dx\,\overline{f(x)}g(x), \quad f,g \in L^2((a,b);rdx). \tag{2.2.2}$$

Assuming Hypothesis 2.2.1, the differential expression τ of the form (2.2.1) on the finite interval $(a,b) \subset \mathbb{R}$ is called *regular on* $[a,b]$. The corresponding *maximal operator* T_{max} in $L^2((a,b);rdx)$ associated with τ is defined by

$$\begin{aligned} &T_{max}f = \tau f, \\ &f \in \operatorname{dom}(T_{max}) = \big\{g \in L^2((a,b);rdx) \,\big|\, g, g^{[1]} \in AC([a,b]); \\ &\qquad\qquad\qquad\qquad\qquad \tau g \in L^2((a,b);rdx)\big\}, \end{aligned} \tag{2.2.3}$$

and the corresponding *minimal operator* T_{min} in $L^2((a,b);rdx)$ associated with τ is given by

$$\begin{aligned} &T_{min}f = \tau f, \\ &f \in \operatorname{dom}(T_{min}) = \big\{g \in L^2((a,b);rdx) \,\big|\, g, g^{[1]} \in AC([a,b]); \end{aligned} \tag{2.2.4}$$

$$g(a) = g^{[1]}(a) = g(b) = g^{[1]}(b) = 0;\ \tau g \in L^2((a,b); rdx)\big\}.$$

Here (with $\prime := d/dx$)

$$y^{[1]}(x) = p(x)y'(x), \tag{2.2.5}$$

denotes the first quasi-derivative of a function y on (a,b), assuming that $y, py' \in AC_{loc}((a,b))$.

Assuming Hypothesis 2.2.1 so that τ is regular on $[a,b]$, the following is well-known (see, e.g., [15, Sect. 6.3], [84, Sect. 3.2], [104, Sect. II.5], [149, Ch. V], [179, Sect. 8.4], [180, Sect. 13.2], [182, Ch. 4]): T_{min} is a densely defined, closed operator in $L^2((a,b); rdx)$, moreover, T_{max} is densely defined and closed in $L^2((a,b); rdx)$, and

$$T_{min}^* = T_{max}, \quad T_{min} = T_{max}^*. \tag{2.2.6}$$

Moreover, $T_{min} \subset T_{max} = T_{min}^*$, and hence T_{min} is symmetric, while T_{max} is not.

The next theorem describes all self-adjoint extensions of T_{min} (cf., e.g., [180, Sect. 13.2], [182, Ch. 4]).

Theorem 2.2.2. *Assume Hypothesis* 2.2.1 *so that τ is regular on $[a,b]$. Then the following items (i)–(iii) hold:*

(i) All self-adjoint extensions $T_{\alpha,\beta}$ of T_{min} with separated boundary conditions are of the form

$$\begin{aligned}
&T_{\alpha,\beta} f = \tau f, \quad \alpha, \beta \in [0,\pi),\\
&f \in \operatorname{dom}(T_{\alpha,\beta}) = \big\{g \in \operatorname{dom}(T_{max}) \,\big|\, g(a)\cos(\alpha) + g^{[1]}(a)\sin(\alpha) = 0; \\
&\qquad\qquad\qquad\qquad g(b)\cos(\beta) - g^{[1]}(b)\sin(\beta) = 0\big\}.
\end{aligned} \tag{2.2.7}$$

Special cases: $\alpha = 0$ (i.e., $g(a) = 0$) is called the Dirichlet boundary condition at a; $\alpha = \frac{\pi}{2}$, (i.e., $g^{[1]}(a) = 0$) is called the Neumann boundary condition at a (analogous facts hold at the endpoint b).

(ii) All self-adjoint extensions $T_{\varphi,R}$ of T_{min} with coupled boundary conditions are of

the type

$$T_{\varphi,R}f = \tau f,$$

$$f \in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{pmatrix} g(b) \\ g^{[1]}(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} g(a) \\ g^{[1]}(a) \end{pmatrix} \right\}, \tag{2.2.8}$$

where $\varphi \in [0,\pi)$, *and* R *is a real* 2×2 *matrix with* $\det(R) = 1$ (*i.e.,* $R \in SL(2,\mathbb{R})$). *Special cases:* $\varphi = 0$, $R = I_2$ (*i.e.,* $g(b) = g(a)$, $g^{[1]}(b) = g^{[1]}(a)$) *are called periodic boundary conditions; similarly,* $\varphi = 0$, $R = -I_2$ (*i.e.,* $g(b) = -g(a)$, $g^{[1]}(b) = -g^{[1]}(a)$) *are called antiperiodic boundary conditions.*

(*iii*) *Every self-adjoint extension of* T_{min} *is either of type* (*i*) (*i.e., separated*) *or of type* (*ii*) (*i.e., coupled*).

Next we state some of the most pertinent concepts and results summarized from [74] (in particular, Section 3) and will then illustrate how this permits one to effectively calculate certain values for the spectral ζ-functions of the regular Sturm–Liouville operators considered.

For this purpose we introduce the fundamental system of solutions $\theta(z,x,a)$, $\phi(z,x,a)$ of $\tau y = zy$ defined by

$$\theta(z,a,a) = \phi^{[1]}(z,a,a) = 1, \quad \theta^{[1]}(z,a,a) = \phi(z,a,a) = 0, \tag{2.2.9}$$

such that

$$W(\theta(z,\,\cdot\,,a),\phi(z,\,\cdot\,,a)) = 1, \tag{2.2.10}$$

noting that for fixed x, each is entire with respect to z. Here the Wronskian of f and g, for $f,g \in AC_{loc}((a,b))$, is defined by

$$W(f,g)(x) = f(x)g^{[1]}(x) - f^{[1]}(x)g(x). \tag{2.2.11}$$

Furthermore, we introduce the boundary values for $g, g^{[1]} \in AC([a,b])$, see [148, Ch. I], [182, Sect. 3.2],

$$\begin{aligned} U_{\alpha,\beta,1}(g) &= g(a)\cos(\alpha) + g^{[1]}(a)\sin(\alpha), \\ U_{\alpha,\beta,2}(g) &= g(b)\cos(\beta) - g^{[1]}(b)\sin(\beta), \end{aligned} \tag{2.2.12}$$

in the case (i) of separated boundary conditions in Theorem 2.2.2, and

$$\begin{aligned} V_{\varphi,R,1}(g) &= g(b) - e^{i\varphi}R_{11}g(a) - e^{i\varphi}R_{12}g^{[1]}(a), \\ V_{\varphi,R,2}(g) &= g^{[1]}(b) - e^{i\varphi}R_{21}g(a) - e^{i\varphi}R_{22}g^{[1]}(a), \end{aligned} \tag{2.2.13}$$

in the case (ii) of coupled boundary conditions in Theorem 2.2.2. Moreover, we define the *characteristic functions*

$$F_{\alpha,\beta}(z) = \det\begin{pmatrix} U_{\alpha,\beta,1}(\theta(z,\,\cdot\,,a)) & U_{\alpha,\beta,1}(\phi(z,\,\cdot\,,a)) \\ U_{\alpha,\beta,2}(\theta(z,\,\cdot\,,a)) & U_{\alpha,\beta,2}(\phi(z,\,\cdot\,,a)) \end{pmatrix}, \tag{2.2.14}$$

and

$$F_{\varphi,R}(z) = \det\begin{pmatrix} V_{\varphi,R,1}(\theta(z,\,\cdot\,,a)) & V_{\varphi,R,1}(\phi(z,\,\cdot\,,a)) \\ V_{\varphi,R,2}(\theta(z,\,\cdot\,,a)) & V_{\varphi,R,2}(\phi(z,\,\cdot\,,a)) \end{pmatrix}. \tag{2.2.15}$$

Notational Convention. *To describe all possible self-adjoint boundary conditions associated with self-adjoint extensions of T_{min} effectively, we will frequently employ the notation $T_{A,B}$, $F_{A,B}$, $\lambda_{A,B,j}$, $j \in J$, etc., where A, B represents α, β in the case of separated boundary conditions and φ, R in the context of coupled boundary conditions.*

By construction, eigenvalues of $T_{A,B}$ are determined via $F_{A,B}(z) = 0$, with multiplicity of eigenvalues of $T_{A,B}$ corresponding to multiplicity of zeros of $F_{A,B}$, and $F_{A,B}(z)$ is entire with respect to z. In particular, for $T_{\alpha,\beta}$, that is, for separated boundary conditions, one has

$$\begin{aligned} F_{\alpha,\beta}(z) = \cos(\alpha)&[-\sin(\beta)\ \phi^{[1]}(z,b,a) + \cos(\beta)\ \phi(z,b,a)] \\ &- \sin(\alpha)[-\sin(\beta)\ \theta^{[1]}(z,b,a) + \cos(\beta)\ \theta(z,b,a)], \quad \alpha, \beta \in [0,\pi), \end{aligned} \tag{2.2.16}$$

and for $T_{\varphi,R}$, that is, for coupled boundary conditions, one has for $\varphi \in [0,\pi)$ and $R \in SL(2,\mathbb{R})$,

$$\begin{aligned} F_{\varphi,R}(z) = e^{i\varphi}\big(R_{12}\theta^{[1]}(z,b,a) - R_{22}\theta(z,b,a) + R_{21}\phi(z,b,a) - R_{11}\phi^{[1]}(z,b,a)\big) \\ + e^{2i\varphi} + 1. \end{aligned} \tag{2.2.17}$$

Next we will demonstrate that $F_{A,B}(\,\cdot\,)$ is an entire function of order 1/2 and finite type, independent of the boundary conditions chosen. This result is used when considering convergence of the complex contour integral representation of the spectral ζ-function for large values of the spectral parameter z.

For this purpose we recall the following facts (see, e.g., [20, Ch. 2], [131, Ch. I]): Supposing that $F(\,\cdot\,)$ is entire, one introduces

$$M_F(R) = \sup_{|z|=R} |F(z)|, \quad R \in [0,\infty). \tag{2.2.18}$$

Then the order ρ_F of F is defined by

$$\rho_F = \limsup_{R\to\infty} \ln(\ln(M_F(R)))/\ln(R) \in [0,\infty) \cup \{\infty\}. \tag{2.2.19}$$

In addition, if $\rho_F > 0$, the type τ_F of F is defined as

$$\tau_F = \limsup_{R\to\infty} \ln(M_F(R))/R^{\rho_F} \in [0,\infty) \cup \{\infty\}, \tag{2.2.20}$$

and, in obvious notation, F is called of order $\rho_F > 0$ and of finite type τ_F if $\tau_F \in [0,\infty)$.

Thus, F is of finite order $\rho_F \in [0,\infty)$ if and only if for every $\varepsilon > 0$, but for no $\varepsilon < 0$,

$$M_F(R) \underset{R\to\infty}{=} O\big(\exp\big(R^{\rho_F+\varepsilon}\big)\big), \tag{2.2.21}$$

and F is of positive and finite order $\rho_F \in (0,\infty)$ and finite type $\tau_F \in [0,\infty)$ if and only if for every $\varepsilon > 0$, but for no $\varepsilon < 0$,

$$M_F(R) \underset{R\to\infty}{=} O\big(\exp\big((\tau_F+\varepsilon)R^{\rho_F}\big)\big). \tag{2.2.22}$$

By definition, if F_j are entire of order ρ_j, $j = 1, 2$, then the order of F_1F_2 does not exceed the larger of ρ_1 and ρ_2.

For F entire we also introduce the zero counting function

$$N_F(R) = \#\big(Z_F \cap \overline{D(0;R)}\big), \quad R \in (0,\infty), \tag{2.2.23}$$

where $\#$ denotes cardinality and Z_F represents the set of zeros of F counting multiplicity (i.e., $N_F(R)$ counts the number of zeros of F in the closed disk of radius $R > 0$ centered at the origin).

Remark 2.2.3. Assuming Hypothesis 2.2.1, then all solutions $\psi(z, \cdot\,)$ of the regular Sturm–Liouville problem $(\tau y)(z, x) = zy(z, x)$, $z \in \mathbb{C}$, $x \in [a, b]$, satisfying z-independent initial conditions

$$\psi(z, x_0) = c_0, \quad \psi^{[1]}(z, x_0) = c_1, \tag{2.2.24}$$

for some $x_0 \in [a, b]$ and some $(c_0, c_1) \in \mathbb{C}^2$, together with $\psi^{[1]}(z, \cdot\,)$, for any fixed $x \in [a, b]$, are entire functions of z of order at most $1/2$. Indeed, as shown in [10, Sect. 8.2] (see also [140], [182, Theorem 2.5.3]), upon employing a Prüfer-type transformation, one obtains

$$\begin{aligned} |z||\psi(z,x)|^2 + \big|\psi^{[1]}(z,x)\big|^2 \leqslant C(x_0)\exp\bigg(|z|^{1/2}\int_{\min(x_0,x)}^{\max(x_0,x)} dt\,\big[|p(t)|^{-1} + |r(t)|\big] \\ + |z|^{-1/2}\int_{\min(x_0,x)}^{\max(x_0,x)} dt\,|q(t)|\bigg), \quad z \in \mathbb{C},\ x_0, x \in [a,b]. \end{aligned} \tag{2.2.25}$$

In particular, (2.2.16) and (2.2.17) yield that $F_{A,B}$ is an entire function of order at most $1/2$ for any self-adjoint boundary condition represented by A, B, that is,

$$\rho_{F_{A,B}} \leqslant 1/2. \tag{2.2.26}$$

Given Hypothesis 2.2.1, one infers that $T_{A,B} \geqslant \Lambda_{A,B} I_{L^2_r((a,b))}$ for some $\Lambda_{A,B} \in \mathbb{R}$, with purely discrete spectrum, and hence $Z_{F_{A,B}}(R) \subset [\Lambda_{A,B}, R]$ the elements of $Z_{F_{A,B}}(R)$ being precisely the eigenvalues of $T_{A,B}$ in the interval $[\max(-R, \Lambda_{A,B}), R]$. Employing the theory of Volterra operators in Hilbert spaces (and under some additional lower boundedness hypotheses on q) in [86, Chs. VI, VII], alternatively, using oscillation theoretic methods in [11], it is shown that the eigenvalue counting function $N_{F_{A,B}}$ associated with $T_{A,B}$ satisfies

$$N_{F_{A,B}}(\lambda) \underset{\lambda\to\infty}{=} \pi^{-1} \int_a^b dx\, [r(x)/p(x)]^{1/2} \lambda^{1/2} [1 + o(1)]. \tag{2.2.27}$$

Ignoring finitely many nonpositive eigenvalues of $T_{A,B}$, equivalently, splitting off the factors in the infinite product representation associated with nonpositive zeros of $F_{A,B}$, that is, replacing $F_{A,B}$ by

$$\widetilde{F}_{A,B}(z) = C_{A,B} \prod_{\substack{j\in\mathbb{N}, \\ \lambda_{A,B,j}>0}} [1 - (z/\lambda_{A,B,j})] \tag{2.2.28}$$

with

$$N_{\widetilde{F}_{A,B}}(\lambda) \underset{\lambda\to\infty}{=} \pi^{-1} \int_a^b dx\, [r(x)/p(x)]^{1/2} \lambda^{1/2} [1 + o(1)], \tag{2.2.29}$$

implies (cf. [20, Theorem 4.1.1], [176], [177]),

$$\ln\big(\widetilde{F}_{A,B}(\lambda)\big) \underset{\lambda\to\infty}{=} \int_a^b dx\, [r(x)/p(x)]^{1/2} \lambda^{1/2} [1 + o(1)]. \tag{2.2.30}$$

Thus,

$$\rho_{F_{A,B}} = \rho_{\widetilde{F}_{A,B}} \geqslant 1/2, \tag{2.2.31}$$

and hence by (2.2.26),

$$\rho_{F_{A,B}} = 1/2. \tag{2.2.32}$$

Moreover, by (2.2.25), $F_{A,B}$ is of order $1/2$ and finite type. Finally, we also mention that (2.2.27) implies that

$$\lambda_{A,B,j} \underset{j\to\infty}{=} \left[\int_a^b dx\, [r(x)/p(x)]^{1/2}\right]^{-2} \pi^2 j^2 [1 + o(1)] \tag{2.2.33}$$

(cf. also the discussion in [164, Sects. 1.11, 9.1], [182, Sect. 4.3]). $\diamond$

The following theorem (see [74, Thm. 3.4]) directly relates the function $F_{A,B}$ to Fredholm determinants and traces (see [85, Ch. IV], [158, Sect. XIII.17], [169], [170, Ch. 3], [171, Ch. 3] for background).

Theorem 2.2.4. *Assume Hypothesis* 2.2.1 *and denote by* $T_{\alpha,\beta}$ *and* $T_{\varphi,R}$ *the self-adjoint extensions of* T_{min} *as described in cases* (i) *and* (ii) *of Theorem* 2.2.2*, respectively.*

(i) *Suppose* $z_0 \in \rho(T_{\alpha,\beta})$*, then*

$$\begin{aligned} &\det{}_{L^2_r((a,b))}\big(I_{L^2_r((a,b))} - (z - z_0)(T_{\alpha,\beta} - z_0 I_{L^2_r((a,b))})^{-1}\big) \\ &\quad = F_{\alpha,\beta}(z)/F_{\alpha,\beta}(z_0), \quad z \in \mathbb{C}. \end{aligned} \tag{2.2.34}$$

In particular,

$$\operatorname{tr}_{L^2_r((a,b))}\big((T_{\alpha,\beta} - zI_{L^2_r((a,b))})^{-1}\big) = -(d/dz)\ln(F_{\alpha,\beta}(z)), \quad z \in \rho(T_{\alpha,\beta}). \tag{2.2.35}$$

(ii) *Suppose* $z_0 \in \rho(T_{\varphi,R})$*, then*

$$\begin{aligned} &\det{}_{L^2_r((a,b))}\big(I_{L^2_r((a,b))} - (z - z_0)(T_{\varphi,R} - z_0 I_{L^2_r((a,b))})^{-1}\big) \\ &\quad = F_{\varphi,R}(z)/F_{\varphi,R}(z_0), \quad z \in \mathbb{C}. \end{aligned} \tag{2.2.36}$$

In particular,

$$\operatorname{tr}_{L^2_r((a,b))}\big((T_{\varphi,R} - zI_{L^2_r((a,b))})^{-1}\big) = -(d/dz)\ln(F_{\varphi,R}(z)), \quad z \in \rho(T_{\varphi,R}). \tag{2.2.37}$$

Given these preparations, we let $T_{A,B}$ denote the self-adjoint extension of T_{min} with either separated ($T_{\alpha,\beta}$) or coupled ($T_{\varphi,R}$) boundary conditions as described in cases (i) and (ii) of Theorem 2.2.2. One recalls (see, e.g., [74]), the spectral ζ-function of the operator, $T_{A,B}$, is defined as

$$\zeta(s; T_{A,B}) := \sum_{\substack{j\in J \\ \lambda_j \neq 0}} \lambda_{A,B,j}^{-s}, \tag{2.2.38}$$

with $J \subset \mathbb{Z}$ an appropriate index set counting eigenvalues according to their multiplicity and $\mathrm{Re}(s) > 0$ sufficiently large such that (2.2.38) converges absolutely. Applying Theorem 2.2.4, it was shown in [74] that for $\mathrm{Re}(s) > 0$ sufficiently large,

$$\begin{aligned} \zeta(s; T_{A,B}) &= \frac{1}{2\pi i}\oint_\gamma dz\ z^{-s}\left(\frac{d}{dz}\ln(F_{A,B}(z)) - z^{-1}m(0; T_{A,B})\right) \\ &= \frac{1}{2\pi i}\oint_\gamma dz\ z^{-s}\left(\frac{d}{dz}\ln(F_{A,B}(z)) - z^{-1}m_0\right), \end{aligned} \tag{2.2.39}$$

where $m(0; T_{A,B}) = m_0$ is the multiplicity of zero as an eigenvalue of $T_{A,B}$ and γ is a simple contour enclosing $\sigma(T_{A,B})\backslash\{0\}$ in a counterclockwise manner so as to dip

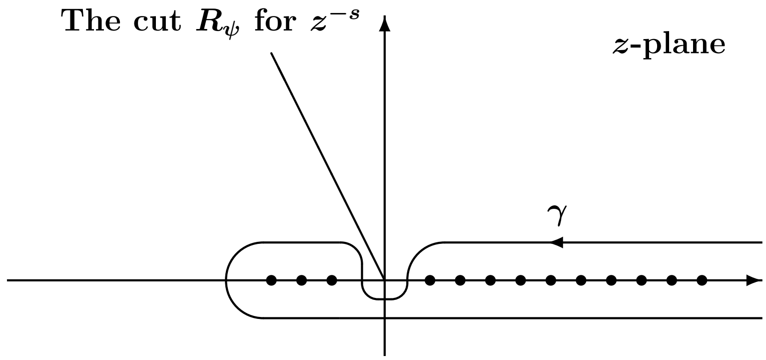

Figure 2.1. Contour γ in the complex z-plane.

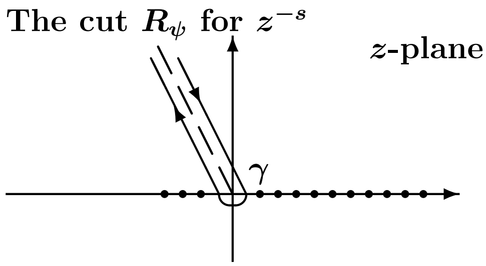

Figure 2.2. Deforming γ.

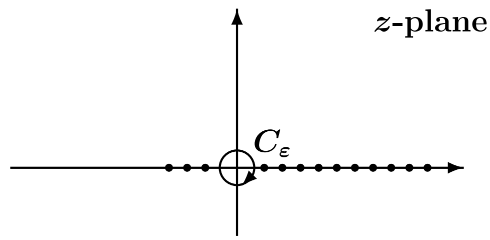

Figure 2.3. Contour C_ε.

under (and hence avoid) the point 0 (cf. Figure 2.1). Here, following [116] (see also [117]), we take

$$R_\psi = \{z = te^{i\psi} \,|\, t \in [0,\infty)\}, \quad \psi \in (\pi/2, \pi), \tag{2.2.40}$$

to be the branch cut of z^{-s}, and, once again, eigenvalues will be determined via $F_{A,B}(z) = 0$, with the multiplicity of eigenvalues of $T_{A,B}$ corresponding to the multiplicity of zeros of $F_{A,B}$.

To continue the computation of (2.2.39) and deform the contour γ as to "hug" the branch cut R_ψ (cf. Figure 2.2) requires knowledge of the asymptotic behavior of $F_{A,B}(z)$ as $|z| \to \infty$, which in turn demands $\mathrm{Re}(s) > 1/2$ for large-z convergence (cf. Remark 2.2.3). Furthermore, if one is interested in the calculation of the value of the spectral zeta function at positive integers, the following method provides a very simple way of obtaining those values. In fact, by letting $s = n$, $n \in \mathbb{N}$, in (2.2.39), one no longer needs a branch cut for the fractional powers of z^{-s} given in Figures 2.1

and 2.2. This reduces the integral along the curve γ to a clockwise oriented integral along the circle C_ε, centered at zero with radius $\varepsilon > 0$ (cf. Figure 2.3). Letting $s = n$ also ensures that m_0 (the multiplicity of zero as an eigenvalue of $T_{A,B}$) does not contribute to the integral in (2.2.39). Hence,

$$\begin{aligned} \zeta(n; T_{A,B}) &= -\frac{1}{2\pi i} \oint_{C_\varepsilon} dz\ z^{-n} \frac{d}{dz} \ln(F_{A,B}(z)) \\ &= -\mathrm{Res}\left[z^{-n} \frac{d}{dz} \ln(F_{A,B}(z));\ z = 0 \right], \quad n \in \mathbb{N}. \end{aligned} \tag{2.2.41}$$

Thus, determining an expansion of $F_{A,B}(z)$ about $z = 0$ enables one to effectively compute $\zeta(n; T_{A,B})$. In addition, by (2.2.16), (2.2.17), $F_{A,B}(z)$ is a linear combination of θ, $\theta^{[1]}$, ϕ, and $\phi^{[1]}$ for each boundary condition considered, so it suffices to find the expansion of each of these functions individually.

2.3 *Expansion in z for Fundamental Solutions, Asymptotic Expansion, and the Zeta Regularized Functional Determinant*

2.3.1 *Expansion in z for Fundamental Solutions*

Assuming Hypothesis 2.2.1 throughout this section, we discuss next the expansion in z about $z = 0$ for the solutions $\phi(z, \cdot\,, a)$ and $\theta(z, \cdot\,, a)$ of $\tau y = zy$,

$$\phi(z, x, a) = \phi(0, x, a) + z \int_a^x r(x')dx'\, g(0, x, x')\phi(z, x', a), \tag{2.3.1}$$

$$\theta(z, x, a) = \theta(0, x, a) + z \int_a^x r(x')dx'\, g(0, x, x')\theta(z, x', a), \tag{2.3.2}$$

$$z \in \mathbb{C},\ x \in [a, b],$$

employing the following expression for the Volterra Green's function

$$g(0, x, x') = \theta(0, x, a)\phi(0, x', a) - \theta(0, x', a)\phi(0, x, a), \quad x, x' \in [a, b]. \tag{2.3.3}$$

That (2.3.1) and (2.3.2) indeed represent solutions of $\tau y = zy$ is clear from applying τ to either side, moreover, the initial conditions (2.2.9) are readily verified.

Iterating these integral equations establishes the power series expansions

$$\phi(z, x, a) = \sum_{m=0}^{\infty} z^m \phi_m(x), \quad z \in \mathbb{C},\ x \in [a, b], \tag{2.3.4}$$

where

$$\begin{aligned}
\phi_0(x) &= \phi(0,x,a), \\
\phi_1(x) &= \int_a^x r(x_1)dx_1 \; g(0,x,x_1)\phi(0,x_1,a), \\
\phi_k(x) &= \int_a^x r(x_1)dx_1 \; g(0,x,x_1) \int_a^{x_1} r(x_2)dx_2 \; g(0,x_1,x_2)\dots \\
&\quad \dots \int_a^{x_{k-1}} r(x_k)dx_k \; g(0,x_{k-1},x_k)\phi(0,x_k,a), \quad k \in \mathbb{N},
\end{aligned} \tag{2.3.5}$$

and

$$\theta(z,x,a) = \sum_{m=0}^{\infty} z^m \theta_m(x), \quad z \in \mathbb{C}, \; x \in [a,b], \tag{2.3.6}$$

where

$$\begin{aligned}
\theta_0(x) &= \theta(0,x,a), \\
\theta_1(x) &= \int_a^x r(x_1)dx_1 \; g(0,x,x_1)\theta(0,x_1,a), \\
\theta_k(x) &= \int_a^x r(x_1)dx_1 \; g(0,x,x_1) \int_a^{x_1} r(x_2)dx_2 \; g(0,x_1,x_2)\dots \\
&\quad \dots \int_a^{x_{k-1}} r(x_k)dx_k \; g(0,x_{k-1},x_k)\theta(0,x_k,a), \quad k \in \mathbb{N}.
\end{aligned} \tag{2.3.7}$$

Analogously one obtains

$$\phi^{[1]}(z,x,a) = \sum_{m=0}^{\infty} z^m \phi_m^{[1]}(x), \quad z \in \mathbb{C}, \; x \in [a,b], \tag{2.3.8}$$

where

$$\begin{aligned}
\phi_0^{[1]}(x) &= \phi^{[1]}(0,x,a), \\
\phi_1^{[1]}(x) &= \int_a^x r(x_1)dx_1 \; g^{[1]}(0,x,x_1)\phi(0,x_1,a), \\
\phi_k^{[1]}(x) &= \int_a^x r(x_1)dx_1 \; g^{[1]}(0,x,x_1) \int_a^{x_1} r(x_2)dx_2 \; g(0,x_1,x_2)\dots \\
&\quad \dots \int_a^{x_{k-1}} r(x_k)dx_k \; g(0,x_{k-1},x_k)\phi(0,x_k,a), \quad k \in \mathbb{N},
\end{aligned} \tag{2.3.9}$$

using the abbreviation

$$g^{[1]}(0,x,x_1) = \theta^{[1]}(0,x,a)\phi(0,x_1,a) - \theta(0,x_1,a)\phi^{[1]}(0,x,a). \tag{2.3.10}$$

Similarly, one finds from (2.3.6)

$$\theta^{[1]}(z,x,a) = \sum_{m=0}^{\infty} z^m \theta_m^{[1]}(x), \quad z \in \mathbb{C},\ x \in [a,b], \tag{2.3.11}$$

where

$$\begin{aligned}
\theta_0^{[1]}(x) &= \theta^{[1]}(0,x,a), \\
\theta_1^{[1]}(x) &= \int_a^x r(x_1)dx_1\ g^{[1]}(0,x,x_1)\theta(0,x_1,a), \\
\theta_k^{[1]}(x) &= \int_a^x r(x_1)dx_1\ g^{[1]}(0,x,x_1) \int_a^{x_1} r(x_2)dx_2\ g(0,x_1,x_2)\dots \\
&\qquad \dots \int_a^{x_{k-1}} r(x_k)dx_k\ g(0,x_{k-1},x_k)\theta(0,x_k,a), \quad k \in \mathbb{N}.
\end{aligned} \tag{2.3.12}$$

2.3.2 Asymptotic Expansion of the Characteristic Function

Next we investigate the $|z| \to \infty$ asymptotic expansion of the function $F_{A,B}(z)$ in order to provide an analytic continuation of the spectral ζ-function, $\zeta(s;T_{A,B})$, and compute the zeta regularized functional determinant. We first strengthen Hypothesis 2.2.1 by introducing the following assumptions on p,q,r following [74, Sect. 3]. These additional assumptions are necessary in order to perform a Liouville-type transformation.

Hypothesis 2.3.1. *Let $(a,b) \subset \mathbb{R}$ be a finite interval and suppose that p,q,r are (Lebesgue) measurable functions on (a,b) such that the following items (i)–(iv) hold:*

(i) $r > 0$ a.e. on (a,b), $r \in L^1((a,b);dx)$.

(ii) $p > 0$ a.e. on (a,b), $1/p \in L^1((a,b);dx)$.

(iii) q is real-valued a.e. on (a,b), $q \in L^1((a,b);dx)$.

(iv) pr and $(pr)'/r$ are absolutely continuous on $[a,b]$, and for some $\varepsilon > 0$, $pr \geqslant \varepsilon$ on $[a,b]$.

The variable transformations (cf. [133, p. 2]),

$$\xi(x) = \frac{1}{c}\int_a^x dt\ [r(t)/p(t)]^{1/2}, \quad \xi(x) \in [0,1] \text{ for } x \in [a,b], \tag{2.3.13}$$

$$\xi'(x) = c^{-1}[r(x)/p(x)]^{1/2} > 0 \text{ a.e. on } (a,b), \tag{2.3.14}$$

$$u(z,\xi) = [p(x(\xi))r(x(\xi))]^{1/4} y(z,x(\xi)), \tag{2.3.15}$$

with $c > 0$ given by

$$c = \int_a^b dt\ [r(t)/p(t)]^{1/2}, \tag{2.3.16}$$

transform the Sturm–Liouville problem $(\tau y(z,\,\cdot\,))(x) = zy(z,x)$, $x \in (a,b)$, into

$$-\ddot{u}(z,\xi) + V(\xi)u(z,\xi) = c^2 z u(z,\xi), \quad \xi \in (0,1), \tag{2.3.17}$$

and abbreviating

$$\nu(\xi) = [p(x(\xi))r(x(\xi))]^{1/4}, \tag{2.3.18}$$

one verifies that

$$\begin{aligned} V(\xi) &= \frac{\ddot{\nu}(\xi)}{\nu(\xi)} + c^2 \frac{q(x)}{r(x)} \\ &= -\frac{c^2}{16} \frac{1}{p(x)r(x)} \left[\frac{(p(x)r(x))'}{r(x)}\right]^2 + \frac{c^2}{4} \frac{1}{r(x)} \left[\frac{(p(x)r(x))'}{r(x)}\right]' + c^2 \frac{q(x)}{r(x)}, \end{aligned} \tag{2.3.19}$$

and

$$V \in L^1((0,1);d\xi), \tag{2.3.20}$$

as guaranteed by Hypothesis 2.3.1.

In order to construct the asymptotic expansion of $F_{A,B}(z)$ we begin by assuming Hypothesis 2.3.1, but note that throughout the construction of the expansion stronger assumptions will be necessary, all of which will be addressed once the final asymptotic expansion is given.

When applying the Liouville transformation the boundary conditions undergo a similar transformation. In fact, setting

$$Q(\xi) = [(pr)'/r](x(\xi)) \tag{2.3.21}$$

one can write

$$\begin{pmatrix} u(z,\xi) \\ \dot{u}(z,\xi) \end{pmatrix} = M(\xi) \begin{pmatrix} y(z,x(\xi)) \\ y^{[1]}(z,x(\xi)) \end{pmatrix}, \tag{2.3.22}$$

where

$$M(\xi) = \begin{pmatrix} \nu(\xi) & 0 \\ (c/4)\nu(\xi)^{-1}Q(\xi) & c\nu(\xi)^{-1} \end{pmatrix}, \quad \xi \in [0,1], \quad \det_{\mathbb{C}^2}(M(\,\cdot\,)) = c. \quad (2.3.23)$$

Employing relation (2.3.22), the separated boundary conditions for the function $g(\,\cdot\,)$ in Theorem 2.2.2 (i) transform into separated boundary conditions for the transformed function $v(\,\cdot\,)$ as follows,

$$\begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ 0 & 0 \end{pmatrix} M(0)^{-1} \begin{pmatrix} v(0) \\ \dot{v}(0) \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \cos(\beta) & -\sin(\beta) \end{pmatrix} M(1)^{-1} \begin{pmatrix} v(1) \\ \dot{v}(1) \end{pmatrix}, \quad (2.3.24)$$

where $\alpha, \beta \in [0, \pi)$, and the inverse matrix $M^{-1}(\,\cdot\,)$ has the form

$$M(\xi)^{-1} = \begin{pmatrix} \nu(\xi)^{-1} & 0 \\ -(1/4)\nu(\xi)^{-1}Q(\xi) & c^{-1}\nu(\xi) \end{pmatrix}, \quad \xi \in [0,1], \quad (2.3.25)$$

or, more explicitly,

$$\begin{aligned} c^{-1}\nu(0)\sin(\alpha)\dot{v}(0) + \nu(0)^{-1}\left[\cos(\alpha) - 4^{-1}\sin(\alpha)Q(0)\right]v(0) = 0, \\ -c^{-1}\nu(1)\sin(\beta)\dot{v}(1) + \nu(1)^{-1}\left[\cos(\beta) + 4^{-1}\sin(\beta)Q(1)\right]v(1) = 0. \end{aligned} \quad (2.3.26)$$

With the help of relation (2.3.22) the coupled boundary conditions for $g(\,\cdot\,)$ in Theorem 2.2.2 (ii) transform into coupled boundary conditions for $v(\,\cdot\,)$ via

$$\begin{pmatrix} v(1) \\ \dot{v}(1) \end{pmatrix} = e^{i\varphi}\widetilde{R} \begin{pmatrix} v(0) \\ \dot{v}(0) \end{pmatrix}, \quad \varphi \in [0, \pi), \quad (2.3.27)$$

where

$$\widetilde{R} = M(1)^{-1}RM(0) \in SL(2, \mathbb{R}) \quad (2.3.28)$$

is of the form

$$\begin{aligned} &\widetilde{R}_{11} = \nu(0)^{-1}\nu(1)\left[R_{11} - 4^{-1}Q(0)R_{12}\right], \quad \widetilde{R}_{12} = c^{-1}\nu(0)\nu(1)R_{12}, \\ &\widetilde{R}_{21} = c\nu(0)^{-1}\nu(1)^{-1}\left[R_{21} - 4^{-1}Q(0)R_{22} + 4^{-1}Q(1)R_{11} - (16)^{-1}Q(0)Q(1)R_{12}\right], \\ &\widetilde{R}_{22} = \nu(0)\nu(1)^{-1}\left[R_{22} + 4^{-1}Q(1)R_{12}\right]. \end{aligned} \quad (2.3.29)$$

The fundamental system of solutions $\phi(z,\,\cdot\,,a)$ and $\theta(z,\,\cdot\,,a)$ of $\tau y = zy$ satisfying (2.2.9) is transformed into the set of solutions $\Phi(z,\,\cdot\,,0)$ and $\Theta(z,\,\cdot\,,0)$ of (2.3.17) satisfying the conditions

$$\Phi(z,0,0) = 0, \qquad \dot{\Phi}(z,0,0) = c\nu(0)^{-1}, \tag{2.3.30}$$

$$\Theta(z,0,0) = \nu(0), \quad \dot{\Theta}(z,0,0) = 4^{-1}c\nu(0)^{-1}Q(0), \tag{2.3.31}$$

where, once again, the derivatives of $\Phi(z,\xi,0)$ and $\Theta(z,\xi,0)$ are understood with respect to the variable ξ (cf. (2.3.17)) and one notes that for fixed ξ, each is entire with respect to z. By writing a generic solution of (2.3.17) as a linear combination of $\Phi(z,\xi,0)$ and $\Theta(z,\xi,0)$ and by imposing the separated boundary conditions in (2.3.26) one obtains the following characteristic function

$$\begin{aligned}
\mathcal{F}_{\alpha,\beta}(z) = \sin(\alpha)\big\{& c^{-1}\nu(1)\sin(\beta)\dot{\Theta}(z,1,0) \\
&- \nu(1)^{-1}\big[\cos(\beta) + 4^{-1}\sin(\beta)Q(1)\big]\,\Theta(z,1,0)\big\} \\
&+ \cos(\alpha)\big\{-c^{-1}\nu(1)\sin(\beta)\dot{\Phi}(z,1,0) \\
&+ \nu(1)^{-1}\big[\cos(\beta) + 4^{-1}\sin(\beta)Q(1)\big]\,\Phi(z,1,0)\big\}, \quad z \in \mathbb{C}.
\end{aligned} \tag{2.3.32}$$

The zeros of $\mathcal{F}_{\alpha,\beta}(z)$ represent, including multiplicity, the eigenvalues $\lambda_{A,B,j}$, $j \in J$, of the original Sturm–Liouville problem $\tau y = zy$ endowed with the separated boundary conditions in (2.2.7). By repeating this argument for coupled boundary conditions (2.2.8) one obtains the characteristic function

$$\begin{aligned}
\mathcal{F}_{\varphi,\widetilde{R}}(z) = e^{i\varphi}\big\{& 2\cos(\varphi) - \big[c^{-1}\nu(0)\widetilde{R}_{11} + 4^{-1}\nu(0)^{-1}Q(0)\widetilde{R}_{12}\big]\dot{\Phi}(z,1,0) \\
&+ \big[c^{-1}\nu(0)\widetilde{R}_{21} + 4^{-1}\nu(0)^{-1}Q(0)\widetilde{R}_{22}\big]\Phi(z,1,0) \\
&+ \widetilde{R}_{12}\nu(0)^{-1}\dot{\Theta}(z,1,0) - \widetilde{R}_{22}\nu(0)^{-1}\Theta(z,1,0)\big\}, \quad z \in \mathbb{C}.
\end{aligned} \tag{2.3.33}$$

Remark 2.3.2. Explicit computations confirm that in the case of separated as well as coupled boundary conditions one finds

$$F_{\alpha,\beta}(z) = \mathcal{F}_{\alpha,\beta}(z), \quad z \in \mathbb{C}, \tag{2.3.34}$$

$$F_{\varphi,R}(z) = \mathcal{F}_{\varphi,\widetilde{R}}(z), \quad z \in \mathbb{C}. \tag{2.3.35}$$

As an example we now consider the case of the Krein–von Neumann extension (see, e.g., [68] and the literature cited therein for details):

Example 2.3.3. *The Krein–von Neumann boundary conditions in terms of the variable $x \in [a,b]$ are characterized by imposing the coupled boundary conditions $\varphi = 0$, $R = R_K$ (cf., e.g.,* [74, eq. (3.35)]) *with*

$$R_K = \begin{pmatrix} \theta(0,b,a) & \phi(0,b,a) \\ \theta^{[1]}(0,b,a) & \phi^{[1]}(0,b,a) \end{pmatrix}. \tag{2.3.36}$$

In terms of $\xi \in [0,1]$, these conditions transform into $\varphi = 0$ and $\widetilde{R} = \widetilde{R}_K$ with

$$\widetilde{R}_K = \begin{pmatrix} \nu(0)^{-1}\big[\Theta(0,1,0) - 4^{-1}Q(0)\Phi(0,1,0)\big] & c^{-1}\nu(0)\Phi(0,1,0) \\ \nu(0)^{-1}\big[\dot{\Theta}(0,1,0) - 4^{-1}Q(0)\dot{\Phi}(0,1,0)\big] & c^{-1}\nu(0)\dot{\Phi}(0,1,0) \end{pmatrix}. \tag{2.3.37}$$

Using these parameters in (2.3.33)*, one obtains the characteristic function*

$$\begin{aligned} \mathcal{F}_{0,\widetilde{R}_K}(z) = 2 - c^{-1}\big[&\dot{\Phi}(0,1,0)\Theta(z,1,0) + \Theta(0,1,0)\dot{\Phi}(z,1,0) \\ &- \Phi(0,1,0)\dot{\Theta}(z,1,0) - \dot{\Theta}(0,1,0)\Phi(z,1,0)\big], \quad z \in \mathbb{C}, \end{aligned} \tag{2.3.38}$$

to be compared with (*see* [74, eq. (3.36), (3.37)])

$$\begin{aligned} F_{0,R_K}(z) = 2 - \big[&\phi^{[1]}(0,b,a)\theta(z,b,a) + \theta(0,b,a)\phi^{[1]}(z,b,a) \\ &- \phi(0,b,a)\theta^{[1]}(z,b,a) - \theta^{[1]}(0,b,a)\phi(z,b,a)\big], \quad z \in \mathbb{C}. \end{aligned} \tag{2.3.39}$$

In order to obtain a large-z asymptotic expansion of the functions (2.3.32) and (2.3.33), we need the asymptotic expansion of the transformed fundamental set of solutions $\Phi(z,\xi,0)$ and $\Theta(z,\xi,0)$. To this end, and since the principal results we are focused on in this section are of a local nature with respect to $\xi \in [0,1]$, we now envisage that $V(\,\cdot\,)$ is continued in a sufficiently smooth and compactly supported manner to a function on $\mathbb{R}$ (by a slight abuse of notation still abbreviated by V),

$$V \in C_0^N(\mathbb{R}) \cap C^\infty((-\infty,-1) \cup (2,\infty)), \tag{2.3.40}$$

for $N \in \mathbb{N}$ to be determined later on. In addition, we consider the associated Weyl–Titchmarsh (resp., Jost) solutions $u_\pm(z,\,\cdot\,)$ such that for all $x_0 \in \mathbb{R}$,

$$u_+(z,\,\cdot\,) \in L^2([x_0,\infty); d\xi), \quad u_-(z,\,\cdot\,) \in L^2((-\infty,x_0]; d\xi), \quad \mathrm{Im}\big(z^{1/2}\big) > 0. \tag{2.3.41}$$

Writing

$$u_\pm(z,\xi) = \exp\bigg\{ \int_0^\xi dt\ \mathcal{S}_\pm(z,t) \bigg\}, \quad \mathcal{S}_\pm(z,\xi) = \frac{\dot{u}_\pm(z,\xi)}{u_\pm(z,\xi)}, \quad \xi \in \mathbb{R},\ \mathrm{Im}\big(z^{1/2}\big) \geqslant 0 \tag{2.3.42}$$

(the compact support hypothesis on V on $\mathbb{R}$, more generally, a suitable short-range, i.e., integrability assumption on V, permits the continuous extension of $\mathcal{S}_\pm(z,\,\cdot\,)$ to $\mathrm{Im}\big(z^{1/2}\big) \geqslant 0$), one infers that $\mathcal{S}_\pm(z,\,\cdot\,)$ satisfy the Riccati differential equation

$$\dot{S}(z,\xi) + S_\pm(z,\xi)^2 - V(\xi) + c^2 z = 0, \quad \xi \in \mathbb{R},\ \mathrm{Im}\big(z^{1/2}\big) \geqslant 0. \tag{2.3.43}$$

In addition, $\mathcal{S}_\pm(z,\xi)$ represent the half-line Weyl–Titchmarsh functions on $[\xi,+\infty)$, respectively, $(-\infty,\xi]$, in particular, for each $\xi \in \mathbb{R}$, $\pm S_\pm(\,\cdot\,,\xi)$ are Nevanlinna–Herglotz functions on $\mathbb{C}_+$ (i.e., analytic on $\mathbb{C}_+$ with strictly positive imaginary part on $\mathbb{C}_+$).

Inserting the formal asymptotic expansion

$$\mathcal{S}_\pm(z,\,\cdot\,) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \pm icz^{1/2} + \sum_{j=1}^{\infty} (\mp 1)^j S_j(\,\cdot\,) z^{-j/2} \tag{2.3.44}$$

into the Riccati equation (2.3.43) yields the recursion relation

$$\begin{aligned} &S_1(\xi) = [i/(2c)]V(\xi), \quad S_2(\xi) = [1/4c^2]\dot{V}(\xi), \\ &S_{j+1}(\xi) = -[i/(2c)]\bigg[\dot{S}_j(\xi) + \sum_{k=1}^{j-1} S_k(\xi)S_{j-k}(\xi)\bigg], \quad j \in \mathbb{N},\ \xi \in \mathbb{R}. \end{aligned} \tag{2.3.45}$$

The first few terms $S_j(\,\cdot\,)$ explicitly read

$$\begin{aligned} &S_3(\xi) = \big[i/\big(8c^3\big)\big]\big[V^2(\xi) - \ddot{V}(\xi)\big], \\ &S_4(\xi) = -\big[1/16c^4\big]\big[V^{(3)}(\xi) - 4V(\xi)\dot{V}(\xi)\big], \\ &S_5(\xi) = \big[i/\big(32c^5\big)\big]\big[2V^3(\xi) - 5\dot{V}(\xi)^2 - 6V(\xi)\ddot{V}(\xi) + V^{(4)}(\xi)\big], \\ &\qquad \text{etc.} \end{aligned} \tag{2.3.46}$$

See [72, Sects. 5, 6] for a variety of closely related asymptotic expansions.

Assuming (2.3.40), the formal asymptotic expansion (2.3.43) turns into an actual asymptotic expansion of the the type (see [23]),

$$\mathcal{S}_{\pm}(z,\xi) \underset{\substack{|z|\to\infty \\ \operatorname{Im}(z^{1/2})\geqslant 0}}{=} \pm icz^{1/2} + \sum_{j=1}^{N} (\mp 1)^j S_j(\xi) z^{-j/2} + o\big(|z|^{-N/2}\big), \tag{2.3.47}$$

with the $o\big(|z|^{-N/2}\big)$-term uniform with respect to $\xi \in [0,1]$.

Remark 2.3.4. There is an enormous literature available in connection with asymptotic high-energy expansions of Weyl–Titchmarsh m-functions (see, e.g., the detailed list in [32]) and the associated spectral function, however, much less can be found in connection with (local) uniformity of the error term $o\big(|z|^{-N/2}\big)$ with respect to x in expansions of the type (2.3.47). Notable exceptions are, for instance, [23], [36], [96], [111], [165], [166]. In particular, [23] (see [137, Sects. 1.4, 3.1]) and [36] use the theory of transformation operators, while [96] and [111] employ a detailed analysis of the Riccati equation (2.3.43), and [165], [166] iterate an underlying Volterra integral equation. In addition, we note that the compact support hypothesis on V can be relaxed to the condition

$$\int_{\mathbb{R}} (1+|x|)dx \left|V^{(\ell)}(x)\right| < \infty, \quad 0 \leqslant \ell \leqslant N. \tag{2.3.48}$$

The correct asymptotic behavior as $|z| \to \infty$ of any solution $u(z,\,\cdot\,)$ to (2.3.17) is given as a linear combination of $u_{\pm}(z,\,\cdot\,)$,

$$u(z,\xi) = \mathcal{A}(z)u_+(z,\xi) + \mathcal{B}(z)u_-(z,\xi), \quad \operatorname{Im}(z) > 0,\ \xi \in [0,1], \tag{2.3.49}$$

and one notices that the solutions $u_{\pm}(z,\,\cdot\,)$ satisfy the initial conditions

$$u_{\pm}(z,0) = 1, \quad \dot{u}_{\pm}(z,0) = \mathcal{S}_{\pm}(z,0), \quad \operatorname{Im}(z) > 0. \tag{2.3.50}$$

Since $W(u_+(z,\,\cdot\,),u_-(z,\,\cdot\,))(\xi) \neq 0$, $\xi \in [0,1]$, one infers that

$$\mathcal{S}^+(z,0) - \mathcal{S}^-(z,0) \neq 0, \quad \operatorname{Im}(z) > 0. \tag{2.3.51}$$

Imposing the initial conditions (2.3.30) and (2.3.31) on the function (2.3.49), one obtains an expression for $\Phi(z,\,\cdot\,,0)$ and $\Theta(z,\,\cdot\,,0)$ suitable for an asymptotic expansion. For instance, in the case of $\Phi(z,\xi,0)$ one obtains

$$\begin{aligned}\Phi(z,\xi,0) = {} & \frac{c\nu(0)^{-1}}{\mathcal{S}_-(z,0)-\mathcal{S}_+(z,0)} \exp\biggl(\int_0^\xi d\eta\, \mathcal{S}_-(z,\eta)\biggr) \\ & \times \biggl[1 - \exp\biggl(\int_0^\xi d\eta\, [\mathcal{S}_+(z,\eta)-\mathcal{S}_-(z,\eta)]\biggr)\biggr].\end{aligned} \tag{2.3.52}$$

Furthermore, for large values of z, with $\mathrm{Im}(z) > 0$, (2.3.47) implies

$$\begin{aligned}& \exp\biggl(\int_0^\xi d\eta\, [\mathcal{S}_+(z,\eta)-\mathcal{S}_-(z,\eta)]\biggr) \\ & \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \exp\bigl(2icz^{1/2}\xi\bigr) \exp\biggl(-2\sum_{n=1}^N z^{-n+(1/2)} \int_0^\xi d\eta\, S_{2n-1}(\eta)\biggr) \\ & \qquad \times [1 + o\bigl(z^{-N+1/2}\bigr)].\end{aligned} \tag{2.3.53}$$

Since the integrals on the right-hand side of (2.3.53) are finite, one finds

$$\exp\biggl(-2\sum_{n=1}^N z^{-n+1/2} \int_0^\xi d\eta\, S_{2n-1}(\eta)\biggr) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} O(1), \tag{2.3.54}$$

uniformly in $\xi \in [0,1]$. Relations (2.3.47) and (2.3.53) permit one to conclude that

$$\exp\biggl(\int_0^\xi d\eta\, [\mathcal{S}_+(z,\eta)-\mathcal{S}_-(z,\eta)]\biggr) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} O\bigl(e^{2icz^{1/2}}\bigr), \tag{2.3.55}$$

uniformly for $\xi \in [0,1]$, and therefore,

$$\Phi(z,\xi,0) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \frac{c\nu(0)^{-1}}{\mathcal{S}_-(z,0)-\mathcal{S}_+(z,0)} \exp\biggl(\int_0^\xi d\eta\, \mathcal{S}_-(z,\eta)\biggr) \bigl[1 + O\bigl(e^{2icz^{1/2}}\bigr)\bigr]. \tag{2.3.56}$$

Similar arguments permit one to derive the following expressions:

$$\begin{aligned}\Theta(z,\xi,0) & \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \frac{(c/4)\nu(0)^{-1}Q(0) - \nu(0)S_+(z,0)}{\mathcal{S}_-(z,0)-\mathcal{S}_+(z,0)} \exp\biggl(\int_0^\xi d\eta\, \mathcal{S}_-(z,\eta)\biggr) \\ & \qquad \times \bigl[1 + O\bigl(e^{2icz^{1/2}}\bigr)\bigr],\end{aligned} \tag{2.3.57}$$

$$\dot{\Phi}(z,\xi,0) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \frac{c\nu(0)^{-1}\mathcal{S}_-(z,1)}{\mathcal{S}_-(z,0)-\mathcal{S}_+(z,0)} \exp\biggl(\int_0^\xi d\eta\, \mathcal{S}_-(z,\eta)\biggr) \bigl[1 + O\bigl(e^{2icz^{1/2}}\bigr)\bigr], \tag{2.3.58}$$

$$\dot{\Theta}(z,\xi,0) \underset{\substack{|z|\to\infty \\ \operatorname{Im}(z^{1/2})\geqslant 0}}{=} \frac{[(c/4)\nu(0)^{-1}Q(0) - \nu(0)\mathcal{S}_+(z,0)]\,\mathcal{S}_-(z,1)}{\mathcal{S}_-(z,0) - \mathcal{S}_+(z,0)} \times \exp\bigg(\int_0^\xi d\eta\,\mathcal{S}_-(z,\eta)\bigg)\big[1 + O\big(e^{2icz^{1/2}}\big)\big], \tag{2.3.59}$$

uniformly with respect to $\xi \in [0,1]$.

Utilizing the expressions (2.3.57)–(2.3.59) in (2.3.32) and (2.3.33) we obtain

$$\begin{aligned}\mathcal{F}_{A,B}(z) \underset{\substack{|z|\to\infty \\ \operatorname{Im}(z^{1/2})\geqslant 0}}{=} &\frac{1}{\mathcal{S}^-(z,0) - \mathcal{S}_-(z,0)} \exp\bigg(\int_0^1 d\eta\,\mathcal{S}_-(z,\eta)\bigg) \\ &\times [j_{A,B} + k_{A,B}\mathcal{S}_+(z,0) + \ell_{A,B}\mathcal{S}_-(z,1) + m_{A,B}\mathcal{S}_+(z,0)\mathcal{S}_-(z,1)] \\ &\times \big[1 + O\big(e^{2icz^{1/2}}\big)\big].\end{aligned} \tag{2.3.60}$$

The first line on the right-hand side of (2.3.60) is entirely independent of boundary conditions, in particular, it does not distinguish between separated and coupled boundary conditions. In contrast, the terms $j_{A,B}, k_{A,B}, \ell_{A,B}$, and $m_{A,B}$ in the second line on the right-hand side of (2.3.60) encode the specific information about the boundary conditions imposed. In the case of separated boundary conditions, where A, B represents α, β as in (2.2.7) one obtains

$$\begin{aligned} j_{\alpha,\beta} &= -\frac{c}{\nu(0)\nu(1)}\left[\cos(\beta) + (1/4)\sin(\beta)Q(1)\right]\left[\cos(\alpha) - (1/4)\sin(\alpha)Q(0)\right], \\ k_{\alpha,\beta} &= -\frac{\nu(0)}{\nu(1)}\sin(\alpha)\left[\cos(\beta) + (1/4)\sin(\beta)Q(1)\right], \\ \ell_{\alpha,\beta} &= \frac{\nu(1)}{\nu(0)}\sin(\beta)\left[\cos(\alpha) - (1/4)\sin(\alpha)Q(0)\right], \\ m_{\alpha,\beta} &= (1/c)\nu(0)\nu(1)\sin(\alpha)\sin(\beta). \end{aligned} \tag{2.3.61}$$

In the case of coupled boundary conditions, where A, B represents $\varphi, \widetilde{R}$ as in (2.3.27), (2.3.29), one infers

$$j_{\varphi,\widetilde{R}} = -e^{i\varphi}\widetilde{R}_{21}, \quad k_{\varphi,\widetilde{R}} = -e^{i\varphi}\widetilde{R}_{22}, \quad \ell_{\varphi,\widetilde{R}} = e^{i\varphi}\widetilde{R}_{11}, \quad m_{\varphi,\widetilde{R}} = e^{i\varphi}\widetilde{R}_{12}. \tag{2.3.62}$$

For the purpose of the analytic continuation of the spectral ζ-function, one needs the large-z asymptotic expansion of $\ln(\mathcal{F}_{A,B}(z))$ rather than of $\mathcal{F}_{A,B}(z)$. For this reason we will focus next on the derivation of the large-z asymptotic expansion of the expression

$$\begin{aligned}\ln(\mathcal{F}_{A,B}(z)) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} & -\ln\big(\mathcal{S}_+(z,0)-\mathcal{S}_-(z,0)\big)+\int_0^1 d\eta\,\mathcal{S}_-(z,\eta)\\ & +\ln\big(j_{A,B}+k_{A,B}\mathcal{S}_+(z,0)+\ell_{A,B}\mathcal{S}_-(z,1)+m_{A,B}\mathcal{S}_+(z,0)\mathcal{S}_-(z,1)\big)\\ & +O\big(e^{2icz^{1/2}}\big).\end{aligned} \tag{2.3.63}$$

We can now use the expansion (2.3.43) in (2.3.60) to obtain a large-z asymptotic expansion of (2.3.63). We start with the part of (2.3.63) that is independent of the boundary conditions. For the integral in (2.3.63) one finds

$$\int_0^1 d\eta\,\mathcal{S}_-(z,\eta) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} -iz^{1/2}c+\sum_{m=1}^{N} z^{-m/2}\int_0^1 d\eta\,S_m(\eta)+o\big(z^{-N/2}\big). \tag{2.3.64}$$

For the first term in (2.3.63) one concludes that

$$\mathcal{S}_+(z,0)-\mathcal{S}_-(z,0) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} 2icz^{1/2}\left(1+(i/c)\sum_{j=1}^{N} S_{2j-1}(0)z^{-j}\right)+o\big(z^{-N+1/2}\big). \tag{2.3.65}$$

Relation (2.3.65) permits one to write

$$\ln\big(\mathcal{S}_+(z,0)-\mathcal{S}_-(z,0)\big) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \ln(2ic)+2^{-1}\ln(z)+\sum_{m=1}^{N} D_{2m-1}z^{-m}+o\big(z^{-N}\big), \tag{2.3.66}$$

where the terms D_{2m-1} are determined through the formal asymptotic expansion

$$\ln\left(1+(i/c)\sum_{m=1}^{\infty} S_{2m-1}(0)z^{-m}\right)=\sum_{j=1}^{\infty} D_j z^{-j}. \tag{2.3.67}$$

We refer to (2.4.7)–(2.4.9) for a recursive formula for D_j in terms of $(i/c)S_{2m-1}(0)$. The first few D_j explicitly read

$$\begin{aligned}
&D_1 = -V(0)/\big[2c^2\big], \quad D_2 = \big[\ddot{V}(0) - 2V(0)^2\big]/\big[8c^4\big],\\
&D_3 = -\big[3V^{(4)}(0) - 24V(0)\ddot{V}(0) - 15\dot{V}(0)^2 + 16V(0)^3\big]/\big[96c^6\big],\\
&D_4 = \big(128c^8\big)^{-1}\big[V^{(6)}(0) + 48V(0)^2\ddot{V}(0) - 20\ddot{V}(0)^2 - 12V(0)V^{(4)}(0)\\
&\qquad + 60V(0)\dot{V}(0)^2 - 28V^{(3)}(0)\dot{V}(0) - 16V(0)^4\big],
\end{aligned} \tag{2.3.68}$$

etc.

Computing the asymptotic expansion of the last logarithmic term in (2.3.63), namely the term which depends on the boundary conditions, is somewhat more involved. By using the asymptotic expansion (2.3.43) it is not difficult to find

$$\begin{aligned}
&j_{A,B} + k_{A,B}\mathcal{S}^-(z,0) + \ell_{A,B}\mathcal{S}^+(z,1)\\
&\quad \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} -icz^{1/2}(\ell_{A,B} - k_{A,B}) + \sum_{m=0}^{N}\Delta_m z^{-m/2} + o\big(z^{-N/2}\big),
\end{aligned} \tag{2.3.69}$$

where

$$\Delta_0 = j_{A,B}, \quad \Delta_m = \ell_{A,B}S_m(1) + (-1)^m k_{A,B}S_m(0), \quad m \in \mathbb{N}, \tag{2.3.70}$$

and

$$m_{A,B}\mathcal{S}^-(z,0)\mathcal{S}^+(z,1) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} m_{A,B}c^2 z\left(1 + \sum_{m=2}^{N}\Lambda_m z^{-m/2}\right) + o\big(z^{-(N-2)/2}\big), \tag{2.3.71}$$

where

$$\Lambda_m = \sum_{\ell=0}^{m}\Omega_\ell^-(0)\Omega_{m-\ell}^+(1), \quad m \in \mathbb{N},\ m \geqslant 2, \tag{2.3.72}$$

with

$$\Omega_0^-(0) = \Omega_0^+(1) = 1, \quad \Omega_j^+(x) = (-1)^j\Omega_j^-(x) = (i/c)S_{j-1}(x), \quad j \in \mathbb{N}. \tag{2.3.73}$$

The first few Λ_m have the explicit form,

$$\begin{aligned}
&\Lambda_2 = -2^{-1}c^{-2}[V(1)+V(0)], \quad \Lambda_3 = -i4^{-1}c^{-3}\big[\dot{V}(1)+\dot{V}(0)\big],\\
&\Lambda_4 = 8^{-1}c^{-4}\big[\ddot{V}(1)+\ddot{V}(0)-V(0)^2-V(1)^2+2V(1)V(0)\big],\\
&\Lambda_5 = i(16)^{-1}c^{-5}\Big[V^{(3)}(0)-V^{(3)}(1)-2V(0)\big(2\dot{V}(0)+\dot{V}(1)\big)\\
&\qquad +2V(1)\big[\dot{V}(0)+2\dot{V}(1)\big]\Big],
\end{aligned} \tag{2.3.74}$$

etc.

This finally implies

$$\begin{aligned}
&j_{A,B}+k_{A,B}\mathcal{S}^-(z,0)+\ell_{A,B}\mathcal{S}^+(z,1)+m_{A,B}\mathcal{S}^-(z,0)\mathcal{S}^+(z,1)\\
&\quad \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \sum_{m=-2}^{N}\Gamma_m z^{-m/2}+o\big(z^{-N/2}\big),
\end{aligned} \tag{2.3.75}$$

where

$$\begin{aligned}
&\Gamma_{-2} = m_{A,B}c^2, \quad \Gamma_{-1} = -ic(\ell_{A,B}-k_{A,B}),\\
&\Gamma_m = \Delta_m + m_{A,B}c^2\Lambda_{m+2}, \quad m\in\mathbb{N}_0.
\end{aligned} \tag{2.3.76}$$

Let Γ_{k_0} with $k_0\in\mathbb{Z}$ and $k_0\geqslant -2$, be the first non-vanishing term of the series in (2.3.75). Since $\Gamma_{k_0}\neq 0$ one can write

$$\begin{aligned}
&\ln\big(j_{A,B}+k_{A,B}\mathcal{S}^-(z,0)+\ell_{A,B}\mathcal{S}^+(z,1)+m_{A,B}\mathcal{S}^-(z,0)\mathcal{S}^+(z,1)\big)\\
&\quad \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \ln(\Gamma_{k_0})-(k_0/2)\ln(z)+\ln\left(1+\sum_{m=1}^{N}[\Gamma_{m+k_0}/\Gamma_{k_0}]z^{-m/2}+o\big(z^{-N/2}\big)\right),
\end{aligned} \tag{2.3.77}$$

which, in turn, yields

$$\begin{aligned}
&\ln\big(j_{A,B}+k_{A,B}\mathcal{S}^-(z,0)+\ell_{A,B}\mathcal{S}^+(z,1)+m_{A,B}\mathcal{S}^-(z,0)\mathcal{S}^+(z,1)\big)\\
&\quad \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} \ln(\Gamma_{k_0})-(k_0/2)\ln(z)+\sum_{j=1}^{N}\Pi_j z^{-j/2}+o\big(z^{-N/2}\big),
\end{aligned} \tag{2.3.78}$$

where the terms Π_j are obtained via the formal asymptotic expansion

$$\ln\left(1+\sum_{m=1}^{\infty}[\Gamma_{m+k_0}/\Gamma_{k_0}]z^{-m/2}\right) = \sum_{j=1}^{\infty}\Pi_j z^{-j/2}. \tag{2.3.79}$$

Once again we refer to (2.4.7)–(2.4.9) for a recursive determination of Π_j in terms of $\Gamma_{m+k_0}/\Gamma_{k_0}$. The first few Π_m are explicitly of the form,

$$
\begin{aligned}
&\Pi_1 = \Gamma_{1+k_0}/\Gamma_{k_0}, \quad \Pi_2 = 2^{-1}\Gamma_{k_0}^{-2}\big[2\Gamma_{k_0}\Gamma_{k_0+2} - \Gamma_{k_0+1}^2\big], \\
&\Pi_3 = 3^{-1}\Gamma_{k_0}^{-3}\big[\Gamma_{k_0+1}^3 - 3\Gamma_{k_0}\Gamma_{k_0+2}\Gamma_{k_0+1} + 3\Gamma_{k_0}^2\Gamma_{k_0+3}\big], \\
&\Pi_4 = -4^{-1}\Gamma_{k_0}^{-4}\big[\Gamma_{k_0+1}^4 - 4\Gamma_{k_0}\Gamma_{k_0+2}\Gamma_{k_0+1}^2 + 4\Gamma_{k_0}^2\Gamma_{k_0+3}\Gamma_{k_0+1} \\
&\qquad + 2\Gamma_{k_0}^2\left(\Gamma_{k_0+2}^2 - 2\Gamma_{k_0}\Gamma_{k_0+4}\right)\big], \\
&\quad \text{etc.}
\end{aligned}
\tag{2.3.80}
$$

More explicit expressions for Π_m in terms of the potential V and its derivatives can be obtained with a simple computer program once the index k_0 has been determined.

Finally, we can provide the large-z asymptotic expansion of the logarithm of the characteristic function in the form

$$
\begin{aligned}
\ln(\mathcal{F}_{A,B}(z)) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} & -icz^{1/2} - 2^{-1}(k_0+1)\ln(z) + \ln(\Gamma_{k_0}/(2ic)) \\
& + \sum_{m=1}^{N} \Psi_m z^{-m/2} + o\big(z^{-N/2}\big),
\end{aligned}
\tag{2.3.81}
$$

where

$$
\begin{aligned}
\Psi_{2n} &= \int_0^1 d\eta\, S_{2n}(\eta) - D_{2n-1} + \Pi_{2n}, \quad n \in \mathbb{N}, \\
\Psi_{2n+1} &= \int_0^1 d\eta\, S_{2n+1}(\eta) + \Pi_{2n+1}, \quad n \in \mathbb{N}_0.
\end{aligned}
\tag{2.3.82}
$$

2.3.3 Analytic Continuation of the Spectral Zeta Function and the Zeta Regularized Functional Determinant

In order to perform the analytic continuation of the spectral ζ-function, we need investigate the specific behavior for $z \downarrow 0$ and $|z| \to \infty$. The characteristic function $\mathcal{F}_{A,B}(z)$ is constructed as a linear combination of the basis functions $\phi(z,\,\cdot\,,a)$ and $\theta(z,\,\cdot\,,a)$ (or equivalently the transformed basis functions $\Phi(z,\,\cdot\,,0)$ and $\Theta(z,\,\cdot\,,0)$) and their first quasi-derivatives. We have proved that $\phi(z,\,\cdot\,,a)$ and $\theta(z,\,\cdot\,,a)$, and consequently $\Phi(z,\,\cdot\,,0)$ and $\Theta(z,\,\cdot\,,0)$, have a small-z asymptotic expansion in the form of a power series in the variable z in Section 2.3.1. This implies that $\mathcal{F}_{A,B}(z)$ has a small-z asymptotic expansion of the form

$$\mathcal{F}_{A,B}(z) = \mathcal{F}_{m_0} z^{m_0} + \sum_{m=m_0+1}^{\infty} \mathcal{F}_m z^m, \tag{2.3.83}$$

where $m_0 \in \{0,1,2\}$ represents the multiplicity of the zero eigenvalue and $\mathcal{F}_{m_0} \neq 0$. The asymptotic expansion (2.3.83) suggests that the appropriate characteristic function to use in the integral representation of the spectral ζ-function is $z^{-m_0}\mathcal{F}_{A,B}(z)$ rather than simply $\mathcal{F}_{A,B}(z)$ (obviously the two coincide when no zero eigenvalue is present). In this case it is easy to verify that

$$\frac{d}{dz} \ln\left(\mathcal{F}_{A,B}(z) z^{-m_0}\right) \underset{|z|\downarrow 0}{=} O(1). \tag{2.3.84}$$

From the large-z asymptotic expansion (2.3.81) of the characteristic function, namely,

$$\begin{aligned} \ln(\mathcal{F}_{A,B}(z)) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} & -icz^{1/2} - [(k_0+1)/2]\ln(z) + \ln(\Gamma_{k_0}/(2ic)) \\ & + \sum_{m=1}^{N} \Psi_m z^{-m/2} + o\big(|z|^{-N/2}\big), \end{aligned} \tag{2.3.85}$$

one readily infers that

$$\frac{d}{dz}\ln(\mathcal{F}_{A,B}(z) z^{-m_0}) \underset{\substack{|z|\to\infty \\ \mathrm{Im}(z^{1/2})\geqslant 0}}{=} O\big(|z|^{-1/2}\big). \tag{2.3.86}$$

The asymptotic behaviors in (2.3.84) and (2.3.86) justify deforming the contour γ in the integral representation (2.2.39) to one that surrounds the branch cut R_ψ as shown in Figure 2.2. This contour deformation leads to the following integral representation (with ψ introduced in (2.2.40))

$$\zeta(s; T_{A,B}) = e^{is(\pi-\psi)}\pi^{-1}\sin(\pi s)\int_0^\infty dt\, t^{-s}\frac{d}{dt}\ln\left(\mathcal{F}_{A,B}(te^{i\psi})t^{-m_0}e^{-im_0\psi}\right), \tag{2.3.87}$$

which is valid in the region $1/2 < \mathrm{Re}(s) < 1$. To obtain the analytic continuation of (2.3.87) to the left of the abscissa of convergence $\mathrm{Re}(s) = 1/2$ we subtract and then add N terms of the large-z asymptotic expansion of $\ln\big(\mathcal{F}_{A,B}(te^{i\psi})t^{-m_0}e^{-im_0\psi}\big)$.

This process leads to the following expression of the spectral ζ-function

$$\zeta(s;T_{A,B}) = Z(s,A,B) + \sum_{j=-1}^{N} h_j(s,A,B), \tag{2.3.88}$$

which is valid in the region $-(N+1)/2 < \mathrm{Re}(s) < 1$. The explicit form of the functions in the analytically continued expression of $\zeta(s;T_{A,B})$ in (2.3.88) is

$$\begin{aligned} Z(s,A,B) = e^{is(\pi-\psi)}\pi^{-1}\sin(\pi s)\int_0^\infty dt\, t^{-s}\frac{d}{dt}\Big\{ \ln\big(\mathcal{F}_{A,B}(te^{i\psi})t^{-m_0}e^{-im_0\psi}\big) \\ - H(t-1)\Big[-ict^{1/2}e^{i\psi/2} - [((k_0+1)/2)+m_0]\ln(t) \\ - \big[((k_0+1)/2)+m_0\big]i\psi + \ln(\Gamma_{k_0}/(2ic)) + \sum_{n=1}^{N}\Psi_n e^{-in\psi/2}t^{-n/2}\Big]\Big\}, \end{aligned} \tag{2.3.89}$$

where $H(s) = \begin{cases} 1, & s > 0, \\ 0, & s < 0, \end{cases}$ represents the Heaviside function, and

$$\begin{aligned} h_{-1}(s,A,B) &= -ie^{is(\pi-\psi)}\pi^{-1}\sin(\pi s)c\, e^{i\psi/2}/(2s-1), \\ h_0(s,A,B) &= -(k_0+1+2m_0)e^{is(\pi-\psi)}(2\pi s)^{-1}\sin(\pi s), \\ h_n(s,A,B) &= -e^{is(\pi-\psi)}\pi^{-1}\sin(\pi s)[n/(2s+n)]e^{-in\psi/2}\Psi_n, \quad n\in\mathbb{N}. \end{aligned} \tag{2.3.90}$$

Given the expression (2.3.88) we are now able to compute the zeta regularized functional determinant in terms of $\zeta'(0;T_{A,B})$ as in [74, Thm. 2.9]. For the purpose of computing $\zeta'(0;T_{A,B})$, it is sufficient to set $N=0$ in (2.3.88) to obtain

$$\zeta'(0;T_{A,B}) = Z'(0,A,B) + h'_{-1}(0,A,B) + h'_0(0,A,B). \tag{2.3.91}$$

By computing the derivative with respect to s of (2.3.89) and the first two expressions in (2.3.90) at $s=0$ one obtains the remarkably simple formula

$$\zeta'(0;T_{A,B}) = i\pi n - \ln(2c|\mathcal{F}_{m_0}/\Gamma_{k_0}|), \tag{2.3.92}$$

where n is the number of strictly negative eigenvalues of $T_{A,B}$.

2.4 Computing Spectral Zeta Function Values and Traces for Regular Sturm–Liouville Operators

We have now completed the necessary preparations to give the main theorem for computing values of the spectral ζ-function for self-adjoint regular Sturm–Liouville operators when imposing either separated or coupled boundary conditions. When zero is not an eigenvalue we also find an expression for computing the trace of the inverse Sturm–Liouville operator.

Theorem 2.4.1. *Assume Hypothesis* 2.2.1*, denote by $T_{A,B}$ the self-adjoint extension of T_{min} with either separated or coupled boundary conditions as described in Theorem* 2.2.2*, and let $m_0 = 0, 1, 2,$ denote the multiplicity of zero as an eigenvalue of $T_{A,B}$* (*with $m_0 = 0$ denoting zero is not an eigenvalue*)*. Suppose that $F_{A,B}(z)$ given in* (2.2.39) *has the series expansion,*

$$F_{A,B}(z) = \sum_{j=0}^{\infty} a_j z^j, \quad 0 \leqslant |z| \text{ sufficiently small.} \tag{2.4.1}$$

Then,

$$\zeta(n; T_{A,B}) = -\mathrm{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{A,B}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.2}$$

where

$$\begin{aligned} &b_1 = a_{1+m_0}/a_{m_0}, \\ &b_j = [a_{j+m_0}/a_{m_0}] - \sum_{\ell=1}^{j-1}[\ell/j][a_{j-\ell+m_0}/a_{m_0}]b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2. \end{aligned} \tag{2.4.3}$$

In particular, if zero is not an eigenvalue of $T_{A,B}$, then

$$\mathrm{tr}_{L_r^2((a,b))}\big(T_{A,B}^{-1}\big) = \zeta(1; T_{A,B}) = -a_1/a_0. \tag{2.4.4}$$

Proof. The residue in equation (2.4.2) coincides with the z^{-1} coefficient of the Laurent expansion, in the neighborhood of $z = 0$, of the integrand in (2.2.41). By using the expansion (2.4.1) one obtains, for $|z| \geqslant 0$ sufficiently small and for $n \in \mathbb{N}$, that

$$z^{-n}\frac{d}{dz}\ln(F_{A,B}(z)) = z^{-n}\frac{d}{dz}\ln\left(\sum_{j=0}^{\infty} a_j z^j\right). \tag{2.4.5}$$

Since $z = 0$ can be an eigenvalue of multiplicity at most 2, the expansion can be rewritten as follows,

$$\begin{aligned} z^{-n}\frac{d}{dz}\ln(F_{A,B}(z)) &= z^{-n}\frac{d}{dz}\ln\left(\sum_{j=m_0}^{\infty} a_j z^j\right) \\ &= z^{-n}\frac{d}{dz}\left(\ln\left(a_{m_0} z^{m_0}\right) + \ln\left(1 + \sum_{j=1}^{\infty}[a_{j+m_0}/a_{m_0}]z^j\right)\right) \\ &= m_0 z^{-n-1} + z^{-n}\frac{d}{dz}\ln\left(1 + \sum_{j=1}^{\infty}[a_{j+m_0}/a_{m_0}]z^j\right). \end{aligned} \tag{2.4.6}$$

Since $n \in \mathbb{N}$, the term $m_0 z^{-n-1}$ never contributes to the residue and the only contribution comes from the z^n coefficient of the small-$|z|$ asymptotic expansion of the logarithm on the right-hand side. This expansion can be obtained by making use of the fact that if F has the analytic expansion

$$F(z) = \sum_{m=1}^{\infty} c_m z^m, \quad 0 \leqslant |z| \text{ sufficiently small,} \tag{2.4.7}$$

then

$$\ln(1 + F(z)) = \sum_{m=1}^{\infty} d_m z^m, \quad 0 \leqslant |z| \text{ sufficiently small,} \tag{2.4.8}$$

where

$$d_1 = c_1, \quad d_j = c_j - \sum_{\ell=1}^{j-1}[\ell/j]c_{j-\ell}d_\ell, \quad j \in \mathbb{N},\ j \geqslant 2. \tag{2.4.9}$$

By using (2.4.8) one obtains

$$\ln\left(1 + \sum_{j=1}^{\infty}[a_{j+m_0}/a_{m_0}]z^j\right) = \sum_{j=1}^{\infty} b_j z^j, \tag{2.4.10}$$

with the coefficients b_j given by equation (2.4.3). From the last expansion one finally obtains

$$z^{-n}\frac{d}{dz}\ln(F_{A,B}(z)) = z^{-n}\frac{d}{dz}\ln\left(\sum_{j=1}^{\infty} a_j z^j\right) = \sum_{j=1}^{\infty} j b_j z^{j-n-1}. \tag{2.4.11}$$

This is the Laurent expansion, and from it one can deduce that

$$\operatorname{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{A,B}(z));\ z = 0\right] = n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.12}$$

proving (2.4.2).

Assertion (2.4.4) about the trace of the inverse operator when $z = 0$ is not an eigenvalue is obtained by noting

$$-\frac{d}{dz}\ln(F_{A,B}(z))\bigg|_{z=0} = -d_1 = -a_1/a_0 \tag{2.4.13}$$

from the analytic expansions (2.4.7) and (2.4.8), and applying Theorem 2.2.4. $\square$

This theorem allows one to utilize the series expansions found in the previous section in order to express the ζ-function values for each of the boundary conditions considered.

2.4.1 Computing Spectral Zeta Function Values and Traces for Separated Boundary Conditions

We begin by applying Theorem 2.4.1 to find an expression for $\zeta(n; T_{\alpha,\beta})$ when imposing separated boundary conditions.

Theorem 2.4.2. *Assume Hypothesis* 2.2.1, *consider* $T_{\alpha,\beta}$ *as described in Theorem* 2.2.2 (*i*), *and let* $m_0 = 0, 1$, *denote the multiplicity of zero as an eigenvalue of* $T_{\alpha,\beta}$. *Then,*

$$\zeta(n; T_{\alpha,\beta}) = -\text{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{\alpha,\beta}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.14}$$

where

$$b_1 = \frac{\cos(\alpha)\big[\cos(\beta)\phi_{1+m_0}(b) - \sin(\beta)\phi^{[1]}_{1+m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{1+m_0}(b) - \sin(\beta)\theta^{[1]}_{1+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi^{[1]}_{m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b) - \sin(\beta)\theta^{[1]}_{m_0}(b)\big]},$$

$$\begin{aligned} b_j = {} & \frac{\cos(\alpha)\big[\cos(\beta)\phi_{j+m_0}(b) - \sin(\beta)\phi^{[1]}_{j+m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{j+m_0}(b) - \sin(\beta)\theta^{[1]}_{j+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi^{[1]}_{m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b) - \sin(\beta)\theta^{[1]}_{m_0}(b)\big]} \\ & - \sum_{\ell=1}^{j-1}\left(\frac{\ell}{j}\right) \frac{\cos(\alpha)\big[\cos(\beta)\phi_{j-\ell+m_0}(b) - \sin(\beta)\phi^{[1]}_{j-\ell+m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{j-\ell+m_0}(b) - \sin(\beta)\theta^{[1]}_{j-\ell+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi^{[1]}_{m_0}(b)\big] - \sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b) - \sin(\beta)\theta^{[1]}_{m_0}(b)\big]} b_\ell, \\ & j \in \mathbb{N},\ j \geqslant 2. \end{aligned} \tag{2.4.15}$$

In particular, if zero is not an eigenvalue of $T_{\alpha,\beta}$, *then*

$$\text{tr}_{L^2_r((a,b))}\big(T^{-1}_{\alpha,\beta}\big) = \zeta(1; T_{\alpha,\beta}) \tag{2.4.16}$$

$$= -\frac{\cos(\alpha)\big[\cos(\beta)\ \phi_1(b) - \sin(\beta)\ \phi_1^{[1]}(b)\big] - \sin(\alpha)\big[\cos(\beta)\ \theta_1(b) - \sin(\beta)\ \theta_1^{[1]}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\ \phi_0(b) - \sin(\beta)\ \phi_0^{[1]}(b)\big] - \sin(\alpha)\big[\cos(\beta)\ \theta_0(b) - \sin(\beta)\ \theta_0^{[1]}(b)\big]}.$$

Proof. One substitutes (2.3.4), (2.3.6), (2.3.8), and (2.3.11) into equation (2.2.16) for $\alpha, \beta \in [0, \pi)$ to find

$$\begin{aligned} F_{\alpha,\beta}(z) = \sum_{m=0}^{\infty} \big\{ &\cos(\alpha)\big[\cos(\beta)\ \phi_m(b) - \sin(\beta)\ \phi_m^{[1]}(b)\big] \\ &- \sin(\alpha)\big[\cos(\beta)\ \theta_m(b) - \sin(\beta)\ \theta_m^{[1]}(b)\big]\big\} z^m. \end{aligned} \tag{2.4.17}$$

From (2.4.17) one proves the assertion by applying Theorem 2.4.1 with

$$\begin{aligned} a_k = &\cos(\alpha)\big[\cos(\beta)\ \phi_k(b) - \sin(\beta)\ \phi_k^{[1]}(b)\big] \\ &- \sin(\alpha)\big[-\sin(\beta)\ \theta_k^{[1]}(b) + \cos(\beta)\ \theta_k(b)\big], \quad k \in \mathbb{N}. \end{aligned} \tag{2.4.18}$$

□

We now give a few corollaries that will be of use in the context of specific boundary conditions. One notes that for Dirichlet boundary conditions one has $\alpha = \beta = 0$ and for Neumann boundary conditions one has $\alpha = \beta = \pi/2$.

Corollary 2.4.3 (Dirichlet boundary conditions). *Assume Hypothesis* 2.2.1*, consider* $T_{0,0}$ *as described in case Theorem* 2.2.2 (*i*)*, and let* $m_0 = 0, 1$*, denote the multiplicity of zero as an eigenvalue of* $T_{0,0}$*. Then,*

$$\zeta(n; T_{0,0}) = -\mathrm{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{0,0}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.19}$$

where

$$\begin{aligned} &b_1 = \phi_{1+m_0}(b)/\phi_{m_0}(b), \\ &b_j = [\phi_{j+m_0}(b)/\phi_{m_0}(b)] - \sum_{\ell=1}^{j-1}[\ell/j][\phi_{j-\ell+m_0}(b)/\phi_{m_0}(b)]b_\ell, \quad j \in \mathbb{N}, \geqslant 2. \end{aligned} \tag{2.4.20}$$

In particular, if zero is not an eigenvalue of $T_{0,0}$*, then*

$$\mathrm{tr}_{L_r^2((a,b))}\big(T_{0,0}^{-1}\big) = \zeta(1; T_{0,0}) = -\phi_1(b)/\phi_0(b). \tag{2.4.21}$$

Proof. Take $\alpha = \beta = 0$ in Theorem 2.4.2. □

In particular, one finds explicitly for $n = 2, 3, 4$, when zero is not an eigenvalue of $T_{0,0}$:

$$\begin{aligned}
\zeta(2;T_{0,0}) &= -2b_2 = -2\left[\frac{\phi_2(b)}{\phi_0(b)} - \frac{[\phi_1(b)]^2}{2[\phi_0(b)]^2}\right], \\
\zeta(3;T_{0,0}) &= -3b_3 = -3\left[\frac{\phi_3(b)}{\phi_0(b)} - \frac{\phi_1(b)\phi_2(b)}{[\phi_0(b)]^2} + \frac{[\phi_1(b)]^3}{3[\phi_0(b)]^3}\right], \\
\zeta(4;T_{0,0}) &= -4b_4 = -4\left[\frac{\phi_4(b)}{\phi_0(b)} - \frac{\phi_1(b)\phi_3(b)}{[\phi_0(b)]^2} - \frac{[\phi_2(b)]^2}{2[\phi_0(b)]^2} + \frac{[\phi_1(b)]^2\phi_2(b)}{[\phi_0(b)]^3} - \frac{[\phi_1(b)]^4}{4[\phi_0(b)]^4}\right].
\end{aligned} \tag{2.4.22}$$

One also finds explicitly for $n = 2, 3, 4$, when zero is a simple eigenvalue of $T_{0,0}$:

$$\begin{aligned}
\zeta(2;T_{0,0}) &= -2b_2 = -2\left[\frac{\phi_3(b)}{\phi_1(b)} - \frac{[\phi_2(b)]^2}{2[\phi_1(b)]^2}\right], \\
\zeta(3;T_{0,0}) &= -3b_3 = -3\left[\frac{\phi_4(b)}{\phi_1(b)} - \frac{\phi_2(b)\phi_3(b)}{[\phi_1(b)]^2} + \frac{[\phi_2(b)]^3}{3[\phi_1(b)]^3}\right], \\
\zeta(4;T_{0,0}) &= -4b_4 = -4\left[\frac{\phi_5(b)}{\phi_1(b)} - \frac{\phi_2(b)\phi_4(b)}{[\phi_1(b)]^2} - \frac{[\phi_3(b)]^2}{2[\phi_1(b)]^2} + \frac{[\phi_2(b)]^2\phi_3(b)}{[\phi_1(b)]^3} - \frac{[\phi_2(b)]^4}{4[\phi_1(b)]^4}\right].
\end{aligned} \tag{2.4.23}$$

Corollary 2.4.4 (Dirichlet boundary condition at a). *Assume Hypothesis* 2.2.1*, consider $T_{0,\beta}$ as described in Theorem* 2.2.2 *(i), and let $m_0 = 0, 1$, denote the multiplicity of zero as an eigenvalue of $T_{0,\beta}$. Then,*

$$\zeta(n;T_{0,\beta}) = -\mathrm{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{0,\beta}(z));\ z=0\right] = -n\,b_n, \quad n \in \mathbb{N}, \tag{2.4.24}$$

where

$$\begin{aligned}
b_1 &= \frac{\cos(\beta)\phi_{1+m_0}(b) - \sin(\beta)\phi_{1+m_0}^{[1]}(b)}{\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi_{m_0}^{[1]}(b)}, \\
b_j &= \frac{\cos(\beta)\phi_{j+m_0}(b) - \sin(\beta)\phi_{j+m_0}^{[1]}(b)}{\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi_{m_0}^{[1]}(b)} \\
&\quad - \sum_{\ell=1}^{j-1}[\ell/j]\frac{\cos(\beta)\phi_{j-\ell+m_0}(b) - \sin(\beta)\phi_{j-\ell+m_0}^{[1]}(b)}{\cos(\beta)\phi_{m_0}(b) - \sin(\beta)\phi_{m_0}^{[1]}(b)}b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2.
\end{aligned} \tag{2.4.25}$$

In particular, if zero is not an eigenvalue of $T_{0,\beta}$, then

$$\mathrm{tr}_{L^2_r((a,b))}\big(T_{0,\beta}^{-1}\big) = \zeta(1;T_{0,\beta}) = -\frac{\cos(\beta)\phi_1(b) - \sin(\beta)\phi_1^{[1]}(b)}{\cos(\beta)\phi_0(b) - \sin(\beta)\phi_0^{[1]}(b)}. \tag{2.4.26}$$

Proof. Take $\alpha = 0$ in Theorem 2.4.2. □

Corollary 2.4.5 (Dirichlet boundary condition at b). *Assume Hypothesis* 2.2.1*, consider* $T_{\alpha,0}$ *as described in Theorem* 2.2.2 (i)*, and let* $m_0 = 0, 1$*, denote the multiplicity of zero as an eigenvalue of* $T_{\alpha,0}$*. Then,*

$$\zeta(n;T_{\alpha,0}) = -\text{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{\alpha,0}(z));\ z=0\right] = -n\,b_n, \quad n\in\mathbb{N}, \tag{2.4.27}$$

where

$$\begin{aligned} b_1 &= \frac{\cos(\alpha)\phi_{1+m_0}(b)-\sin(\alpha)\theta_{1+m_0}(b)}{\cos(\alpha)\phi_{m_0}(b)-\sin(\alpha)\theta_{m_0}(b)}, \\ b_j &= \frac{\cos(\alpha)\phi_{j+m_0}(b)-\sin(\alpha)\theta_{j+m_0}(b)}{\cos(\alpha)\phi_{m_0}(b)-\sin(\alpha)\theta_{m_0}(b)} \\ &\quad -\sum_{\ell=1}^{j-1}[\ell/j]\frac{\cos(\alpha)\phi_{j-\ell+m_0}(b)-\sin(\alpha)\theta_{j-\ell+m_0}(b)}{\cos(\alpha)\phi_{m_0}(b)-\sin(\alpha)\theta_{m_0}(b)}b_\ell, \quad j\in\mathbb{N},\ j\geqslant 2. \end{aligned} \tag{2.4.28}$$

In particular, if zero is not an eigenvalue of $T_{\alpha,0}$*, then*

$$\text{tr}_{L^2_r((a,b))}\big(T_{\alpha,0}^{-1}\big) = \zeta(1;T_{\alpha,0}) = -\frac{\cos(\alpha)\phi_1(b)-\sin(\alpha)\theta_1(b)}{\cos(\alpha)\phi_0(b)-\sin(\alpha)\theta_0(b)}. \tag{2.4.29}$$

Proof. Take $\beta = 0$ in Theorem 2.4.2. □

Corollary 2.4.6 (Neumann boundary conditions). *Assume Hypothesis* 2.2.1*, consider* $T_{\pi/2,\pi/2}$ *as described in Theorem* 2.2.2 (i)*, and let* $m_0 = 0, 1$*, denote the multiplicity of zero as an eigenvalue of* $T_{\pi/2,\pi/2}$*. Then,*

$$\zeta(n;T_{\pi/2,\pi/2}) = -\text{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{\pi/2,\pi/2}(z));\ z=0\right] = -n\,b_n, \quad n\in\mathbb{N}, \tag{2.4.30}$$

where

$$\begin{aligned} b_1 &= \theta^{[1]}_{1+m_0}(b)/\theta^{[1]}_{m_0}(b), \\ b_j &= \theta^{[1]}_{j+m_0}/(b)\theta^{[1]}_{m_0}(b) - \sum_{\ell=1}^{j-1}[\ell/j]\big[\theta^{[1]}_{j-\ell+m_0}(b)/\theta^{[1]}_{m_0}(b)\big]b_\ell, \quad j\in\mathbb{N},\ j\geqslant 2. \end{aligned} \tag{2.4.31}$$

In particular, if zero is not an eigenvalue of $T_{\pi/2,\pi/2}$*, then*

$$\text{tr}_{L^2_r((a,b))}\big(T_{\pi/2,\pi/2}^{-1}\big) = \zeta(1;T_{\pi/2,\pi/2}) = -\theta_1^{[1]}(b)/\theta_0^{[1]}(b). \tag{2.4.32}$$

Proof. Take $\alpha = \beta = \pi/2$ in Theorem 2.4.2. □

These are only a few of the most considered separated boundary conditions that have been singled out. One can also consider Neumann boundary conditions at only one endpoint, or any other combination of separated boundary conditions, by referring back to Theorem 2.4.2 with the appropriate values chosen for $\alpha, \beta \in [0, \pi)$.

2.4.2 Computing Spectral Zeta Function Values and Traces for Coupled Boundary Conditions

We now apply Theorem 2.4.1 to find values of $\zeta(n; T_{\varphi,R})$ when imposing coupled boundary conditions. Notice that according to [68], zero is an eigenvalue of multiplicity 2 only for the Krein–von Neumann extension.

Theorem 2.4.7. *Assume Hypothesis* 2.2.1*, consider $T_{\varphi,R}$ as described in Theorem* 2.2.2 *(ii), and let $m_0 = 0, 1$, denote the multiplicity of zero as an eigenvalue of $T_{\varphi,R}$. Then,*

$$\zeta(n; T_{\varphi,R}) = -\mathrm{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{\varphi,R}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.33}$$

where for $m_0 = 0$,

$$\begin{aligned}
b_1 &= \frac{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b) - R_{22}\theta_1(b) + R_{21}\phi_1(b) - R_{11}\phi_1^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1},\\
b_j &= \frac{e^{i\varphi}\big(R_{12}\theta_j^{[1]}(b) - R_{22}\theta_j(b) + R_{21}\phi_j(b) - R_{11}\phi_j^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1}\\
&\quad - \sum_{\ell=1}^{j-1}\frac{\ell}{j}\frac{e^{i\varphi}\big(R_{12}\theta_{j-\ell}^{[1]}(b) - R_{22}\theta_{j-\ell}(b) + R_{21}\phi_{j-\ell}(b) - R_{11}\phi_{j-\ell}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1} b_\ell,\\
&\qquad j \in \mathbb{N},\ j \geqslant 2,
\end{aligned} \tag{2.4.34}$$

and for $m_0 = 1$,

$$\begin{aligned}
b_1 &= \frac{e^{i\varphi}\big(R_{12}\theta_2^{[1]}(b) - R_{22}\theta_2(b) + R_{21}\phi_2(b) - R_{11}\phi_2^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b) - R_{22}\theta_1(b) + R_{21}\phi_1(b) - R_{11}\phi_1^{[1]}(b)\big)},\\
b_j &= \frac{e^{i\varphi}\big(R_{12}\theta_{j+1}^{[1]}(b) - R_{22}\theta_{j+1}(b) + R_{21}\phi_{j+1}(b) - R_{11}\phi_{j+1}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b) - R_{22}\theta_1(b) + R_{21}\phi_1(b) - R_{11}\phi_1^{[1]}(b)\big)}\\
&\quad - \sum_{\ell=1}^{j-1}\frac{\ell}{j}\frac{e^{i\varphi}\big(R_{12}\theta_{j-\ell+1}^{[1]}(b) - R_{22}\theta_{j-\ell+1}(b) + R_{21}\phi_{j-\ell+1}(b) - R_{11}\phi_{j-\ell+1}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b) - R_{22}\theta_1(b) + R_{21}\phi_1(b) - R_{11}\phi_1^{[1]}(b)\big)} b_\ell,\\
&\qquad j \in \mathbb{N},\ j \geqslant 2.
\end{aligned} \tag{2.4.35}$$

In particular, if zero is not an eigenvalue of $T_{\varphi,R}$, then

$$\begin{aligned}
&\operatorname{tr}_{L^2_r((a,b))}\big(T_{\varphi,R}^{-1}\big) = \zeta(1;T_{\varphi,R}) \\
&\quad = \frac{-e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b) - R_{22}\theta_1(b) + R_{21}\phi_1(b) - R_{11}\phi_1^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1}.
\end{aligned} \tag{2.4.36}$$

Proof. Substituting (2.3.4), (2.3.6), (2.3.8), and (2.3.11) into equation (2.2.17) yields

$$F_{\varphi,R}(0) = e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1. \tag{2.4.37}$$

Thus, the coefficient of the z^m term for $m \geqslant 1$ in the series is given by

$$e^{i\varphi}\big(R_{12}\theta_m^{[1]}(b) - R_{22}\theta_m(b) + R_{21}\phi_m(b) - R_{11}\phi_m^{[1]}(b)\big). \tag{2.4.38}$$

Hence, assertions (2.4.34) and (2.4.35) follow from Theorem 2.4.1 with

$$\begin{aligned}
a_0 &= e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b) - R_{22}\theta_0(b) + R_{21}\phi_0(b) - R_{11}\phi_0^{[1]}(b)\big) + e^{2i\varphi} + 1, \\
a_k &= e^{i\varphi}\big(R_{12}\theta_k^{[1]}(b) - R_{22}\theta_k(b) + R_{21}\phi_k(b) - R_{11}\phi_k^{[1]}(b)\big), \quad k \in \mathbb{N}.
\end{aligned} \tag{2.4.39}$$

□

Next, we provide corollaries regarding the most common coupled boundary conditions, periodic and antiperiodic as well as the Krein-von Neumann extension.

Corollary 2.4.8 (Periodic boundary conditions). *Assume Hypothesis* 2.2.1*, consider T_{0,I_2} as described in Theorem* 2.2.2 *(ii), and let $m_0 = 0, 1$, denote the multiplicity of zero as an eigenvalue of T_{0,I_2}. Then,*

$$\zeta(n;T_{0,I_2}) = -\operatorname{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{0,I_2}(z));\ z=0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.40}$$

where for $m_0 = 0$,

$$b_1 = \big[-\theta_1(b) - \phi_1^{[1]}(b)\big]\big/\big[-\theta_0(b) - \phi_0^{[1]}(b) + 2\big], \tag{2.4.41}$$

$$b_j = \frac{-\theta_j(b) - \phi_j^{[1]}(b)}{-\theta_0(b) - \phi_0^{[1]}(b) + 2} - \sum_{\ell=1}^{j-1} \frac{\ell}{j}\, \frac{-\theta_{j-\ell}(b) - \phi_{j-\ell}^{[1]}(b)}{-\theta_0(b) - \phi_0^{[1]}(b) + 2} b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2,$$

and for $m_0 = 1$,

$$b_1 = \big[\theta_2(b) + \phi_2^{[1]}(b)\big]\big/\big[\theta_1(b) + \phi_1^{[1]}(b)\big], \tag{2.4.42}$$

$$b_j = \frac{\theta_{j+1}(b) + \phi_{j+1}^{[1]}(b)}{\theta_1(b) + \phi_1^{[1]}(b)} - \sum_{\ell=1}^{j-1} \frac{\ell}{j} \frac{\theta_{j-\ell+1}(b) + \phi_{j-\ell+1}^{[1]}(b)}{\theta_1(b) + \phi_1^{[1]}(b)} b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2.$$

In particular, if zero is not an eigenvalue of T_{0,I_2}*, then*

$$\operatorname{tr}_{L^2_r((a,b))}\big(T_{0,I_2}^{-1}\big) = \zeta(1; T_{0,I_2}) = \big[\theta_1(b) + \phi_1^{[1]}(b)\big] / \big[-\theta_0(b) - \phi_0^{[1]}(b) + 2\big]. \quad (2.4.43)$$

Proof. Take $\varphi = 0$ and $R = I_2$ in Theorem 2.4.7. □

Corollary 2.4.9 (Antiperiodic boundary conditions). *Assume Hypothesis* 2.2.1*, consider* $T_{0,-I_2}$ *as described in Theorem* 2.2.2 *(ii), and let* $m_0 = 0, 1$*, denote the multiplicity of zero as an eigenvalue of* $T_{0,-I_2}$*. Then,*

$$\zeta(n; T_{0,-I_2}) = -\operatorname{Res}\left[z^{-n} \frac{d}{dz} \ln(F_{0,-I_2}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \qquad (2.4.44)$$

where for $m_0 = 0$*,*

$$b_1 = \big[\theta_1(b) + \phi_1^{[1]}(b)\big] / \big[\theta_0(b) + \phi_0^{[1]}(b) + 2\big], \qquad (2.4.45)$$

$$b_j = \frac{\theta_j(b) + \phi_j^{[1]}(b)}{\theta_0(b) + \phi_0^{[1]}(b) + 2} - \sum_{\ell=1}^{j-1} \frac{\ell}{j} \frac{\theta_{j-\ell}(b) + \phi_{j-\ell}^{[1]}(b)}{\theta_0(b) + \phi_0^{[1]}(b) + 2} b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2,$$

and for $m_0 = 1$*,*

$$b_1 = \big[\theta_2(b) + \phi_2^{[1]}(b)\big] / \big[\theta_1(b) + \phi_1^{[1]}(b)\big], \qquad (2.4.46)$$

$$b_j = \frac{\theta_{j+1}(b) + \phi_{j+1}^{[1]}(b)}{\theta_1(b) + \phi_1^{[1]}(b)} - \sum_{\ell=1}^{j-1} \frac{\ell}{j} \frac{\theta_{j-\ell+1}(b) + \phi_{j-\ell+1}^{[1]}(b)}{\theta_1(b) + \phi_1^{[1]}(b)} b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2.$$

In particular, if zero is not an eigenvalue of $T_{0,-I_2}$*, then*

$$\operatorname{tr}_{L^2_r((a,b))}\big(T_{0,-I_2}^{-1}\big) = \zeta(1; T_{0,-I_2}) = -\big[\theta_1(b) + \phi_1^{[1]}(b)\big] / \big[\theta_0(b) + \phi_0^{[1]}(b) + 2\big]. \quad (2.4.47)$$

Proof. Take $\varphi = 0$ and $R = -I_2$ in Theorem 2.4.7. □

Corollary 2.4.10 (Krein-von Neumann extension). *Assume Hypothesis* 2.2.1*, consider* T_{0,R_K} *the Krein-von Neumann extension of* T_{min} *with*

$$\varphi = 0, \quad R_K = \begin{pmatrix} \theta(0,b,a) & \phi(0,b,a) \\ \theta^{[1]}(0,b,a) & \phi^{[1]}(0,b,a) \end{pmatrix}, \qquad (2.4.48)$$

and let $m_0 = 2$, denote the multiplicity of zero as an eigenvalue of T_{0,R_K}. Then,

$$\zeta(n; T_{0,R_K}) = -\text{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{0,R_K}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{2.4.49}$$

where

$$b_1 = \frac{\phi_0(b)\theta_3^{[1]}(b) - \phi_0^{[1]}(b)\theta_3(b) + \theta_0^{[1]}(b)\phi_3(b) - \theta_0(b)\phi_3^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)},$$

$$\begin{aligned} b_j = {} & \frac{\phi_0(b)\theta_{j+2}^{[1]}(b) - \phi_0^{[1]}(b)\theta_{j+2}(b) + \theta_0^{[1]}(b)\phi_{j+2}(b) - \theta_0(b)\phi_{j+2}^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)} \\ & - \sum_{\ell=1}^{j-1}\frac{\ell}{j}\,\frac{\phi_0(b)\theta_{j-\ell+2}^{[1]}(b) - \phi_0^{[1]}(b)\theta_{j-\ell+2}(b) + \theta_0^{[1]}(b)\phi_{j-\ell+2}(b) - \theta_0(b)\phi_{j-\ell+2}^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)}\, b_\ell, \\ & \qquad j \in \mathbb{N},\ j \geqslant 2. \end{aligned} \tag{2.4.50}$$

Proof. As shown in [34, Example 3.3], the resulting operator T_{0,R_K} represents the Krein–von Neumann extension of T_{min}. Take $\varphi = 0$ and $R = R_K$ (as defined by (2.4.48)) in Theorem 2.4.7, denoting $\phi_0(b) = \phi(0,b,a)$, $\phi_0^{[1]}(b) = \phi^{[1]}(0,b,a)$, $\theta_0(b) = \theta(0,b,a)$, and $\theta_0^{[1]}(b) = \theta^{[1]}(0,b,a)$ as before, for simplicity. □

2.5 Examples

In this section, we provide an array of examples illustrating our approach for computing spectral ζ-function values of regular Schrödinger operators starting with the simplest case of $q = 0$, then a positive (piecewise) constant potential, followed by a constant negative potential, and ending with the case of a linear potential.

Throughout this section we suppose that

$$p = r = 1 \text{ a.e. on } (a,b) \tag{2.5.1}$$

which leaves the potential coefficient $q \in L^1((a,b);dx)$, q real-valued, and hence leaves us with the differential expression

$$\tau = -\big(d^2/dx^2\big) + q(x), \quad x \in (a,b). \tag{2.5.2}$$

2.5.1 The Example q=0

We start by providing examples for calculating spectral ζ-function values for the simple case $q(x) = 0$, $x \in (a, b)$, imposing various boundary conditions. In this case $\tau y = -y'' = zy$ has the following linearly independent solutions,

$$\phi(z,x,a) = z^{-1/2} \sin\big(z^{1/2}(x-a)\big), \quad \theta(z,x,a) = \cos\big(z^{1/2}(x-a)\big), \quad z \in \mathbb{C}. \tag{2.5.3}$$

Hence,

$$\begin{aligned}
\phi(z,b,a) &= \sum_{m=0}^{\infty} z^m \phi_m(b), \quad z \in \mathbb{C}, \quad \phi_k(b) = \frac{(-1)^k}{(2k+1)!}(b-a)^{2k+1}, \ k \in \mathbb{N}, \\
\theta(z,b,a) &= \sum_{m=0}^{\infty} z^m \theta_m(b), \quad z \in \mathbb{C}, \quad \theta_k(b) = \frac{(-1)^k}{(2k)!}(b-a)^{2k}, \ k \in \mathbb{N}, \\
\phi'(z,b,a) &= \sum_{m=0}^{\infty} z^m \phi'_m(b), \quad z \in \mathbb{C}, \quad \phi'_k(b) = -\frac{(-1)^k}{(k+1)!}(b-a)^{k+1}, \quad k \in \mathbb{N}, \\
\theta'(z,b,a) &= \sum_{m=0}^{\infty} z^m \theta'_m(b), \quad z \in \mathbb{C}, \quad \theta'_k(b) = \frac{(-1)^k}{k!}(b-a)^{k}, \quad k \in \mathbb{N}.
\end{aligned} \tag{2.5.4}$$

One can explicitly write the corresponding expressions for $F_{\alpha,\beta}(z)$ and $F_{\varphi,R}(z)$ for this example to find for $\alpha, \beta \in [0, \pi)$,

$$\begin{aligned}
F_{\alpha,\beta}(z) &= \cos(\alpha)\big[- \sin(\beta) \ \cos\big(z^{1/2}(b-a)\big) + \cos(\beta) z^{-1/2} \sin\big(z^{1/2}(b-a)\big)\big] \\
&\quad - \sin(\alpha)\big[\sin(\beta) \ z^{1/2} \sin\big(z^{1/2}(b-a)\big) + \cos(\beta) \ \cos\big(z^{1/2}(b-a)\big)\big],
\end{aligned} \tag{2.5.5}$$

and for $\varphi \in [0, \pi)$, $R \in SL(2, \mathbb{R})$,

$$\begin{aligned}
F_{\varphi,R}(z) &= e^{i\varphi}\big[- R_{12} z^{1/2} \sin\big(z^{1/2}(b-a)\big) - R_{22} \cos\big(z^{1/2}(b-a)\big) \\
&\quad + R_{21} z^{-1/2} \sin\big(z^{1/2}(b-a)\big) - R_{11} \cos\big(z^{1/2}(b-a)\big)\big] + e^{2i\varphi} + 1.
\end{aligned} \tag{2.5.6}$$

We provide an explicit expression for $\zeta(1; T_{A,B})$ since it only involves the first few coefficients of the small-z expansion. In the case of separated boundary conditions one obtains

$$
\begin{aligned}
a_0 &= \cos(\alpha)((b-a)\cos(\beta) - \sin(\beta)) - \sin(\alpha)\cos(\beta),\\
a_1 &= \cos(\alpha)\left(\frac{1}{2}(b-a)^2\sin(\beta) - \frac{1}{6}(b-a)^3\cos(\beta)\right)\\
&\quad + \sin(\alpha)\left(\frac{1}{2}(b-a)^2\cos(\beta) - (b-a)\sin(\beta)\right),\\
a_2 &= \sin(\alpha)\left(\frac{1}{6}(b-a)^3\sin(\beta) - \frac{1}{24}(b-a)^4\cos(\beta)\right)\\
&\quad + \cos(\alpha)\left(\frac{1}{120}(b-a)^5\cos(\beta) - \frac{1}{24}(b-a)^4\sin(\beta)\right).
\end{aligned} \tag{2.5.7}
$$

If $T_{\alpha,\beta}$ does not have a zero eigenvalue, then $a_0 \neq 0$ and, hence, one finds from (2.4.4),

$$
\begin{aligned}
&\operatorname{tr}_{L^2_r((0,b))}\big(T^{-1}_{\alpha,\beta}\big) = \zeta(1;T_{\alpha,\beta}) = \\
&\frac{\cos(\alpha)\left(3(b-a)^2\sin(\beta) - (b-a)^3\cos(\beta)\right) + \sin(\alpha)\left(3(b-a)^2\cos(\beta) - 6(b-a)\sin(\beta)\right)}{6\sin(\alpha)\cos(\beta) - 6\cos(\alpha)((b-a)\cos(\beta) - \sin(\beta))}.
\end{aligned} \tag{2.5.8}
$$

If, instead, $T_{\alpha,\beta}$ has a zero eigenvalue then $a_0 = 0$ and one finds

$$
\begin{aligned}
&\zeta(1;T_{\alpha,\beta}) = \\
&\frac{-\sin(\alpha)\left(20(b-a)^3\sin(\beta) - 5(b-a)^4\cos(\beta)\right) - \cos(\alpha)\left((b-a)^5\cos(\beta) - 5(b-a)^4\sin(\beta)\right)}{\cos(\alpha)\left(60(b-a)^2\sin(\beta) - 20(b-a)^3\cos(\beta)\right) + \sin(\alpha)\left(60(b-a)^2\cos(\beta) - 120(b-a)\sin(\beta)\right)}.
\end{aligned} \tag{2.5.9}
$$

In the case of coupled boundary conditions one finds

$$
\begin{aligned}
a_0 &= e^{i\varphi}((b-a)R_{21} - R_{11} - R_{22}) + e^{2i\varphi} + 1,\\
a_1 &= e^{i\varphi}\left(-\frac{1}{6}(b-a)^3R_{21} + \frac{1}{2}(b-a)^2R_{11} + \frac{1}{2}(b-a)^2R_{22} + (a-b)R_{12}\right),\\
a_2 &= e^{i\varphi}\left(\frac{1}{120}(b-a)^5R_{21} - \frac{1}{24}(b-a)^4R_{11} - \frac{1}{24}(b-a)^4R_{22} + \frac{1}{6}(b-a)^3R_{12}\right).
\end{aligned} \tag{2.5.10}
$$

Once again, if zero is not an eigenvalue of $T_{\varphi,R}$, $a_0 \neq 0$ and one finds

$$
\begin{aligned}
&\operatorname{tr}_{L^2_r((0,b))}\big(T^{-1}_{\varphi,R}\big) = \zeta(1;T_{\varphi,R})\\
&\quad = \frac{e^{i\varphi}\left(R_{21}(b-a)^3 - 3(b-a)^2R_{11} - 3(b-a)^2R_{22} + 6(b-a)R_{12}\right)}{6e^{i\varphi}((b-a)R_{21} - R_{11} - R_{22}) + 6e^{2i\varphi} + 6}.
\end{aligned} \tag{2.5.11}
$$

If, on the other hand, zero is an eigenvalue of $T_{\varphi,R}$ with multiplicity one, then $a_0 = 0$ and

$$\zeta(1; T_{\varphi,R}) = \frac{(b-a)^5 R_{21} - 5(b-a)^4 R_{11} - 5(b-a)^4 R_{22} + 20(b-a)^3 R_{12}}{20(b-a)^3 R_{21} - 60(b-a)^2 R_{11} - 60(b-a)^2 R_{22} + 120(b-a) R_{12}}. \tag{2.5.12}$$

If zero is an eigenvalue of $T_{\varphi,R}$ with multiplicity two, we refer to the Krein–von Neumann extension, see Example 2.5.5.

Finally we give the form of the zeta regularized functional determinant for this example. As $z \downarrow 0$, one obtains

$$F_{\alpha,\beta}(z) = (b-a)\cos(\alpha)\cos(\beta) - \sin(\alpha+\beta) + O(z), \tag{2.5.13}$$

which implies that for particular values of α and β one finds a zero eigenvalue. For now we will assume that no zero eigenvalue is present and hence we consider the following set of parameters

$$\mathcal{A} = \{(\alpha,\beta) \in (0,\pi) \times (0,\pi) \,|\, (b-a)\cos(\alpha)\cos(\beta) - \sin(\alpha+\beta) \neq 0\}. \tag{2.5.14}$$

For $(\alpha,\beta) \in \mathcal{A}$ one infers, by construction, that $m_0 = 0$ and hence, $\sin(\alpha)\sin(\beta) \neq 0$. The latter condition implies that in (2.3.92) one must set $k_0 = -2$. By using (2.5.13), one obtains

$$\begin{aligned} \zeta'(0; T_{\alpha,\beta}) &= -\ln\left(\left|\frac{2\mathcal{F}_{\alpha,\beta}(0)}{\sin(\alpha)\sin(\beta)}\right|\right) \\ &= -\ln\left(\left|\frac{2(b-a)\cos(\alpha)\cos(\beta) - 2\sin(\alpha+\beta)}{\sin(\alpha)\sin(\beta)}\right|\right), \end{aligned} \tag{2.5.15}$$

which coincides with [74, Eq. (3.72)].

Furthermore, as $z \downarrow 0$, one obtains

$$F_{\varphi,R}(z) = e^{i\varphi}[(b-a)R_{21} - R_{11} - R_{22}] + e^{2i\varphi} + 1 + O(z), \tag{2.5.16}$$

which implies that for particular choices of φ and R one finds a zero eigenvalue. For now we will assume that no zero eigenvalue is present and hence we consider the following set of parameters

$$\mathcal{B} = \{\varphi \in (0,\pi), R \in SL(2,\mathbb{R}) \,|\, e^{i\varphi}[(b-a)R_{21} - R_{11} - R_{22}] + e^{2i\varphi} + 1 \neq 0\}. \tag{2.5.17}$$

For $(\varphi, R) \in \mathcal{B}$ we have, by construction, that $m_0 = 0$. Making the additional assumption $R_{12} \neq 0$ implies that in (2.3.92) one must set $k_0 = -2$. By using (2.5.16), one obtains

$$\begin{aligned}\zeta'(0; T_{\varphi,\widetilde{R}}) &= -\ln\left(\left|2\mathcal{F}_{\varphi,\widetilde{R}}(0)/R_{12}\right|\right) \\ &= -\ln\left(\left|\frac{2[(b-a)R_{21} - R_{11} - R_{22}] + 4\cos(\varphi)}{R_{12}}\right|\right).\end{aligned} \tag{2.5.18}$$

If $R_{12} = 0$, then since $R \in SL(2,\mathbb{R})$, by assumption $R_{11} \neq -R_{22}$ which implies that in (2.3.92) one must set $k_0 = -1$. By once again using (2.5.16), one obtains

$$\begin{aligned}\zeta'(0; T_{\varphi,\widetilde{R}}) &= -\ln\left(\left|\frac{2\mathcal{F}_{\varphi,\widetilde{R}}(0)}{R_{11} + R_{22}}\right|\right) \\ &= -\ln\left(\left|\frac{2[(b-a)R_{21} - R_{11} - R_{22}] + 4\cos(\varphi)}{R_{11} + R_{22}}\right|\right).\end{aligned} \tag{2.5.19}$$

The following examples, each with different boundary conditions, will illustrate how the main theorems and corollaries of the previous section can be used to effectively compute the spectral ζ-function values of the operator, $T_{A,B}$, for $n \in \mathbb{N}$.

Example 2.5.1 (Dirichlet boundary conditions). *Consider the case $\alpha = \beta = 0$. Then the operator $T_{0,0}$ has eigenvalues and eigenfunctions given by*

$$\lambda_k = k^2\pi^2\big/(b-a)^2, \quad y_k(x) = \lambda_k^{-1/2}\sin\left(\lambda_k^{1/2}(x-a)\right), \quad k \in \mathbb{N} \tag{2.5.20}$$

(*in particular, $z = 0$ is not an eigenvalue of $T_{0,0}$*), *and*

$$F_{0,0}(z) = z^{-1/2}\sin\left(z^{1/2}(b-a)\right), \quad z \in \mathbb{C}. \tag{2.5.21}$$

Applying Corollary 2.4.3 *with* $m_0 = 0$ *one finds for* $n = 1, 2, 3, 4$,

$$\begin{aligned}
\zeta(1; T_{0,0}) &= (b-a)^2 \pi^{-2} \sum_{k=1}^{\infty} k^{-2} = \operatorname{tr}_{L^2_r((a,b))}\big(T_{0,0}^{-1}\big) = (b-a)^2/6, \\
\zeta(2; T_{0,0}) &= (b-a)^4/90, \\
\zeta(3; T_{0,0}) &= (b-a)^6/945, \\
\zeta(4; T_{0,0}) &= (b-a)^8/9450.
\end{aligned} \tag{2.5.22}$$

Next, we explicitly compute the zeta regularized functional determinant with Dirichlet boundary conditions. Since no zero eigenvalue is present and $\Gamma_0 = -(b-a)$, *one obtains*

$$\zeta'(0; T_{0,0}) = -\ln[2F_{0,0}(0)] = -\ln[2(b-a)]. \tag{2.5.23}$$

One can corroborate the values found in Example 2.5.1 by utilizing the following relation of $\zeta(s; T_{0,0})$ with the Riemann ζ-function (see, e.g., [13], [47] for some background)

$$\zeta(s; T_{0,0}) = (b-a)^{2s} \pi^{-2s} \zeta(2s), \quad \operatorname{Re}(s) > 1/2. \tag{2.5.24}$$

By using [87, 0.2333], the last expression allows us to find for $s = n \in \mathbb{N}$,

$$\zeta(n; T_{0,0}) = 2^{2n-1}(b-a)^{2n} |B_{2n}|/[(2n)!], \tag{2.5.25}$$

where B_{2n} is the $2n$th Bernoulli number (cf. [1, Ch. 23]).

Example 2.5.2 (Neumann boundary conditions). *Consider the case* $\alpha = \beta = \pi/2$. *Then the operator* $T_{\pi/2,\pi/2}$ *has eigenvalues and eigenfunctions given by*

$$\lambda_k = k^2\pi^2/(b-a)^2, \quad y_k(x) = \cos\big(\lambda_k^{1/2}(x-a)\big), \quad k \in \mathbb{N}_0 \tag{2.5.26}$$

(*in particular,* $z = 0$ *is a simple eigenvalue of* $T_{\pi/2,\pi/2}$) *and*

$$F_{\pi/2,\pi/2}(z) = -z^{1/2} \sin\big(z^{1/2}(b-a)\big), \quad z \in \mathbb{C}. \tag{2.5.27}$$

Applying Corollary 2.4.6 *with* $m_0 = 1$ *one finds for* $n = 1, 2, 3, 4$,

$$\begin{aligned}
\zeta(1; T_{\pi/2,\pi/2}) &= (b-a)^2\pi^{-2}\sum_{k=1}^{\infty} k^{-2} = (b-a)^2/6, \\
\zeta(2; T_{\pi/2,\pi/2}) &= (b-a)^4/90, \\
\zeta(3; T_{\pi/2,\pi/2}) &= (b-a)^6/945, \\
\zeta(4; T_{\pi/2,\pi/2}) &= (b-a)^8/9450.
\end{aligned} \tag{2.5.28}$$

Noting that the series expression for $\zeta(s; T_{\pi/2,\pi/2})$ in (2.2.38) sums only over non-zero eigenvalues, and that the eigenvalues for Dirichlet and Neumann boundary conditions only differ by zero being an eigenvalue for the latter, but not the former, the same expressions apply as in Example 2.5.1, which is reflected in equations (2.5.22) and (2.5.28) yielding the same values.

Example 2.5.3 (Periodic boundary conditions). *Consider the case* $\varphi = 0$, $R = I_2$. *Then the operator* T_{0,I_2} *has eigenvalues given by*

$$\lambda_k = (2k)^2\pi^2/(b-a)^2, \quad k \in \mathbb{N}_0. \tag{2.5.29}$$

In particular, $z = 0$ *is a simple eigenvalue of* T_{0,I_2} *and all other eigenvalues of* T_{0,I_2} *are of multiplicity 2, and*

$$F_{0,I_2}(z) = -2\cos\left(z^{1/2}(b-a)\right) + 2, \quad z \in \mathbb{C}. \tag{2.5.30}$$

Applying Corollary 2.4.8 *with* $m_0 = 1$ *one finds for* $n = 1, 2, 3, 4$,

$$\begin{aligned}
\zeta(1; T_{0,I_2}) &= 2(b-a)^2\pi^{-2}\sum_{k=1}^{\infty}(2k)^{-2} = (b-a)^2/12, \\
\zeta(2; T_{0,I_2}) &= (b-a)^4/720, \\
\zeta(3; T_{0,I_2}) &= (b-a)^6/30240, \\
\zeta(4; T_{0,I_2}) &= (b-a)^8/1209600.
\end{aligned} \tag{2.5.31}$$

Here, once again, one can verify the values found in Example 2.5.3 by utilizing the following relation of $\zeta(s; T_{0,I_2})$ with the Riemann ζ-function,

$$\zeta(s; T_{0,I_2}) = 2^{1-2s}\pi^{-2s}(b-a)^{2s}\zeta(2s), \quad \mathrm{Re}(s) > 1/2. \tag{2.5.32}$$

By using [87, 0.2333], the last expression allows one to find for $s = n \in \mathbb{N}$,

$$\zeta(n; T_{0,I_2}) = (b-a)^{2n}|B_{2n}|/[(2n)!]. \tag{2.5.33}$$

Example 2.5.4 (Antiperiodic boundary conditions). *Consider the case* $\varphi = 0$, $R = -I_2$. *Then the operator* $T_{0,-I_2}$ *has eigenvalues given by*

$$\lambda_k = (2k-1)^2\pi^2/(b-a)^2, \quad k \in \mathbb{N}. \tag{2.5.34}$$

In particular, $z = 0$ *is not an eigenvalue of* $T_{0,-I_2}$ *and all eigenvalues of* $T_{0,-I_2}$ *are of multiplicity 2, and*

$$F_{0,-I_2}(z) = 2\cos\big(z^{1/2}(b-a)\big) + 2, \quad z \in \mathbb{C}. \tag{2.5.35}$$

Applying Corollary 2.4.9 *with* $m_0 = 0$ *one finds for* $n = 1, 2, 3, 4$,

$$\begin{aligned}
&\zeta(1; T_{0,-I_2}) = 2(b-a)^2\pi^{-2}\sum_{k=1}^{\infty}(2k-1)^{-2} = \operatorname{tr}_{L^2_r((a,b))}\big(T_{0,-I_2}^{-1}\big) = (b-a)^2/4, \\
&\zeta(2; T_{0,-I_2}) = (b-a)^4/48, \\
&\zeta(3; T_{0,-I_2}) = (b-a)^6/480, \\
&\zeta(4; T_{0,-I_2}) = [17/80640](b-a)^8.
\end{aligned} \tag{2.5.36}$$

One can verify the values found in Example 2.5.4 by utilizing the following relation,

$$\zeta(s; T_{0,-I_2}) = 2(b-a)^{2s}\pi^{-2s}\sum_{k\in\mathbb{N}}(2k-1)^{-2s} = \big(1 - 2^{-2s}\big)2(b-a)^{2s}\pi^{-2s}\zeta(2s),$$
$$\operatorname{Re}(s) > 1/2, \tag{2.5.37}$$

which in turn by using either [87, 0.2335] on the first equality or [87, 0.2333] on the second allows one to find for $s = n \in \mathbb{N}$,

$$\zeta(n; T_{0,-I_2}) = (2^{2n}-1)(b-a)^{2n}|B_{2n}|/[(2n)!]. \tag{2.5.38}$$

Example 2.5.5 (Krein–von Neumann boundary conditions). *Consider the case* $\varphi = 0$, $R = R_K$, *with*

$$R_K = \begin{pmatrix} \theta(0,b,a) & \phi(0,b,a) \\ \theta^{[1]}(0,b,a) & \phi^{[1]}(0,b,a) \end{pmatrix} = \begin{pmatrix} 1 & b-a \\ 0 & 1 \end{pmatrix}. \tag{2.5.39}$$

As shown in [34, Example 3.3], *the resulting operator* T_{0,R_K} *represents the Krein–von Neumann extension of* T_{min}. *For more on the Krein–von Neumann extension, including an extensive discussion of eigenvalues and eigenfunctions, see* [3] *or* [7]. *From* (2.2.17) *with* $\varphi = 0$, $R = R_K$ *defined as in* (2.5.39),

$$F_{0,R_K}(z) = (a-b)z^{1/2}\sin\big(z^{1/2}(b-a)\big) - 2\cos\big(z^{1/2}(b-a)\big) + 2, \quad z \in \mathbb{C}. \tag{2.5.40}$$

Using the series expansions in (2.5.40), *one finds*

$$F_{0,R_K}(z) \underset{z\downarrow 0}{=} \big[(b-a)^4/12\big]z^2 + O\big(z^3\big), \tag{2.5.41}$$

so that $z = 0$ *is a zero of multiplicity two of* $F_{0,R_K}(z)$ *and hence an eigenvalue of multiplicity two of* T_{0,R_K} (*coinciding with what was found in* [7] *and noted in* [74, Example 3.7]). *Applying Corollary* 2.4.10 *with* $m_0 = 2$ *gives*

$$\begin{aligned} \zeta(1;T_{0,R_K}) &= (b-a)^2/15, \\ \zeta(2;T_{0,R_K}) &= [11/12600](b-a)^4, \\ \zeta(3;T_{0,R_K}) &= (b-a)^6/54000, \\ \zeta(4;T_{0,R_K}) &= [457/317520000](b-a)^8. \end{aligned} \tag{2.5.42}$$

2.5.2 Examples of Nonnegative (Piecewise) Constant Potentials

Next we provide examples for calculating spectral ζ-function values considering a positive (piecewise) constant potential q, imposing Dirichlet boundary conditions.

Example 2.5.6. *Let* $V_0 \in (0,\infty)$, *consider* $q(x) = V_0$, $x \in (a,b)$, *and denote by* $T_{0,0}$ *the associated Schrödinger operator with Dirichlet boundary conditions at* a *and* b

(*i.e.*, $\alpha = \beta = 0$). *Then,*

$$\begin{aligned}
&\phi(z,x,a) = (z - V_0)^{-1/2} \sin\big((z-V_0)^{1/2}(x-a)\big), \\
&\theta(z,x,a) = \cos\big((z-V_0)^{1/2}(x-a)\big), \quad x \in (a,b),\ z \in \mathbb{C}.
\end{aligned} \tag{2.5.43}$$

Furthermore, the eigenvalues and eigenfunctions for $T_{0,0}$ *with* $q(x) = V_0 > 0,\ x \in (a,b)$, *are given by*

$$\begin{aligned}
&\lambda_k = k^2\pi^2/(b-a)^{-2} + V_0, \\
&y_k(x) = (\lambda_k - V_0)^{-1/2} \sin\big((\lambda_k - V_0)^{1/2}(x-a)\big), \quad k \in \mathbb{N}
\end{aligned} \tag{2.5.44}$$

(*in particular,* $z = 0$ *is not an eigenvalue of* $T_{0,0}$), *and*

$$F_{0,0}(z) = (z-V_0)^{-1/2} \sin\big((z-V_0)^{1/2}(b-a)\big), \quad z \in \mathbb{C}. \tag{2.5.45}$$

Applying Corollary 2.4.3 *with* $m_0 = 0$ *one finds for* $n = 1,2,3$ (*the expression for* $n = 4$ *is significantly longer and hence is omitted here*),

$$\begin{aligned}
\zeta(1;T_{0,0}) &= \sum_{k=1}^{\infty} \bigg[\frac{k^2\pi^2}{(b-a)^2} + V_0\bigg]^{-1} = \operatorname{tr}_{L_r^2((a,b))}\big(T_{0,0}^{-1}\big) \\
&= \big[V_0^{1/2}(b-a)\coth\big(V_0^{1/2}(b-a)\big) - 1\big]/(2V_0), \\
\zeta(2;T_{0,0}) &= \frac{V_0^{1/2}(b-a)\sinh\big(2V_0^{1/2}(b-a)\big) - 2\cosh\big(2V_0^{1/2}(b-a)\big) + 2V_0(b-a)^2 + 2}{8V_0^2\sinh^2\big(V_0^{1/2}(b-a)\big)}, \\
\zeta(3;T_{0,0}) &= \big(64V_0^3\sinh^2\big(V_0^{1/2}(b-a)\big)\big)^{-1}\big[12V_0(b-a)^2 - 16\cosh\big(2V_0^{1/2}(b-a)\big) \\
&\quad + 16 + V_0^{1/2}(b-a)\big(8a^2V_0 - 16abV_0 + 8b^2V_0 - 3\big)\coth\big(V_0^{1/2}(b-a)\big) \\
&\quad - 3aV_0^{1/2}\cosh\big(3V_0^{1/2}(b-a)\big)\big(\sinh\big(V_0^{1/2}(b-a)\big)\big)^{-1} \\
&\quad + 3bV_0^{1/2}\cosh\big(3V_0^{1/2}(b-a)\big)\big(\sinh\big(V_0^{1/2}(b-a)\big)\big)^{-1}\big].
\end{aligned} \tag{2.5.46}$$

Taking the limit $V_0 \downarrow 0$ of (2.5.46) recovers the expressions in Example 2.5.1.

Remark 2.5.7. One can also verify the expressions found in Example 2.5.6 by means of the one-dimensional Epstein ζ-function given by

$$\zeta_E(s;m^2) = \sum_{k=-\infty}^{\infty} \big(k^2 + m^2\big)^{-s}, \quad m^2 \neq 0,\ s > 1/2 \tag{2.5.47}$$

(see, e.g., the classical sources [56], [57], [113], and [53, Sect. 1.1.3], [55, Sects. 1.2.2, 5.3.2], [114], [115, Ch. 3, App. A], and the extensive list of references therein). Now one finds that $\zeta(s; T_{0,0})$ in Example 2.5.6 can be written in the form

$$\begin{aligned}\zeta(s; T_{0,0}) &= \sum_{k=1}^{\infty} \left[\frac{k^2\pi^2}{(b-a)^2} + V_0\right]^{-s} = (b-a)^{2s}\pi^{-2s}\sum_{k=1}^{\infty}\left[k^2+m^2\right]^{-s} \\ &= 2^{-1}(b-a)^{2s}\pi^{-2s}\big[\zeta_E(s;m^2) - m^{-2s}\big], \quad s > 1/2,\end{aligned} \tag{2.5.48}$$

where

$$m^2 = (b-a)^2 V_0 \pi^{-2} > 0. \tag{2.5.49}$$

Then the following formula for the analytic continuation of $\zeta_E(s; m^2)$ in s for $m \neq 0, -1, -2, \dots$ (see [53, Sect. 4.1.1])

$$\begin{aligned}\zeta_E(s; m^2) = \pi^{1/2}\frac{\Gamma(s-\frac{1}{2})}{\Gamma(s)}m^{1-2s} + \frac{4\pi^s}{\Gamma(s)}m^{1/2-s}\sum_{n=1}^{\infty} n^{s-1/2}K_{s-1/2}(2\pi m n), \\ s \neq (1/2) - \ell,\ \ell \in \mathbb{N}_0,\ s \in \mathbb{C},\end{aligned} \tag{2.5.50}$$

where $K_\mu(\,\cdot\,)$ is the modified Bessel function of the second kind (see for example [1, Chs. 9-10]), can be used to explicitly verify the expressions found in Example 2.5.6.

We verify the expressions for $\zeta(1; T_{0,0})$ and $\zeta(2; T_{0,0})$ next. From (2.5.50) one has, using the fact that $K_{1/2}(z) = \pi^{1/2}(2z)^{-1/2}e^{-z}$,

$$\begin{aligned}\zeta_E(1; m^2) &= \pi m^{-1} + 4\pi m^{-1/2}\sum_{n=1}^{\infty} n^{1/2}\pi^{1/2}(4\pi m n)^{-1/2}e^{-2\pi m n} \\ &= \pi m^{-1} + 2\pi m^{-1}\sum_{n=1}^{\infty} e^{-2\pi m n} = \pi m^{-1} + 2\pi m^{-1}\frac{1}{e^{2\pi m} - 1} \\ &= \frac{\pi}{m}\coth(\pi m).\end{aligned} \tag{2.5.51}$$

Thus, from (2.5.48) and (2.5.49) one obtains, in accordance with Example 2.5.6,

$$\begin{aligned}\zeta(1; T_{0,0}) &= \frac{(b-a)^2}{2\pi^2}\big(\zeta_E(1;m^2) - m^{-2}\big) = \frac{(b-a)^2}{2\pi^2}\left(\frac{\pi m\coth(\pi m) - 1}{m^2}\right) \\ &= \big[V_0^{1/2}(b-a)\coth\big(V_0^{1/2}(b-a)\big) - 1\big]\big/(2V_0).\end{aligned} \tag{2.5.52}$$

Next we verify the expression for $\zeta(2;T_{0,0})$ by first noting that

$$\frac{d}{dm}\big(\zeta_E(s;m^2)\big) = -2sm\zeta_E(s+1;m^2), \tag{2.5.53}$$

which implies the functional equation

$$\zeta_E(s+1;m^2) = -\frac{1}{2sm}\frac{d}{dm}\big(\zeta_E(s;m^2)\big). \tag{2.5.54}$$

From (2.5.51) and (2.5.54) with $s=1$ one has

$$\zeta_E(2;m^2) = -\frac{\pi}{2m}\frac{d}{dm}\left(\frac{\coth(\pi m)}{m}\right) = \frac{\pi\sinh(2\pi m)+2\pi^2 m}{4m^3\sinh^2(\pi m)}. \tag{2.5.55}$$

Thus from (2.5.48) and (2.5.49) one obtains

$$\begin{aligned}
\zeta(2;T_{0,0}) &= \frac{(b-a)^4}{2\pi^4}\big(\zeta_E(2;m^2)-m^{-4}\big)\\
&= \frac{(b-a)^4}{2\pi^4}\left(\frac{\pi\sinh(2\pi m)+2\pi^2 m}{4m^3\sinh^2(\pi m)}-\frac{1}{m^4}\right)\\
&= \frac{V_0^{1/2}(b-a)\sinh\big(2V_0^{1/2}(b-a)\big)-2\cosh\big(2V_0^{1/2}(b-a)\big)+2V_0(b-a)^2+2}{8V_0^2\sinh^2\big(V_0^{1/2}(b-a)\big)},
\end{aligned} \tag{2.5.56}$$

again in accordance with Example 2.5.6. All other positive integer values can be found recursively by means of (2.5.51) and the functional equation (2.5.54). $\diamond$

Next, we turn to the case of a nonnegative piecewise constant potential (a potential well):

Example 2.5.8. *Let $c,d\in(a,b)$, $c<d$, $V_0\in(0,\infty)$, consider*

$$q(x) = \begin{cases} 0 & x\in(a,c),\\ V_0 & x\in(c,d),\\ 0 & x\in(d,b), \end{cases} \tag{2.5.57}$$

and denote by $T_{0,0}$ the associated Schrödinger operator with Dirichlet boundary conditions at a and b. Then, for $z\in\mathbb{C}$,

$$\phi(z,x,a) = z^{-1/2}\sin\big(z^{1/2}(x-a)\big), \quad x\in(a,c),$$

$$\theta(z,x,a) = \cos\big(z^{1/2}(x-a)\big), \quad x\in(a,c),$$

$$\phi(z,x,a) = \cos\big(z^{1/2}(c-a)\big)(z-V_0)^{-1/2}\sin\big((z-V_0)^{1/2}(x-c)\big)$$

$$
\begin{aligned}
&\quad + z^{-1/2}\sin\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(x-c)\big), \quad x\in(c,d),\\
\theta(z,x,a) &= -z^{1/2}\sin\big(z^{1/2}(c-a)\big)(z-V_0)^{-1/2}\sin\big((z-V_0)^{1/2}(x-c)\big)\\
&\quad + \cos\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(x-c)\big), \quad x\in(c,d),\\
\phi(z,x,a) &= \Big[\cos\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)\\
&\quad - (z-V_0)^{1/2}z^{-1/2}\sin\big(z^{1/2}(c-a)\big)\sin\big((z-V_0)^{1/2}(d-c)\big)\Big]\\
&\quad \times z^{-1/2}\sin\big(z^{1/2}(x-d)\big) \qquad (2.5.58)\\
&\quad + \Big[\cos\big(z^{1/2}(c-a)\big)(z-V_0)^{-1/2}\sin\big((z-V_0)^{1/2}(d-c)\big)\\
&\quad + z^{-1/2}\sin\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)\Big]\cos\big(z^{1/2}(x-d)\big),\\
&\qquad x\in(d,b),\\
\theta(z,x,a) &= -\Big[z^{1/2}\sin\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)\\
&\quad + (z-V_0)^{1/2}\cos\big(z^{1/2}(c-a)\big)\sin\big((z-V_0)^{1/2}(d-c)\big)\Big]\\
&\quad \times z^{-1/2}\sin\big(z^{1/2}(x-d)\big)\\
&\quad + \Big[-z^{1/2}\sin\big(z^{1/2}(c-a)\big)(z-V_0)^{-1/2}\sin\big((z-V_0)^{1/2}(d-c)\big)\\
&\quad + \cos\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)\Big]\cos\big(z^{1/2}(x-d)\big),\\
&\qquad x\in(d,b).
\end{aligned}
$$

In particular,

$$
\phi(z,b,a) = \sum_{m=0}^{\infty} z^m \phi_m(b), \quad z\in\mathbb{C}, \qquad (2.5.59)
$$

where

$$
\begin{aligned}
\phi_0(b) &= \Big[\cosh\big(V_0^{1/2}(d-c)\big) + V_0^{1/2}(c-a)\sinh\big(V_0^{1/2}(d-c)\big)\Big](b-d)\\
&\quad + V_0^{-1/2}\sinh\big(V_0^{1/2}(d-c)\big) + (c-a)\cosh\big(V_0^{1/2}(d-c)\big),\\
\phi_1(b) &= \big(6V_0^{3/2}\big)^{-1}\big\{3\big[\big(aV_0(c-d) - c^2V_0 + cdV_0 - 1\big)\sinh\big(V_0^{1/2}(c-d)\big) \qquad (2.5.60)\\
&\quad + V_0^{1/2}(c-d)\cosh\big(V_0^{1/2}(c-d)\big)\big] + V_0\big[\sinh\big(V_0^{1/2}(d-c)\big)\big(aV_0(b-d)
\end{aligned}
$$

$$- bcV_0 + cdV_0 - 3) + V_0^{1/2}(3a - b - 3c + d)\cosh\big(V_0^{1/2}(d-c)\big)\big]$$

$$\times (b-d)^2\big[V_0^{1/2}\sinh\big(2V_0^{1/2}(d-c)\big) + \cosh\big(2V_0^{1/2}(d-c)\big)\big]$$

$$+ V_0^{3/2}(a-c)^3\big\},$$

etc.

By construction, $\phi(z,a,a) = 0$*, so eigenvalues are given by solving* $\phi(z,b,a) = 0$*, or, equivalently, by solving*

$$\tan\big(z^{1/2}(b-d)\big) \tag{2.5.61}$$
$$= \frac{-z\cos\big(z^{1/2}(c-a)\big)\sin\big((z-V_0)^{1/2}(d-c)\big) - \sqrt{z(z-V_0)}\sin\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)}{\sqrt{z(z-V_0)}\cos\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big) - (z-V_0)\sin\big(z^{1/2}(c-a)\big)\sin\big((z-V_0)^{1/2}(d-c)\big)}.$$

From (2.2.16)*, one has*

$$\begin{aligned} F_{0,0}(z) = \bigg[&\cos\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big) \\ &- (z-V_0)^{1/2}\frac{\sin\big(z^{1/2}(c-a)\big)}{z^{1/2}}\sin\big((z-V_0)^{1/2}(d-c)\big)\bigg]\frac{\sin\big(z^{1/2}(b-d)\big)}{z^{1/2}} \\ &+ \bigg[\cos\big(z^{1/2}(c-a)\big)(z-V_0)^{-1/2}\sin\big((z-V_0)^{1/2}(d-c)\big) \\ &\quad + z^{-1/2}\sin\big(z^{1/2}(c-a)\big)\cos\big((z-V_0)^{1/2}(d-c)\big)\bigg]\cos\big(z^{1/2}(b-d)\big), \\ &\qquad z \in \mathbb{C}. \end{aligned} \tag{2.5.62}$$

Hence, applying Corollary 2.4.3 *with* $m_0 = 0$ *one explicitly finds the sum of the inverse of these eigenvalues, namely*

$$\zeta(1; T_{0,0}) = \operatorname{tr}_{L_r^2((a,b))}\big(T_{0,0}^{-1}\big) = -\phi_1(b)/\phi_0(b) \tag{2.5.63}$$
$$= -\big\{6V_0\big[(V_0(c-a)(b-d)+1)\sinh\big(V_0^{1/2}(d-c)\big) - V_0^{1/2}(a-b-c+d)\cosh\big(V_0^{1/2}(d-c)\big)\big]\big\}^{-1}$$
$$\times\big\{3\big[\big(aV_0(c-d) - c^2V_0 + cdV_0 - 1\big)\sinh\big(V_0^{1/2}(c-d)\big) + V_0^{1/2}(c-d)\cosh\big(V_0^{1/2}(c-d)\big)\big]$$
$$+ V_0\big[\sinh\big(V_0^{1/2}(d-c)\big)(aV_0(b-d) - bcV_0 + cdV_0 - 3) + V_0^{1/2}(3a-b-3c+d)\cosh\big(V_0^{1/2}(d-c)\big)\big]$$
$$\times(b-d)^2\big[V_0^{1/2}\sinh\big(2V_0^{1/2}(d-c)\big) + \cosh\big(2V_0^{1/2}(d-c)\big)\big] + V_0^{3/2}(a-c)^3\big\}.$$

Taking the limits $c \downarrow a$ and $d \uparrow b$ of (2.5.63) recovers the expression in Example 2.5.6. Furthermore, taking the limit $V_0 \downarrow 0$ recovers the same expression as in Example 2.5.1. The expression for $n = 2$ is significantly longer and hence it is omitted here.

2.5.3 Example of a Negative Constant Potential

Next, we derive spectral ζ-function values for the case of a negative constant potential. This case is dealt with separately since the question as to whether $z = 0$ is an eigenvalue of $T_{0,0}$ depends on the actual constant value of the potential.

Example 2.5.9. *Let $V_0 \in (0, \infty)$, consider $q(x) = -V_0$, $x \in (a, b)$, and denote by $T_{0,0}$ the associated Schrödinger operator with Dirichlet boundary conditions at a and b. Then,*

$$\begin{aligned} \phi(z, x, a) &= (z + V_0)^{-1/2} \sin\big((z + V_0)^{1/2}(x - a)\big), \\ \theta(z, x, a) &= \cos\big((z + V_0)^{1/2}(x - a)\big), \quad z \in \mathbb{C}. \end{aligned} \tag{2.5.64}$$

Furthermore, eigenvalues and eigenfunctions for $T_{0,0}$ with $q(x) = -V_0 < 0$, $x \in (a, b)$, are given by

$$\lambda_k = \frac{k^2\pi^2}{(b - a)^2} - V_0, \quad y_k(x) = (\lambda_k + V_0)^{-1/2} \sin\big((\lambda_k + V_0)^{1/2}(x - a)\big), \quad k \in \mathbb{N}, \tag{2.5.65}$$

where one notes that due to $q(x) = -V_0 < 0$, $z = 0$ is an eigenvalue of $T_{0,0}$ for certain values of V_0. Specifically, if one has

$$V_0 = k^2\pi^2/(b - a)^2, \text{ for some } k \in \mathbb{N}, \tag{2.5.66}$$

then $z = 0$ is a simple eigenvalue of $T_{0,0}$. Otherwise, $z = 0$ is not an eigenvalue of $T_{0,0}$. Moreover,

$$F_{0,0}(z) = (z + V_0)^{-1/2} \sin\big((z + V_0)^{1/2}(b - a)\big), \quad z \in \mathbb{C}. \tag{2.5.67}$$

Applying Corollary 2.4.3 with $m_0 = 0$ when $V_0 \neq k^2\pi^2/(b-a)^2$, $k \in \mathbb{N}$, one finds for $n = 1, 2, 3$ (the expression for $n = 4$ is significantly longer and hence is omitted),

$$\zeta(1; T_{0,0}) = \sum_{k=1}^{\infty} \left[\frac{k^2\pi^2}{(b-a)^2} - V_0\right]^{-1} = \operatorname{tr}_{L_r^2((a,b))}\big(T_{0,0}^{-1}\big)$$
$$= \big[V_0^{1/2}(a-b)\cot\big(V_0^{1/2}(b-a)\big) + 1\big]/(2V_0),$$
$$\zeta(2; T_{0,0}) = \frac{V_0^{1/2}(b-a)\sin\big(2V_0^{1/2}(b-a)\big) + 2\cos\big(2V_0^{1/2}(b-a)\big) + 2V_0(b-a)^2 - 2}{8V_0^2\sin^2\big(V_0^{1/2}(b-a)\big)},$$
$$\zeta(3; T_{0,0}) = \big(64V_0^3\sin^2\big(V_0^{1/2}(b-a)\big)\big)^{-1}\big[-12V_0(b-a)^2 - 16\cos\big(2V_0^{1/2}(b-a)\big)$$
$$+ 16 - V_0^{1/2}(b-a)\big(8a^2V_0 - 16abV_0 + 8b^2V_0 - 3\big)\cot\big(V_0^{1/2}(b-a)\big)$$
$$- 3aV_0^{1/2}\cos\big(3V_0^{1/2}(b-a)\big)\big(\sin\big(V_0^{1/2}(b-a)\big)\big)^{-1}$$
$$+ 3bV_0^{1/2}\cos\big(3V_0^{1/2}(b-a)\big)\big(\sin\big(V_0^{1/2}(b-a)\big)\big)^{-1}\big]. \tag{2.5.68}$$

When $V_0 = k_0^2\pi^2/(b-a)^2$ for some $k_0 \in \mathbb{N}$, applying Corollary 2.4.3 with $m_0 = 1$ one finds for $n = 1, 2$ (the expressions for $n = 3, 4$ are significantly longer and hence are omitted here),

$$\zeta(1; T_{0,0}) = \sum_{\substack{k=1 \\ k\neq k_0}}^{\infty} \left[\frac{k^2\pi^2}{(b-a)^2} - V_0\right]^{-1} = \frac{\pi^2}{(b-a)^2}\sum_{\substack{k=1 \\ k\neq k_0}}^{\infty}\big[k^2 - k_0^2\big]^{-1}$$
$$= \frac{\big(V_0(b-a)^2 - 3\big)\sin\big(V_0^{1/2}(a-b)\big) + 3V_0^{1/2}(a-b)\cos\big(V_0^{1/2}(a-b)\big)}{4V_0\big(\sin\big(V_0^{1/2}(b-a)\big) + V_0^{1/2}(a-b)\cos\big(V_0^{1/2}(b-a)\big)\big)},$$
$$\zeta(2; T_{0,0}) = \frac{1}{24V_0^2\big(\sin\big(V_0^{1/2}(b-a)\big) + V_0^{1/2}(a-b)\cos\big(V_0^{1/2}(b-a)\big)\big)}$$
$$\times \big\{2\big[3\big(5 - 2V_0(b-a)^2\big)\sin\big(V_0^{1/2}(a-b)\big)$$
$$- V_0^{1/2}(b-a)(V_0(b-a)^2 - 15)\cos\big(V_0^{1/2}(a-b)\big)\big]$$
$$+ 3\big(\sin\big(V_0^{1/2}(b-a)\big)\big)^{-1}\big[\big(V_0(b-a)^2 - 3\big)\sin\big(V_0^{1/2}(a-b)\big)$$
$$- 3V_0^{1/2}(b-a)\cos\big(V_0^{1/2}(a-b)\big)\big]$$
$$\times\big[\sin\big(V_0^{1/2}(b-a)\big) - V_0^{1/2}(b-a)\cos\big(V_0^{1/2}(b-a)\big)\big]\big\}. \tag{2.5.69}$$

Taking the limit $V_0 \downarrow 0$ of (2.5.68) recovers the expressions in Example 2.5.1.

Remark 2.5.10. In the case $z = 0$ is not an eigenvalue, one can verify these results via the method outlined in Remark 2.5.7. Namely, letting

$$m^2 = -(b-a)^2 V_0 \pi^{-2} < 0 \tag{2.5.70}$$

so that

$$m = (i/\pi)(b-a)V_0^{1/2} \tag{2.5.71}$$

in (2.5.52) and (2.5.56), one verifies the expressions for $n = 1, 2$ as before. ⋄

2.5.4 Example of a Linear Potential

We finish with an example for calculating spectral ζ-function values for the linear potential, $q(x) = x$, $x \in (a, b)$.

Example 2.5.11. *Consider $q(x) = x$, $x \in (a, b)$, and denote by $T_{0,0}$ the associated Schrödinger operator with Dirichlet boundary conditions at a and b. Then, noting that $W(\mathrm{Ai}, \mathrm{Bi})(x) = \pi^{-1}$ (cf. [1, Eq. 10.4.10]), one finds*

$$\phi(z, x, a) = \pi[\mathrm{Ai}(a - z)\,\mathrm{Bi}(x - z) - \mathrm{Bi}(a - z)\,\mathrm{Ai}(x - z)], \tag{2.5.72}$$

$$\theta(z, x, a) = -\pi[\mathrm{Ai}'(a - z)\,\mathrm{Bi}(x - z) - \mathrm{Bi}'(a - z)\,\mathrm{Ai}(x - z)], \quad z \in \mathbb{C}, \tag{2.5.73}$$

where $\mathrm{Ai}(\,\cdot\,)$ and $\mathrm{Bi}(\,\cdot\,)$ represent the Airy functions of the first and second kind, respectively (cf. [1, Sect. 10.4]). In particular, substituting $z = 0$ in (2.5.72) yields

$$\phi_0(x) = \pi[\mathrm{Ai}(a)\,\mathrm{Bi}(x) - \mathrm{Bi}(a)\,\mathrm{Ai}(x)], \quad \theta_0(x) = -\pi[\mathrm{Ai}'(a)\,\mathrm{Bi}(x) - \mathrm{Bi}'(a)\,\mathrm{Ai}(x)], \tag{2.5.74}$$

and thus the Volterra Green's function becomes

$$g(0, x, x') = \pi[\mathrm{Ai}(x)\,\mathrm{Bi}(x') - \mathrm{Ai}(x')\,\mathrm{Bi}(x)]. \tag{2.5.75}$$

Hence,

$$\phi(z, b, a) = \sum_{m=0}^{\infty} z^m \phi_m(b), \quad z \in \mathbb{C}, \tag{2.5.76}$$

where

$$\phi_0(b) = \pi[\mathrm{Ai}(a)\,\mathrm{Bi}(b) - \mathrm{Bi}(a)\,\mathrm{Ai}(b)],$$

$$\begin{aligned}\phi_1(b) &= \pi^2 \int_a^b dx_1\; [\mathrm{Ai}(b)\,\mathrm{Bi}(x_1) - \mathrm{Ai}(x_1)\,\mathrm{Bi}(b)][\mathrm{Ai}(a)\,\mathrm{Bi}(x_1) - \mathrm{Bi}(a)\,\mathrm{Ai}(x_1)] \\ &= \pi^2\big\{\,\mathrm{Ai}(a)\,\mathrm{Ai}(b)\big[\,\mathrm{Bi}'(a)^2 - \mathrm{Bi}'(b)^2\big] + \mathrm{Bi}(a)\,\mathrm{Bi}(b)\big[\,\mathrm{Ai}'(a)^2 - \mathrm{Ai}'(b)^2\big] \qquad (2.5.77) \\ &\quad + [\mathrm{Ai}'(b)\,\mathrm{Bi}'(b) - \mathrm{Ai}'(a)\,\mathrm{Bi}'(a)][\mathrm{Bi}(a)\,\mathrm{Ai}(b) + \mathrm{Ai}(a)\,\mathrm{Bi}(b)]\big\},\end{aligned}$$

etc.

Furthermore, one has by construction, $\phi(z,a,a) = 0$*, so eigenvalues are given by solving* $\phi(z,b,a) = 0$*, or, equivalently, by solving* $\mathrm{Ai}(a-z)\,\mathrm{Bi}(b-z) = \mathrm{Bi}(a-z)\,\mathrm{Ai}(b-z)$*. In particular, the characteristic function is given by*

$$F_{0,0}(z) = \pi[\mathrm{Ai}(a-z)\,\mathrm{Bi}(b-z) - \mathrm{Bi}(a-z)\,\mathrm{Ai}(b-z)], \quad z \in \mathbb{C}. \qquad (2.5.78)$$

If zero is not an eigenvalue, applying Corollary 2.4.3 *with* $m_0 = 0$ *one does find the sum of the inverse of these eigenvalues, namely*

$$\begin{aligned}\zeta(1;T_{0,0}) &= \mathrm{tr}_{L^2_r((a,b))}\left(T_{0,0}^{-1}\right) = -\phi_1(b)/\phi_0(b) \\ &= \pi[\mathrm{Bi}(a)\,\mathrm{Ai}(b) - \mathrm{Ai}(a)\,\mathrm{Bi}(b)]^{-1}\big\{\,\mathrm{Ai}(a)\,\mathrm{Ai}(b)\big[\,\mathrm{Bi}'(a)^2 - \mathrm{Bi}'(b)^2\big] \\ &\quad + \mathrm{Bi}(a)\,\mathrm{Bi}(b)\big[\,\mathrm{Ai}'(a)^2 - \mathrm{Ai}'(b)^2\big] \qquad (2.5.79) \\ &\quad + [\mathrm{Ai}'(b)\,\mathrm{Bi}'(b) - \mathrm{Ai}'(a)\,\mathrm{Bi}'(a)][\mathrm{Bi}(a)\,\mathrm{Ai}(b) + \mathrm{Ai}(a)\,\mathrm{Bi}(b)]\big\}.\end{aligned}$$

CHAPTER THREE

Donoghue m-functions for Singular Sturm–Liouville Operators

The content of this chapter relies on (but is not identical to) the paper submitted as: F. Gesztesy, L. L. Littlejohn, R. Nichols, M. Piorkowski, and J. Stanfill, *Donoghue m-functions for Singular Sturm–Liouville Operators*, 35pp.

3.1 Introduction

To set the stage we briefly discuss abstract Donoghue m-functions following [78] (see also [73], [77]). Given a self-adjoint extension A of a densely defined, closed, symmetric operator $\dot{A}$ in $\mathcal{H}$ (a complex, separable Hilbert space) with equal deficiency indices and the deficiency subspace $\mathcal{N}_i$ of $\dot{A}$ in $\mathcal{H}$, with

$$\mathcal{N}_i = \ker\big((\dot{A})^* - iI_{\mathcal{H}}\big), \quad \dim(\mathcal{N}_i) = k \in \mathbb{N} \cup \{\infty\}, \tag{3.1.1}$$

the Donoghue m-operator $M_{A,\mathcal{N}_i}^{Do}(\,\cdot\,) \in \mathcal{B}(\mathcal{N}_i)$ associated with the pair $(A, \mathcal{N}_i)$ is given by

$$\begin{aligned} M_{A,\mathcal{N}_i}^{Do}(z) &= P_{\mathcal{N}_i}(zA + I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1} P_{\mathcal{N}_i}\big|_{\mathcal{N}_i} \\ &= zI_{\mathcal{N}_i} + (z^2+1) P_{\mathcal{N}_i}(A - zI_{\mathcal{H}})^{-1} P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{3.1.2}$$

with $I_{\mathcal{N}_i}$ the identity operator in $\mathcal{N}_i$, and $P_{\mathcal{N}_i}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}_i$. The special case $k = 1$, was discussed in detail by Donoghue [49]; for the case $k \in \mathbb{N}$ we refer to [82].

More generally, given a self-adjoint extension A of $\dot{A}$ in $\mathcal{H}$ and a closed, linear subspace $\mathcal{N}$ of $\mathcal{N}_i$, the Donoghue m-operator $M_{A,\mathcal{N}}^{Do}(\,\cdot\,) \in \mathcal{B}(\mathcal{N})$ associated with the pair $(A, \mathcal{N})$ is defined by

$$\begin{aligned} M_{A,\mathcal{N}}^{Do}(z) &= P_{\mathcal{N}}(zA + I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1} P_{\mathcal{N}}\big|_{\mathcal{N}} \\ &= zI_{\mathcal{N}} + (z^2+1) P_{\mathcal{N}}(A - zI_{\mathcal{H}})^{-1} P_{\mathcal{N}}\big|_{\mathcal{N}}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{3.1.3}$$

with $I_{\mathcal{N}}$ the identity operator in $\mathcal{N}$ and $P_{\mathcal{N}}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}$.

Since $M_{A,\mathcal{N}}^{Do}(z)$ is analytic for $z \in \mathbb{C}\backslash\mathbb{R}$ and satisfies (see [78, Theorem 5.3])

$$[\mathrm{Im}(z)]^{-1}\mathrm{Im}\big(M_{A,\mathcal{N}}^{Do}(z)\big) \geqslant 2\Big[\big(|z|^2+1\big) + \big[\big(|z|^2-1\big)^2 + 4(\mathrm{Re}(z))^2\big]^{1/2}\Big]^{-1} I_{\mathcal{N}},$$
$$z \in \mathbb{C}\backslash\mathbb{R}, \qquad (3.1.4)$$

$M_{A,\mathcal{N}}^{Do}(\,\cdot\,)$ is a $\mathcal{B}(\mathcal{N})$-valued Nevanlinna–Herglotz function. Thus, $M_{A,\mathcal{N}}^{Do}(\,\cdot\,)$ admits the representation

$$M_{A,\mathcal{N}}^{Do}(z) = \int_{\mathbb{R}} d\Omega_{A,\mathcal{N}}^{Do}(\lambda)\bigg[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2+1}\bigg], \quad z \in \mathbb{C}\backslash\mathbb{R}, \qquad (3.1.5)$$

where the $\mathcal{B}(\mathcal{N})$-valued measure $\Omega_{A,\mathcal{N}}^{Do}(\,\cdot\,)$ satisfies

$$\Omega_{A,\mathcal{N}}^{Do}(\lambda) = (\lambda^2+1)(P_{\mathcal{N}}E_A(\lambda)P_{\mathcal{N}}\big|_{\mathcal{N}}), \qquad (3.1.6)$$

$$\int_{\mathbb{R}} d\Omega_{A,\mathcal{N}}^{Do}(\lambda)\,(1+\lambda^2)^{-1} = I_{\mathcal{N}}, \qquad (3.1.7)$$

$$\int_{\mathbb{R}} d(\xi, \Omega_{A,\mathcal{N}}^{Do}(\lambda)\xi)_{\mathcal{N}} = \infty \text{ for all } \xi \in \mathcal{N}\backslash\{0\}, \qquad (3.1.8)$$

with $E_A(\,\cdot\,)$ the family of strongly right-continuous spectral projections of A in $\mathcal{H}$.

Operators of the type $M_{A,\mathcal{N}}^{Do}(\,\cdot\,)$ and some of its variants have attracted considerable attention in the literature. They appear to go back to Krein [122] (see also [123]), Saakjan [168], and independently, Donoghue [49]. The interested reader can find a wealth of additional information in the context of (3.1.2)–(3.1.8) in [4], [6], [16]– [19], [24], [25]– [29], [38]– [44], [73]– [82], [83], [93], [124], [126], [134], [135], [136], [138], [142], [145]– [147], [154], [156], [167], and the references therein.

Without going into further details (see [78, Corollary 5.8] for details) we note that the prime reason for the interest in $M_{A,\mathcal{N}_i}^{Do}(\,\cdot\,)$ lies in the fundamental fact that the entire spectral information of A contained in its family of spectral projections $E_A(\,\cdot\,)$, is already encoded in the $\mathcal{B}(\mathcal{N}_i)$-valued measure $\Omega_{A,\mathcal{N}_i}^{Do}(\,\cdot\,)$ (including multiplicity properties of the spectrum of A) if and only if $\dot{A}$ is completely non-self-adjoint in $\mathcal{H}$ (that is, if and only if $\dot{A}$ has no invariant subspace on which it is self-adjoint, see [78, Lemma 5.4]).

We also note that a particularly attractive feature of the Donoghue m-operator, that distinguishes it from the Weyl–Titchmarsh–Kodaira m-operator, consists of the explicit appearance of the resolvent $(A - zI_{\mathcal{H}})^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$, in its definition (3.1.2) (resp., (3.1.3)).

We conclude these introductory remarks with a brief sketch of the relation between $M_{A,\mathcal{N}}^{Do}(\,\cdot\,)$ and an associated γ-field, familiar from the abstract theory of self-adjoint extensions of closed symmetric operators in connection with the notion of boundary triplets. To keep the discussion as short as possible, we restrict ourselves in the following to a relatively prime pair (A_1, A_2) of self-adjoint extensions of a closed symmetric operator $\dot{A}$ with equal (finite or infinite) deficiency indices $\big($such that $\operatorname{dom}(A_1) \cap \operatorname{dom}(A_2) = \operatorname{dom}\big(\dot{A}\big)\big)$. We start by recalling Krein's resolvent formula as described in [77],

$$\begin{aligned}
(A_2 - zI_{\mathcal{H}})^{-1} &= (A_1 - zI_{\mathcal{H}})^{-1} \\
&\quad + \gamma_{A_1,\mathcal{N}_i}(z)\big[\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_i}^{Do}(z)\big]^{-1}\gamma_{A_1,\mathcal{N}_i}(\overline{z})^*, \quad z \in \rho(A_1) \cap \rho(A_2),
\end{aligned} \tag{3.1.9}$$

where the γ-field $\gamma_{A_1,\mathcal{N}_i}(\,\cdot\,)$ is given by

$$\begin{aligned}
\gamma_{A_1,\mathcal{N}_i}(z) &= (A_1 - iI_{\mathcal{H}})(A_1 - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}_i}, \quad z \in \rho(A_1), \\
\gamma_{A_1,\mathcal{N}_i}(\overline{z})^* &= P_{\mathcal{N}_i}(A_1 + iI_{\mathcal{H}})(A_1 - zI_{\mathcal{H}})^{-1}, \quad z \in \rho(A_1),
\end{aligned} \tag{3.1.10}$$

and the operator $\alpha_{1,2}$ in $\mathcal{N}_i$ is introduced via

$$e^{-2i\alpha_{1,2}} = -C_{A_2}C_{A_1}^{-1}\big|_{\mathcal{N}_i}, \tag{3.1.11}$$

where C_B denotes the (unitary) Cayley transform of the self-adjoint operator B in $\mathcal{H}$, that is,

$$C_B = (B + iI_{\mathcal{H}})(B - iI_{\mathcal{H}})^{-1}, \tag{3.1.12}$$

and one notes that $\mathcal{N}_i$ is an invariant subspace for $C_{A_2}C_{A_1}^{-1}$.

One then verifies the following formulas, familiar from the theory of boundary triplets (see, e.g., [15, Sect. 2.3]),

$$\gamma_{A_1,\mathcal{N}_i}(z) = (A_1 - \zeta I_{\mathcal{H}})(A_1 - zI_{\mathcal{H}})^{-1}\gamma_{A_1,\mathcal{N}_i}(\zeta), \quad z,\zeta \in \rho(A_1), \tag{3.1.13}$$

$$M_{A_1,\mathcal{N}_i}^{Do}(z) - M_{A_1,\mathcal{N}_i}^{Do}(\zeta)^* = \big(z - \overline{\zeta}\big)\gamma_{A_1,\mathcal{N}_i}(\zeta)^*\gamma_{A_1,\mathcal{N}_i}(z), \quad z,\zeta \in \rho(A_1), \tag{3.1.14}$$

$$M_{A_1,\mathcal{N}_i}^{Do}(z)^* = M_{A_1,\mathcal{N}_i}^{Do}(\overline{z}), \quad z \in \rho(A_1), \tag{3.1.15}$$

$$\begin{aligned}&(z-\zeta_1)(\zeta_1-\zeta_2)(\zeta_2-z)\,\gamma_{A_1,\mathcal{N}_i}(\overline{\zeta}_1)^*(A_1 - zI_{\mathcal{H}})^{-1}\gamma_{A_1,\mathcal{N}_i}(\zeta_2)\\ &\quad = (\zeta_1-\zeta_2)M_{A_1,\mathcal{N}_i}^{Do}(z) + (z-\zeta_2)M_{A_1,\mathcal{N}_i}^{Do}(\zeta_1) + (\zeta_1 - z)M_{A_1,\mathcal{N}_i}^{Do}(\zeta_2),\\ &\hspace{6cm} z,\zeta_1,\zeta_2 \in \rho(A_1).\end{aligned} \tag{3.1.16}$$

In the remainder of this chapter and the next, we will exclusively focus on the particular case $\mathcal{N} = \mathcal{N}_i = \ker\big((\dot{A})^* - iI_{\mathcal{H}}\big)$ and develop a self-contained approach to constructing Donoghue m-functions (resp., 2×2 matrices) for singular Sturm–Liouville operators on arbitrary intervals $(a,b) \subseteq \mathbb{R}$. More precisely, assuming the standard local integrability hypotheses on the coefficients p, q, r (cf. Hypothesis 3.2.1) we study all self-adjoint $L^2((a,b);rdx)$-realizations corresponding to the differential expression

$$\tau = \frac{1}{r(x)}\left[-\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] \text{ for a.e. } x \in (a,b) \subseteq \mathbb{R}, \tag{3.1.17}$$

and systematically determine the underlying Donoghue m-functions in all cases where τ is in the limit circle case at least at one interval endpoint a or b.

Turning to the content of each section, we discuss the necessary background in connection with minimal T_{min} and maximal T_{max} operators, self-adjoint extensions, etc., corresponding to (3.1.17) in the underlying Hilbert space $L^2((a,b);rdx)$ in Section 3.2. In particular, we recall the discussion of boundary values in terms of appropriate Wronskians, especially, in the case where T_{min} is bounded from below (utilizing principal and nonprincipal solutions). Our strategy for the construction of Donoghue m-functions consists of first constructing them for the Friedrichs extension of T_{min} and then employing Krein-type resolvent formulas to derive Donoghue m-functions for the remaining self-adjoint extensions of T_{min}. These Krein-type resolvent formulas use the Friedrichs extension as a reference operator and then explicitly characterize the resolvents of all the remaining self-adjoint extensions of T_{min} in terms of the Friedrichs extension and the deficiency subspaces for T_{min}. Hence Sections 3.3 and 3.4 derive Krein-type resolvent formulas for singular Sturm–Liouville operators in the case where τ has one, respectively, two, interval endpoints in the limit circle case. Donoghue m-functions corresponding to the case where τ is in the limit circle case in precisely one interval endpoint are derived in Section 3.5; the case where τ is in the limit circle case at a and b is treated in detail in Section 3.6. We conclude this chapter with an illustration of a generalized Bessel operator in Section 3.7 where $a = 0$, $b \in (0, \infty) \cup \{\infty\}$, and τ takes on the explicit form,

$$\begin{aligned} &\tau_{\delta,\nu,\gamma} = x^{-\delta}\left[-\frac{d}{dx}x^{\nu}\frac{d}{dx} + \frac{(2+\delta-\nu)^2\gamma^2 - (1-\nu)^2}{4}x^{\nu-2}\right], \\ &\qquad\qquad \delta > -1,\ \nu < 1,\ \gamma \geqslant 0,\ x \in (0,b). \end{aligned} \tag{3.1.18}$$

Finally, we comment on some of the basic notation used throughout this chapter and the next. If T is a linear operator mapping (a subspace of) a Hilbert space into another, then $\operatorname{dom}(T)$ and $\ker(T)$ denote the domain and kernel (i.e., null space) of T. The spectrum and resolvent set of a closed linear operator in a Hilbert space will be denoted by $\sigma(\,\cdot\,)$ and $\rho(\,\cdot\,)$, respectively. Moreover, we typically abbreviate $L^2((a,b); rdx)$ as $L^2_r((a,b))$ in various subscripts involving the identity operator $I_{L^2_r((a,b))}$ and the scalar product $(\,\cdot\,,\,\cdot\,)_{L^2_r((a,b))}$ (linear in the second argument) and associated norm $\|\cdot\|_{L^2_r((a,b))}$ in $L^2((a,b); rdx)$.

3.2 Some Background

In this section we briefly recall the basics of singular Sturm–Liouville operators. The material is standard and can be found, for instance, in [15, Ch. 6], [35, Chs. 8, 9], [51, Sects. 13.6, 13.9, 13.10], [52], [84, Ch. 4], [104, Ch. III], [149, Ch. V], [150], [155, Ch. 6], [175, Ch. 9], [179, Sect. 8.3], [180, Ch. 13], [182, Chs. 4, 6–8].

Throughout this section we make the following assumptions:

Hypothesis 3.2.1. *Let $(a, b) \subseteq \mathbb{R}$ and suppose that p, q, r are (Lebesgue) measurable functions on (a, b) such that the following items (i)–(iii) hold:*

(i) $r > 0$ a.e. on (a, b), $r \in L^1_{loc}((a, b); dx)$.

(ii) $p > 0$ a.e. on (a, b), $1/p \in L^1_{loc}((a, b); dx)$.

(iii) q is real-valued a.e. on (a, b), $q \in L^1_{loc}((a, b); dx)$.

Given Hypothesis 3.2.1, we study Sturm–Liouville operators associated with the general, three-coefficient differential expression τ of the form

$$\tau = \frac{1}{r(x)} \left[-\frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right] \text{ for a.e. } x \in (a, b) \subseteq \mathbb{R}. \tag{3.2.1}$$

If $f \in AC_{loc}((a, b))$, then the quasi-derivative of f is defined to be $f^{[1]} := pf'$. Moreover, the Wronskian of two functions $f, g \in AC_{loc}((a, b))$ is defined by

$$W(f, g)(x) = f(x)g^{[1]}(x) - f^{[1]}(x)g(x) \text{ for a.e. } x \in (a, b). \tag{3.2.2}$$

The following result is useful for computing weighted integrals of products of solutions of $(\tau - z)y = 0$: Assume Hypothesis 3.2.1 and let $z_1, z_2 \in \mathbb{C}$ with $z_1 \neq z_2$. If $y(z_j, \cdot)$ is a solution of $(\tau - z_j)y = 0$, $j \in \{1, 2\}$, then for all $a < \alpha < \beta < b$,

$$\int_\alpha^\beta r(x)dx\, y(z_1, x)y(z_2, x) = \frac{W(y(z_1, \cdot), y(z_2, \cdot))\big|_\alpha^\beta}{z_1 - z_2}. \tag{3.2.3}$$

Definition 3.2.2. *Assume Hypothesis 3.2.1. Given τ as in (3.2.1), the maximal operator T_{max} in $L^2((a, b); rdx)$ associated with τ is defined by*

$$\begin{aligned} &T_{max} f = \tau f, \\ &f \in \operatorname{dom}(T_{max}) = \big\{ g \in L^2((a, b); rdx) \,\big|\, g, g^{[1]} \in AC_{loc}((a, b)); \\ &\qquad\qquad\qquad\qquad\qquad \tau g \in L^2((a, b); rdx) \big\}. \end{aligned} \tag{3.2.4}$$

The preminimal operator $\dot{T}_{min}$ *in* $L^2((a,b);rdx)$ *associated with* τ *is defined by*

$$\begin{aligned}
&\dot{T}_{min} f = \tau f, \\
&f \in \operatorname{dom}\big(\dot{T}_{min}\big) = \big\{ g \in L^2((a,b);rdx) \,\big|\, g, g^{[1]} \in AC_{loc}((a,b)); \\
&\qquad\qquad \operatorname{supp}(g) \subset (a,b) \textit{ is compact; } \tau g \in L^2((a,b);rdx) \big\}.
\end{aligned} \tag{3.2.5}$$

One can prove that $\dot{T}_{min}$ *is closable, and one then defines the minimal operator* T_{min} *as the closure of* $\dot{T}_{min}$.

For $f, g \in \operatorname{dom}(T_{max})$, one can prove that the following limits exist:

$$W(f,g)(a) = \lim_{x \downarrow a} W(f,g)(x) \quad \text{and} \quad W(f,g)(b) = \lim_{x \uparrow b} W(f,g)(x). \tag{3.2.6}$$

In addition, one can prove the following basic fact:

Theorem 3.2.3. *Assume Hypothesis* 3.2.1. *Then*

$$\big(\dot{T}_{min}\big)^* = T_{max}, \tag{3.2.7}$$

and hence T_{max} *is closed and* $T_{min} = \overline{\dot{T}_{min}}$ *is given by*

$$\begin{aligned}
&T_{min} f = \tau f, \\
&f \in \operatorname{dom}(T_{min}) = \big\{ g \in L^2((a,b);rdx) \,\big|\, g, g^{[1]} \in AC_{loc}((a,b)); \\
&\qquad \textit{for all } h \in \operatorname{dom}(T_{max}),\ W(h,g)(a) = 0 = W(h,g)(b);\ \tau g \in L^2((a,b);rdx) \big\} \\
&\quad = \big\{ g \in \operatorname{dom}(T_{max}) \,\big|\, W(h,g)(a) = 0 = W(h,g)(b) \textit{ for all } h \in \operatorname{dom}(T_{max}) \big\}.
\end{aligned} \tag{3.2.8}$$

Moreover, $\dot{T}_{min}$ *is essentially self-adjoint if and only if* T_{max} *is symmetric, and then* $\overline{\dot{T}_{min}} = T_{min} = T_{max}$.

Regarding self-adjoint extensions of T_{min} one has the following first result.

Theorem 3.2.4. *Assume Hypothesis* 3.2.1. *An extension* $\widetilde{T}$ *of* $\dot{T}_{min}$ *or of* $T_{min} = \overline{\dot{T}_{min}}$ *is self-adjoint if and only if*

$$\begin{aligned}
&\widetilde{T} f = \tau f, \\
&f \in \operatorname{dom}\big(\widetilde{T}\big) = \big\{ g \in \operatorname{dom}(T_{max}) \,\big|\, W(f,g)(a) = W(f,g)(b) \textit{ for all } f \in \operatorname{dom}\big(\widetilde{T}\big) \big\}.
\end{aligned} \tag{3.2.9}$$

The celebrated Weyl alternative then can be stated as follows:

Theorem 3.2.5 (Weyl's Alternative).

Assume Hypothesis 3.2.1*. Then the following alternative holds: Either*

(i) *for every* $z \in \mathbb{C}$*, all solutions* u *of* $(\tau - z)u = 0$ *are in* $L^2((a,b); rdx)$ *near* b $($*resp., near* $a)$*,*

or,

(ii) *for every* $z \in \mathbb{C}$*, there exists at least one solution* u *of* $(\tau - z)u = 0$ *which is not in* $L^2((a,b); rdx)$ *near* b $($*resp., near* $a)$*. In this case, for each* $z \in \mathbb{C}\backslash\mathbb{R}$*, there exists precisely one solution* u_b $($*resp.,* $u_a)$ *of* $(\tau - z)u = 0$ $($*up to constant multiples*$)$ *which lies in* $L^2((a,b); rdx)$ *near* b $($*resp., near* $a)$*.*

This yields the limit circle/limit point classification of τ at an interval endpoint as follows.

Definition 3.2.6. *Assume Hypothesis* 3.2.1*.*

In case (i) *in Theorem* 3.2.5*,* τ *is said to be in the limit circle case at* b $($*resp.,* $a)$*.* $($*Frequently,* τ *is then called quasi-regular at* b $($*resp.,* $a).)$

In case (ii) *in Theorem* 3.2.5*,* τ *is said to be in the limit point case at* b $($*resp.,* $a)$*.*

If τ *is in the limit circle case at* a *and* b *then* τ *is also called quasi-regular on* (a,b)*.*

The next result links self-adjointness of T_{min} (resp., T_{max}) and the limit point property of τ at both endpoints. Here, and throughout, we shall employ the notation

$$\mathcal{N}_z = \ker\left(T_{max} - zI_{L^2_r((a,b))}\right), \quad z \in \mathbb{C}. \tag{3.2.10}$$

Theorem 3.2.7. *Assume Hypothesis* 3.2.1*, then the following items* (i) *and* (ii) *hold:*

(i) *If* τ *is in the limit point case at* a $($*resp.,* $b)$*, then*

$$W(f,g)(a) = 0 \, (\textit{resp., } W(f,g)(b) = 0) \textit{ for all } f,g \in \operatorname{dom}(T_{max}). \tag{3.2.11}$$

(ii) *Let* $T_{min} = \overline{\dot{T}_{min}}$. *Then*

$$n_\pm(T_{min}) = \dim\big(\mathcal{N}_{\pm i}\big)$$
$$= \begin{cases} 2 & \text{if } \tau \text{ is in the limit circle case at } a \text{ and } b, \\ 1 & \text{if } \tau \text{ is in the limit circle case at } a \\ & \text{and in the limit point case at } b, \text{ or vice versa}, \\ 0 & \text{if } \tau \text{ is in the limit point case at } a \text{ and } b. \end{cases} \tag{3.2.12}$$

In particular, $T_{min} = T_{max}$ *is self-adjoint if and only if* τ *is in the limit point case at* a *and* b.

All self-adjoint extensions of T_{min} are then described as follows:

Theorem 3.2.8. *Assume Hypothesis* 3.2.1 *and that* τ *is in the limit circle case at* a *and* b *(i.e.,* τ *is quasi-regular on* (a,b)*). In addition, assume that* $v_j \in \operatorname{dom}(T_{max})$, $j = 1,2$, *satisfy*

$$W(\overline{v_1}, v_2)(a) = W(\overline{v_1}, v_2)(b) = 1, \quad W(\overline{v_j}, v_j)(a) = W(\overline{v_j}, v_j)(b) = 0,\ j = 1,2. \tag{3.2.13}$$

(E.g., real-valued solutions v_j, $j = 1,2$, *of* $(\tau - \lambda)u = 0$ *with* $\lambda \in \mathbb{R}$, *such that* $W(v_1, v_2) = 1$.*) For* $g \in \operatorname{dom}(T_{max})$ *we introduce the generalized boundary values*

$$\begin{aligned} \widetilde{g}_1(a) &= -W(v_2, g)(a), \quad & \widetilde{g}_1(b) &= -W(v_2, g)(b), \\ \widetilde{g}_2(a) &= W(v_1, g)(a), \quad & \widetilde{g}_2(b) &= W(v_1, g)(b). \end{aligned} \tag{3.2.14}$$

Then the following items (i)–(iii) hold:

(i) *All self-adjoint extensions* $T_{\alpha,\beta}$ *of* T_{min} *with separated boundary conditions are of the form*

$$T_{\alpha,\beta} f = \tau f, \quad \alpha, \beta \in [0, \pi), \tag{3.2.15}$$

$$f \in \operatorname{dom}(T_{\alpha,\beta}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{matrix} \cos(\alpha)\widetilde{g}_1(a) + \sin(\alpha)\widetilde{g}_2(a) = 0, \\ \cos(\beta)\widetilde{g}_1(b) + \sin(\beta)\widetilde{g}_2(b) = 0 \end{matrix} \right\}.$$

(ii) All self-adjoint extensions $T_{\varphi,R}$ *of* T_{min} *with coupled boundary conditions are of the type*

$$T_{\varphi,R} f = \tau f,$$

$$f \in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{pmatrix} \widetilde{g}_1(b) \\ \widetilde{g}_2(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} \widetilde{g}_1(a) \\ \widetilde{g}_2(a) \end{pmatrix} \right\}, \tag{3.2.16}$$

where $\varphi \in [0, \pi)$, *and* R *is a real* 2×2 *matrix with* $\det(R) = 1$ *(i.e.,* $R \in SL(2, \mathbb{R})$*).*

(iii) Every self-adjoint extension of T_{min} *is either of type (i) (i.e., separated) or of type (ii) (i.e., coupled).*

Remark 3.2.9. *(i)* If τ is in the limit point case at one endpoint, say, at the endpoint b, one omits the corresponding boundary condition involving $\beta \in [0, \pi)$ at b in (3.2.15) to obtain all self-adjoint extensions T_α of T_{min}, indexed by $\alpha \in [0, \pi)$. (In this case item *(iii)* in Theorem 3.2.8 is vacuous.) In the case where τ is in the limit point case at both endpoints, all boundary values and boundary conditions become superfluous as in this case $T_{min} = T_{max}$ is self-adjoint.

(ii) In the special case where τ is regular on the finite interval $[a, b]$, choose $v_j \in \operatorname{dom}(T_{max})$, $j = 1, 2$, such that

$$v_1(x) = \begin{cases} \theta_0(\lambda, x, a), & \text{for } x \text{ near } a, \\ \theta_0(\lambda, x, b), & \text{for } x \text{ near } b, \end{cases} \qquad v_2(x) = \begin{cases} \phi_0(\lambda, x, a), & \text{for } x \text{ near } a, \\ \phi_0(\lambda, x, b), & \text{for } x \text{ near } b, \end{cases} \tag{3.2.17}$$

where $\phi_0(\lambda, \cdot\,, d)$, $\theta_0(\lambda, \cdot\,, d)$, $d \in \{a, b\}$, are real-valued solutions of $(\tau - \lambda)u = 0$, $\lambda \in \mathbb{R}$, satisfying the boundary conditions

$$\begin{aligned} &\phi_0(\lambda, a, a) = \theta_0^{[1]}(\lambda, a, a) = 0, \quad \theta_0(\lambda, a, a) = \phi_0^{[1]}(\lambda, a, a) = 1, \\ &\phi_0(\lambda, b, b) = \theta_0^{[1]}(\lambda, b, b) = 0, \quad \theta_0(\lambda, b, b) = \phi_0^{[1]}(\lambda, b, b) = 1. \end{aligned} \tag{3.2.18}$$

Then one verifies that

$$\widetilde{g}_1(a) = g(a), \quad \widetilde{g}_1(b) = g(b), \quad \widetilde{g}_2(a) = g^{[1]}(a), \quad \widetilde{g}_2(b) = g^{[1]}(b), \tag{3.2.19}$$

and hence Theorem 3.2.8 recovers the well-known special regular case.

(iii) In connection with (3.2.14), an explicit calculation demonstrates that for $g, h \in \operatorname{dom}(T_{max})$,

$$\widetilde{g}_1(d)\widetilde{h}_2(d) - \widetilde{g}_2(d)\widetilde{h}_1(d) = W(g,h)(d), \quad d \in \{a,b\}, \tag{3.2.20}$$

interpreted in the sense that either side in (3.2.20) has a finite limit as $d \downarrow a$ and $d \uparrow b$. Of course, for (3.2.20) to hold at $d \in \{a,b\}$, it suffices that g and h lie locally in $\operatorname{dom}(T_{max})$ near $x = d$.

(iv) Clearly, $\widetilde{g}_1, \widetilde{g}_2$ depend on the choice of v_j, $j = 1,2$, and a more precise notation would indicate this as $\widetilde{g}_{1,v_2}, \widetilde{g}_{2,v_1}$, etc.

(v) One can supplement the characterization (3.2.8) of $\operatorname{dom}(T_{min})$ by

$$\begin{aligned} &T_{min} f = \tau f, \\ &f \in \operatorname{dom}(T_{min}) = \big\{ g \in \operatorname{dom}(T_{max}) \,\big|\, \widetilde{g}_1(a) = \widetilde{g}_2(a) = \widetilde{g}_1(b) = \widetilde{g}_2(b) = 0 \big\}. \end{aligned} \tag{3.2.21}$$

Next, we determine when two self-adjoint extensions of T_{min} are *relatively prime* with respect to T_{min}.

Definition 3.2.10. *If T and T' are self-adjoint extensions of a symmetric operator S, then the maximal common part of T and T' is the operator $C_{T,T'}$ defined by*

$$C_{T,T'} u = Tu, \quad u \in \operatorname{dom}(C_{T,T'}) = \{ f \in \operatorname{dom}(T) \cap \operatorname{dom}(T') \,|\, Tf = T'f \}. \tag{3.2.22}$$

Moreover, T and T' are said to be relatively prime with respect to S if $C_{T,T'} = S$.

Theorem 3.2.11. *Assume Hypothesis* 3.2.1.

(i) If $\alpha, \alpha', \beta, \beta' \in [0,\pi)$ with $\alpha \neq \alpha'$ and $\beta \neq \beta'$, then $T_{\alpha,\beta}$ and $T_{\alpha',\beta'}$ are relatively prime with respect to T_{min}.

(ii) If $\alpha, \beta, \beta' \in [0,\pi)$ with $\beta \neq \beta'$, then the maximal common part of $T_{\alpha,\beta}$ and $T_{\alpha,\beta'}$ is the restriction of T_{max} to the subspace

$$\big\{ g \in \operatorname{dom}(T_{max}) \,\big|\, \cos(\alpha)\widetilde{g}_1(a) + \sin(\alpha)\widetilde{g}_2(a) = 0,\, \widetilde{g}_1(b) = \widetilde{g}_2(b) = 0 \big\}. \tag{3.2.23}$$

(iii) If $\alpha, \alpha', \beta \in [0, \pi)$ with $\alpha \neq \alpha'$, then the maximal common part of $T_{\alpha,\beta}$ and $T_{\alpha',\beta}$ is the restriction of T_{max} to the subspace

$$\big\{g \in \operatorname{dom}(T_{max}) \,\big|\, \widetilde{g}_1(a) = \widetilde{g}_2(a) = 0,\ \cos(\beta)\widetilde{g}_1(b) + \sin(\beta)\widetilde{g}_2(b) = 0\big\}. \tag{3.2.24}$$

(iv) Let $\alpha, \beta \in [0, \pi)$, $\varphi \in [0, \pi)$, $R = (R_{j,k})_{j,k=1}^2 \in SL(2, \mathbb{R})$, and define

$$\begin{aligned} d(\alpha, \beta, R) = \cos(\alpha)\cos(\beta)R_{1,2} &+ \cos(\alpha)\sin(\beta)R_{2,2} \\ &- \sin(\alpha)\cos(\beta)R_{1,1} - \sin(\alpha)\sin(\beta)R_{2,1}. \end{aligned} \tag{3.2.25}$$

If $d(\alpha, \beta, R) \neq 0$, then $T_{\alpha,\beta}$ and $T_{\varphi,R}$ are relatively prime with respect to T_{min}. If $d(\alpha, \beta, R) = 0$, then the maximal common part of $T_{\alpha,\beta}$ and $T_{\varphi,R}$ is the restriction of T_{max} to the subspace

$$\big\{g \in \operatorname{dom}(T_{\varphi,R}) \,\big|\, \cos(\alpha)\widetilde{g}_1(a) + \sin(\alpha)\widetilde{g}_2(a) = 0\big\}. \tag{3.2.26}$$

(v) Let $\varphi, \eta \in [0, \pi)$ and $R, S \in SL(2, \mathbb{R})$. If $\det\big(e^{i(\eta-\varphi)}SR^{-1} - I_{\mathbb{C}^2}\big) \neq 0$, then $T_{\varphi,R}$ and $T_{\eta,S}$ are relatively prime with respect to T_{min}. If $\det\big(e^{i(\eta-\varphi)}SR^{-1} - I_{\mathbb{C}^2}\big) = 0$, so that 1 is an eigenvalue of $e^{i(\eta-\varphi)}SR^{-1}$ with corresponding eigenspace $\mathcal{V}_1 \subset \mathbb{C}^2$, then the maximal common part of $T_{\varphi,R}$ and $T_{\eta,S}$ is the restriction of T_{max} to the subspace

$$\big\{g \in \operatorname{dom}(T_{\varphi,R}) \,\big|\, (\widetilde{g}_1(b), \widetilde{g}_2(b))^\top \in \mathcal{V}_1\big\}. \tag{3.2.27}$$

Proof. To prove (i), it suffices to show that $f \in \operatorname{dom}(T_{\alpha,\beta}) \cap \operatorname{dom}(T_{\alpha',\beta'})$ implies $f \in \operatorname{dom}(T_{min})$. If $f \in \operatorname{dom}(T_{\alpha,\beta}) \cap \operatorname{dom}(T_{\alpha',\beta'})$, then

$$\begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ \cos(\alpha') & \sin(\alpha') \end{pmatrix} \begin{pmatrix} \widetilde{f}_1(a) \\ \widetilde{f}_2(a) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{3.2.28}$$

$$\begin{pmatrix} \cos(\beta) & \sin(\beta) \\ \cos(\beta') & \sin(\beta') \end{pmatrix} \begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.2.29}$$

The determinants of the 2×2 coefficient matrices in (3.2.28) and (3.2.29) are $\sin(\alpha - \alpha')$ and $\sin(\beta - \beta')$, respectively. Since the assumptions on α, α', β, and β' imply $\alpha - \alpha', \beta - \beta' \in (-\pi, \pi)\backslash\{0\}$, it follows that the coefficient matrices in (3.2.28) and (3.2.29) are invertible. Hence, $\widetilde{f}_1(a) = \widetilde{f}_2(a) = \widetilde{f}_1(b) = \widetilde{f}_2(b) = 0$, and the characterization of $\mathrm{dom}(T_{min})$ in (3.2.21) implies $f \in \mathrm{dom}(T_{min})$.

The proofs of (ii) and (iii) are similar, so we only provide the proof of (ii) here. Let D denote the set in (3.2.24). To prove (ii), it suffices to show $\mathrm{dom}(T_{\alpha,\beta}) \cap \mathrm{dom}(T_{\alpha,\beta'}) = D$. If $f \in \mathrm{dom}(T_{\alpha,\beta}) \cap \mathrm{dom}(T_{\alpha,\beta'})$, then $\cos(\alpha)\widetilde{f}_1(a) + \sin(\alpha)\widetilde{f}_2(a) = 0$ and (3.2.29) holds. As in the proof of (i), the determinant of the 2×2 coefficient matrix in (3.2.29) is nonzero. Therefore, $\widetilde{f}_1(b) = \widetilde{f}_2(b) = 0$, and it follows that $f \in D$. Conversely, if $f \in D$, then it is clear that f simultaneously belongs to $\mathrm{dom}(T_{\alpha,\beta})$ and $\mathrm{dom}(T_{\alpha,\beta'})$.

The proof of (iv) begins with a general observation about functions in the intersection $\mathrm{dom}(T_{\alpha,\beta}) \cap \mathrm{dom}(T_{\varphi,R})$. If $f \in \mathrm{dom}(T_{\alpha,\beta}) \cap \mathrm{dom}(T_{\varphi,R})$, then

$$\begin{aligned} \cos(\alpha)\widetilde{f}_1(a) + \sin(\alpha)\widetilde{f}_2(a) = 0, \\ \cos(\beta)\widetilde{f}_1(b) + \sin(\beta)\widetilde{f}_2(b) = 0, \end{aligned} \tag{3.2.30}$$

and

$$\begin{aligned} \widetilde{f}_1(b) = e^{i\varphi}R_{1,1}\widetilde{f}_1(a) + e^{i\varphi}R_{1,2}\widetilde{f}_2(a), \\ \widetilde{f}_2(b) = e^{i\varphi}R_{2,1}\widetilde{f}_1(a) + e^{i\varphi}R_{2,2}\widetilde{f}_2(a). \end{aligned} \tag{3.2.31}$$

Applying (3.2.31) in (3.2.30) yields a set of boundary conditions that may be recast in matrix form as

$$\begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ \cos(\beta)R_{1,1} + \sin(\beta)R_{2,1} & \cos(\beta)R_{1,2} + \sin(\beta)R_{2,2} \end{pmatrix} \begin{pmatrix} \widetilde{f}_1(a) \\ \widetilde{f}_2(a) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.2.32}$$

The determinant of the 2×2 coefficient matrix in (3.2.32) is $d(\alpha, \beta, R)$.

If $d(\alpha, \beta, R) \neq 0$, then (3.2.32) implies $\widetilde{f}_1(a) = \widetilde{f}_2(a) = 0$. In turn, (3.2.31) implies $\widetilde{f}_1(b) = \widetilde{f}_2(b) = 0$. Hence, $f \in \mathrm{dom}(T_{min})$, and it follows that $T_{\alpha,\beta}$ and $T_{\varphi,R}$ are relatively prime with respect to T_{min}.

To complete the proof of (iv), it remains to show that the set in (3.2.26), call it D, coincides with $\mathrm{dom}(T_{\alpha,\beta}) \cap \mathrm{dom}(T_{\varphi,R})$ when $d(\alpha, \beta, R) = 0$. The containment

$\operatorname{dom}(T_{\alpha,\beta}) \cap \operatorname{dom}(T_{\varphi,R}) \subset D$ follows immediately from the definitions of $T_{\alpha,\beta}$, $T_{\varphi,R}$, and D. To prove the reverse containment, let $f \in D$, so that $f \in \operatorname{dom}(H_{\varphi,R})$ and f satisfies the boundary condition at a in (3.2.30). The proof is then reduced to showing f satisfies the boundary condition at b in (3.2.30). In order to do this, one distinguishes the cases $\alpha \neq 0$ and $\alpha = 0$. If $\alpha \neq 0$, one uses $d(\alpha, \beta, R) = 0$, the conditions in (3.2.31), and $\sin(\alpha)\widetilde{f}_2(a) = -\cos(\alpha)\widetilde{f}_1(a)$ to compute

$$\begin{aligned}
&e^{-i\varphi}\sin(\alpha)\big[\cos(\beta)\widetilde{f}_1(b) + \sin(\beta)\widetilde{f}_2(b)\big] \\
&\quad= [\cos(\beta)R_{1,1} + \sin(\beta)R_{2,1}]\sin(\alpha)\widetilde{f}_1(a) \\
&\qquad - [\cos(\beta)R_{1,2} + \sin(\beta)R_{2,2}]\cos(\alpha)\widetilde{f}_1(a) \\
&\quad= -d(\alpha, \beta, R)\widetilde{f}_1(a) \\
&\quad= 0.
\end{aligned} \tag{3.2.33}$$

Since $e^{-i\varphi}\sin(\alpha) \neq 0$ when $\alpha \neq 0$, (3.2.33) implies f satisfies the boundary condition at b in (3.2.30). If $\alpha = 0$, then $\widetilde{f}_1(a) = 0$, and (3.2.31) simplifies. One then computes

$$\begin{aligned}
\cos(\beta)\widetilde{f}_1(b) + \sin(\beta)\widetilde{f}_2(b) &= e^{i\varphi}[\cos(\beta)R_{1,2} + \sin(\beta)R_{2,2}]\widetilde{f}_2(a) \\
&= e^{i\varphi}d(0, \beta, R)\widetilde{f}_2(a) \\
&= 0,
\end{aligned} \tag{3.2.34}$$

so f satisfies the boundary condition at b in (3.2.30).

To prove (v), let $f \in \operatorname{dom}(T_{\varphi,R}) \cap \operatorname{dom}(T_{\eta,S})$, so that

$$\begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix} = e^{i\eta}S \begin{pmatrix} \widetilde{f}_1(a) \\ \widetilde{f}_2(a) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix} = e^{i\varphi}R \begin{pmatrix} \widetilde{f}_1(a) \\ \widetilde{f}_2(a) \end{pmatrix}. \tag{3.2.35}$$

Using the invertibility of $e^{i\varphi}R$ to solve the second equation in (3.2.35) for the vector $\big(\widetilde{f}_1(a), \widetilde{f}_2(a)\big)^\top$ and substituting into the first equation in (3.2.35) yields

$$\big[e^{i(\eta-\varphi)}SR^{-1} - I_{\mathbb{C}^2}\big] \begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.2.36}$$

If $\det\left(e^{i(\eta-\varphi)}SR^{-1} - I_{\mathbb{C}^2}\right) \neq 0$, then (3.2.36) implies $\widetilde{f}_1(b) = \widetilde{f}_2(b) = 0$. In turn, the invertibility of $e^{i\varphi}R$ and the second equation in (3.2.35) yields $\widetilde{f}_1(a) = \widetilde{f}_2(a) = 0$. Hence, $f \in \operatorname{dom}(T_{min})$, and it follows that $T_{\varphi,R}$ and $T_{\eta,S}$ are relatively prime with respect to T_{min}.

Now, suppose that $\det\left(e^{i(\eta-\varphi)}SR^{-1} - I_{\mathbb{C}^2}\right) = 0$, so that 1 is an eigenvalue of $e^{i(\eta-\varphi)}SR^{-1}$ with corresponding eigenspace $\mathcal{V}_1$. Let D denote the subspace in (3.2.27). To complete the proof of (v), it suffices to show the subspace D coincides with $\operatorname{dom}(T_{\varphi,R}) \cap \operatorname{dom}(T_{\eta,S})$. To this end, let $f \in \operatorname{dom}(T_{\varphi,R}) \cap \operatorname{dom}(T_{\eta,S})$, so that both equalities in (3.2.35) hold. In particular, (3.2.36) holds due to the invertibility of $e^{i\varphi}R$, and one concludes that $\left(\widetilde{f}_1(b), \widetilde{f}_2(b)\right)^\top \in \mathcal{V}_1$. Therefore, $f \in D$. Conversely, if $f \in D$, then $f \in \operatorname{dom}(T_{\varphi,R})$, and one only needs to show $f \in \operatorname{dom}(T_{\eta,S})$ to complete the proof. Using the boundary conditions implied by the inclusion $f \in \operatorname{dom}(T_{\varphi,R})$ (i.e., the second equality in (3.2.35)), one computes

$$e^{i\eta}S \begin{pmatrix} \widetilde{f}_1(a) \\ \widetilde{f}_2(a) \end{pmatrix} = e^{i(\eta-\varphi)}SR^{-1} \begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix} = \begin{pmatrix} \widetilde{f}_1(b) \\ \widetilde{f}_2(b) \end{pmatrix}, \tag{3.2.37}$$

where the last equality in (3.2.37) follows from the fact that $\left(\widetilde{f}_1(b), \widetilde{f}_2(b)\right)^\top \in \mathcal{V}_1$ by the assumption $f \in D$. The equality in (3.2.37) implies $f \in \operatorname{dom}(T_{\eta,S})$. $\square$

Finally, we turn to the characterization of generalized boundary values in the case where T_{min} is bounded from below following [75] and [150].

We recall the basics of oscillation theory with particular emphasis on principal and nonprincipal solutions, a notion originally due to Leighton and Morse [127] (see also Rellich [159], [160] and Hartman and Wintner [92, Appendix]). Our outline below follows [33], [51, Sects. 13.6, 13.9, 13.10], [84, Ch. 7], [91, Ch. XI], [150], [182, Chs. 4, 6–8].

Definition 3.2.12. *Assume Hypothesis* 3.2.1.

(i) Fix $c \in (a,b)$ and $\lambda \in \mathbb{R}$. Then $\tau - \lambda$ is called nonoscillatory at a (resp., b), if

every real-valued solution $u(\lambda,\,\cdot\,)$ *of* $\tau u = \lambda u$ *has finitely many zeros in* (a,c) *(resp.,* (c,b)*). Otherwise,* $\tau - \lambda$ *is called oscillatory at* a *(resp.,* b*).*

(ii) Let $\lambda_0 \in \mathbb{R}$*. Then* T_{min} *is called bounded from below by* λ_0*, and one writes* $T_{min} \geqslant \lambda_0 I_{L^2_r((a,b))}$*, if*

$$\big(u, [T_{min} - \lambda_0 I_{L^2_r((a,b))}]u\big)_{L^2((a,b);rdx)} \geqslant 0, \quad u \in \operatorname{dom}(T_{min}). \tag{3.2.38}$$

The following is a key result.

Theorem 3.2.13. *Assume Hypothesis* 3.2.1*. Then the following items (i)–(iii) are equivalent:*

(i) T_{min} *(and hence any symmetric extension of* T_{min}*) is bounded from below.*

(ii) There exists a $\nu_0 \in \mathbb{R}$ *such that for all* $\lambda < \nu_0$*,* $\tau - \lambda$ *is nonoscillatory at* a *and* b*.*

(iii) For fixed $c, d \in (a,b)$*,* $c \leqslant d$*, there exists a* $\nu_0 \in \mathbb{R}$ *such that for all* $\lambda < \nu_0$*,* $\tau u = \lambda u$ *has (real-valued) nonvanishing solutions* $u_a(\lambda,\,\cdot\,) \neq 0$*,* $\widehat{u}_a(\lambda,\,\cdot\,) \neq 0$ *in the neighborhood* $(a,c]$ *of* a*, and (real-valued) nonvanishing solutions* $u_b(\lambda,\,\cdot\,) \neq 0$*,* $\widehat{u}_b(\lambda,\,\cdot\,) \neq 0$ *in the neighborhood* $[d,b)$ *of* b*, such that*

$$W(\widehat{u}_a(\lambda,\,\cdot\,), u_a(\lambda,\,\cdot\,)) = 1, \quad u_a(\lambda,x) = o(\widehat{u}_a(\lambda,x)) \text{ as } x \downarrow a, \tag{3.2.39}$$

$$W(\widehat{u}_b(\lambda,\,\cdot\,), u_b(\lambda,\,\cdot\,)) = 1, \quad u_b(\lambda,x) = o(\widehat{u}_b(\lambda,x)) \text{ as } x \uparrow b, \tag{3.2.40}$$

$$\int_a^c dx\, p(x)^{-1} u_a(\lambda,x)^{-2} = \int_d^b dx\, p(x)^{-1} u_b(\lambda,x)^{-2} = \infty, \tag{3.2.41}$$

$$\int_a^c dx\, p(x)^{-1} \widehat{u}_a(\lambda,x)^{-2} < \infty, \quad \int_d^b dx\, p(x)^{-1} \widehat{u}_b(\lambda,x)^{-2} < \infty. \tag{3.2.42}$$

Definition 3.2.14. *Assume Hypothesis* 3.2.1*, suppose that* T_{min} *is bounded from below, and let* $\lambda \in \mathbb{R}$*. Then* $u_a(\lambda,\,\cdot\,)$ *(resp.,* $u_b(\lambda,\,\cdot\,)$*) in Theorem* 3.2.13 *(iii) is called a principal (or minimal) solution of* $\tau u = \lambda u$ *at* a *(resp.,* b*). A real-valued solution* $\breve{u}_a(\lambda,\,\cdot\,)$ *(resp.,* $\breve{u}_b(\lambda,\,\cdot\,)$*) of* $\tau u = \lambda u$ *linearly independent of* $u_a(\lambda,\,\cdot\,)$ *(resp.,* $u_b(\lambda,\,\cdot\,)$*) is called nonprincipal at* a *(resp.,* b*). In particular,* $\widehat{u}_a(\lambda,\,\cdot\,)$ *(resp.,* $\widehat{u}_b(\lambda,\,\cdot\,)$*) in* (3.2.39)–(3.2.42) *are nonprincipal solutions at* a *(resp.,* b*).*

Next, we revisit in Theorem 3.2.8 how the generalized boundary values are utilized in the description of all self-adjoint extensions of T_{min} in the case where T_{min} is bounded from below.

Theorem 3.2.15 ([75, Theorem 4.5]). *Assume Hypothesis* 3.2.1 *and that* τ *is in the limit circle case at* a *and* b *(i.e.,* τ *is quasi-regular on* (a,b)*). In addition, assume that* $T_{min} \geqslant \lambda_0 I$ *for some* $\lambda_0 \in \mathbb{R}$*, and denote by* $u_a(\lambda_0,\,\cdot\,)$ *and* $\widehat{u}_a(\lambda_0,\,\cdot\,)$ *(resp.,* $u_b(\lambda_0,\,\cdot\,)$ *and* $\widehat{u}_b(\lambda_0,\,\cdot\,)$*) principal and nonprincipal solutions of* $\tau u = \lambda_0 u$ *at* a *(resp.,* b*), satisfying*

$$W(\widehat{u}_a(\lambda_0,\,\cdot\,), u_a(\lambda_0,\,\cdot\,)) = W(\widehat{u}_b(\lambda_0,\,\cdot\,), u_b(\lambda_0,\,\cdot\,)) = 1. \tag{3.2.43}$$

Introducing $v_j \in \operatorname{dom}(T_{max})$*,* $j = 1, 2,$ *via*

$$v_1(x) = \begin{cases} \widehat{u}_a(\lambda_0, x), & \text{for } x \text{ near } a, \\ \widehat{u}_b(\lambda_0, x), & \text{for } x \text{ near } b, \end{cases} \qquad v_2(x) = \begin{cases} u_a(\lambda_0, x), & \text{for } x \text{ near } a, \\ u_b(\lambda_0, x), & \text{for } x \text{ near } b, \end{cases} \tag{3.2.44}$$

one obtains for all $g \in \operatorname{dom}(T_{max})$*,*

$$\begin{aligned} \widetilde{g}(a) &= -W(v_2, g)(a) = \widetilde{g}_1(a) = -W(u_a(\lambda_0,\,\cdot\,), g)(a) = \lim_{x \downarrow a} \frac{g(x)}{\widehat{u}_a(\lambda_0, x)}, \\ \widetilde{g}(b) &= -W(v_2, g)(b) = \widetilde{g}_1(b) = -W(u_b(\lambda_0,\,\cdot\,), g)(b) = \lim_{x \uparrow b} \frac{g(x)}{\widehat{u}_b(\lambda_0, x)}, \end{aligned} \tag{3.2.45}$$

$$\begin{aligned} \widetilde{g}'(a) &= W(v_1, g)(a) = \widetilde{g}_2(a) = W(\widehat{u}_a(\lambda_0,\,\cdot\,), g)(a) = \lim_{x \downarrow a} \frac{g(x) - \widetilde{g}(a)\widehat{u}_a(\lambda_0, x)}{u_a(\lambda_0, x)}, \\ \widetilde{g}'(b) &= W(v_1, g)(b) = \widetilde{g}_2(b) = W(\widehat{u}_b(\lambda_0,\,\cdot\,), g)(b) = \lim_{x \uparrow b} \frac{g(x) - \widetilde{g}(b)\widehat{u}_b(\lambda_0, x)}{u_b(\lambda_0, x)}. \end{aligned} \tag{3.2.46}$$

In particular, the limits on the right-hand sides in (3.2.45), (3.2.46) *exist.*

Remark 3.2.16. The notion of "generalized boundary values" in (3.2.14) and (3.2.45), (3.2.46) corresponds to "boundary values for τ" in the sense of [51, p. 1297, 1304–1307], see also [70, Sect. 3], [71, p. 57]. $\diamond$

The Friedrichs extension T_F of T_{min} now permits a particularly simple characterization in terms of the generalized boundary values $\widetilde{g}(a), \widetilde{g}(b)$ as derived by Niessen and Zettl [150](see also [81], [107], [108], [112], [139], [160], [163], [181]):

Theorem 3.2.17. *Assume Hypothesis* 3.2.1 *and that τ is in the limit circle case at a and b (i.e., τ is quasi-regular on (a, b)). In addition, assume that $T_{min} \geqslant \lambda_0 I$ for some $\lambda_0 \in \mathbb{R}$. Then the Friedrichs extension $T_F = T_{0,0}$ of T_{min} is characterized by*

$$T_F f = \tau f, \quad f \in \operatorname{dom}(T_F) = \big\{g \in \operatorname{dom}(T_{max}) \,\big|\, \widetilde{g}(a) = \widetilde{g}(b) = 0\big\}. \tag{3.2.47}$$

Remark 3.2.18. (i) As in (3.2.20), one readily verifies for $g, h \in \operatorname{dom}(T_{max})$,

$$\widetilde{g}(d)\widetilde{h}'(d) - \widetilde{g}'(d)\widetilde{h}(d) = W(g, h)(d), \quad d \in \{a, b\}, \tag{3.2.48}$$

again interpreted in the sense that either side in (3.2.48) has a finite limit as $d \downarrow a$ and $d \uparrow b$.

(ii) As always in this context (cf. Remark 3.2.9 (i)), if τ is in the limit point case at one (or both) interval endpoints, the corresponding boundary conditions at that endpoint are dropped in Theorems 3.2.15 and 3.2.17. ⋄

3.3 Krein Resolvent Identities: One Limit Circle Endpoint

Assuming that τ is in the limit circle case at a and in the limit point case at b, we derive in this section the Krein resolvent formulas for all self-adjoint extensions of T_{min} using the Friedrichs extension as the reference operator.

Hypothesis 3.3.1. *In addition to Hypothesis* 3.2.1 *assume that τ is in the limit circle case at a and in the limit point case at b. Moreover, for $z \in \rho(T_0)$, let $\psi(z, \cdot\,)$ denote the unique solution to $(\tau - z)y = 0$ that satisfies $\psi(z, \cdot\,) \in L^2_r((a, b))$ and $\widetilde{\psi}(z, a) = 1$.*

Assume Hypothesis 3.3.1. By Theorem 3.2.8 or Theorem 3.2.15, the following statements (i) and (ii) hold.

(i) If $\alpha \in [0, \pi)$, then the operator T_α defined by

$$\begin{aligned} &T_\alpha f = T_{max} f, \\ &f \in \operatorname{dom}(T_\alpha) = \{g \in \operatorname{dom}(T_{max}) \,|\, \cos(\alpha)\widetilde{g}(a) + \sin(\alpha)\widetilde{g}'(a) = 0\} \end{aligned} \tag{3.3.1}$$

is a self-adjoint extension of T_{min}.

(ii) If T is a self-adjoint extension of T_{min}, then $T = T_\alpha$ for some $\alpha \in [0, \pi)$.

Statements analogous to (i) and (ii) hold if τ is in the limit point case at a and in the limit circle case at b; for brevity we omit the details.

Choosing $\alpha = 0$ in (3.3.1) yields the self-adjoint extension T_0 with a Dirichlet-type boundary condition at a:

$$\operatorname{dom}(T_0) = \{g \in \operatorname{dom}(T_{max}) \,|\, \widetilde{g}(a) = 0\}. \tag{3.3.2}$$

Since the coefficients p, q, and r are real-valued, the solution $\psi(z, \cdot\,)$ has the following conjugation property:

$$\overline{\psi(z, \cdot\,)} = \psi(\overline{z}, \cdot\,), \quad z \in \rho(T_0). \tag{3.3.3}$$

Theorem 3.3.2. *Assume Hypothesis* 3.3.1. *If $\alpha \in (0, \pi)$, then T_0 and T_α are relatively prime with respect to $T_{\min}$. Moreover, for each $z \in \rho(T_0) \cap \rho(T_\alpha)$, the scalar*

$$k_\alpha(z) = -\cot(\alpha) - \widetilde{\psi}'(z, a) \tag{3.3.4}$$

is nonzero and

$$(T_\alpha - zI_{L^2_r((a,b))})^{-1} = (T_0 - zI_{L^2_r((a,b))})^{-1} + k_\alpha(z)^{-1}(\psi(\overline{z}, \cdot\,), \cdot\,)_{L^2_r((a,b))}\psi(z, \cdot\,). \tag{3.3.5}$$

Proof. The claims follow as a direct application of [2, Theorem 3.4] which is stated in terms of boundary conditions bases and the Lagrange bracket. The condition

$$W(\widehat{u}_a(\lambda_0, \cdot\,), u_a(\lambda_0, \cdot\,)) = 1 \tag{3.3.6}$$

implies

$$\{u_a(\lambda_0, \cdot\,), \widehat{u}_a(\lambda_0, \cdot\,)\} \text{ is a boundary condition basis at } x = a \tag{3.3.7}$$

in the sense of [2, Definition 2.15] and [182, Definition 10.4.3]. The generalized boundary values take the form

$$[g, u_a(\lambda_0, \cdot\,)](a) = \widetilde{g}(a), \quad [g, \widehat{u}_a(\lambda_0, \cdot\,)](a) = -\widetilde{g}'(a), \tag{3.3.8}$$

where $[\,\cdot\,, \cdot\,]$ denotes the Lagrange bracket:

$$[f, g](x) = f(x)\overline{(pg')(x)} - (pf')(x)\overline{g(x)}, \quad x \in (a, b). \tag{3.3.9}$$

Using the boundary condition basis in (3.3.7) and the identities in (3.3.8), the claims now follow from [2, Theorem 3.4] after a standard reparametrizion of the self-adjoint extensions (3.3.1) to fit the parametrization used in [2, Theorem 2.19]. □

3.4 Krein Resolvent Identities: Two Limit Circle Endpoints

Assuming that τ is in the limit circle case at a and b, we now derive the Krein resolvent formulas for all self-adjoint extensions of T_{min} using once more the Friedrichs extension as the reference operator (in this context we also refer to [34]).

Hypothesis 3.4.1. *In addition to Hypothesis* 3.2.1 *assume that* τ *is in the limit circle case at* a *and* b. *Moreover, for* $z \in \rho(T_{0,0})$, *let* $\{u_j(z, \cdot\,)\}_{j=1,2}$ *denote solutions to* $\tau u = zu$ *which satisfy the boundary conditions*

$$\begin{aligned} &\widetilde{u}_1(z, a) = 0, \quad \widetilde{u}_1(z, b) = 1, \\ &\widetilde{u}_2(z, a) = 1, \quad \widetilde{u}_2(z, b) = 0. \end{aligned} \tag{3.4.1}$$

Assume Hypotheses 3.4.1. By Theorem 3.2.8 or Theorem 3.2.15, the following statements (i)–(iii) hold.

(i) If $\alpha, \beta \in [0, \pi)$, then the operator $T_{\alpha,\beta}$ defined by

$$T_{\alpha,\beta} f = T_{max} f, \tag{3.4.2}$$

$$f \in \operatorname{dom}(T_{\alpha,\beta}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{array}{c} \cos(\alpha)\widetilde{g}(a) + \sin(\alpha)\widetilde{g}'(a) = 0, \\ \cos(\beta)\widetilde{g}(b) + \sin(\beta)\widetilde{g}'(b) = 0 \end{array} \right\},$$

is a self-adjoint extension of T_{min}.

(ii) If $\varphi \in [0, \pi)$ and $R \in SL(2, \mathbb{R})$, then the operator $T_{\varphi,R}$ defined by

$$
\begin{aligned}
&T_{\varphi,R} f = T_{max} f, \\
&f \in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{pmatrix} \widetilde{g}(b) \\ \widetilde{g}'(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} \widetilde{g}(a) \\ \widetilde{g}'(a) \end{pmatrix} \right\},
\end{aligned} \tag{3.4.3}
$$

is a self-adjoint extension of T_{min}.

(iii) If T is a self-adjoint extension of T_{min}, then $T = T_{\alpha,\beta}$ for some $\alpha, \beta \in [0, \pi)$ or $T = T_{\varphi,R}$ for some $\varphi \in [0, \pi)$ and some $R \in SL(2, \mathbb{R})$.

Notational Convention. *To describe all possible self-adjoint boundary conditions associated with self-adjoint extensions of T_{min} effectively, we will frequently employ the notation $T_{A,B}$, $M_{A,B}^{Do}(\,\cdot\,)$, etc., where A, B represents α, β in the case of separated boundary conditions and φ, R in the context of coupled boundary conditions.*

Choosing $\alpha = \beta = 0$ in (3.4.2) yields the self-adjoint extension with Dirichlet-type boundary conditions at a and b:

$$
\operatorname{dom}(T_{0,0}) = \{ g \in \operatorname{dom}(T_{max}) \,|\, \widetilde{g}(a) = \widetilde{g}(b) = 0 \}. \tag{3.4.4}
$$

Since the coefficients of the Sturm–Liouville differential expression are real, the following conjugation property holds:

$$
\overline{u_j(z,\,\cdot\,)} = u_j(\overline{z},\,\cdot\,), \quad z \in \rho(T_{0,0}),\ j \in \{1, 2\}. \tag{3.4.5}
$$

Applying (3.4.1), one computes

$$
\begin{aligned}
&W(u_1(z,\,\cdot\,), u_2(z,\,\cdot\,)(a) = -\widetilde{u}_1'(z, a), \\
&W(u_1(z,\,\cdot\,), u_2(z,\,\cdot\,)(b) = \widetilde{u}_2'(z, b), \quad z \in \rho(T_{0,0}).
\end{aligned} \tag{3.4.6}
$$

In particular, since the Wronskian of two solutions is constant,

$$
\widetilde{u}_2'(z, b) = -\widetilde{u}_1'(z, a), \quad z \in \rho(T_{0,0}). \tag{3.4.7}
$$

Theorem 3.4.2. *Assume Hypothesis* 3.4.1. *Then the following statements* (i)–(v) *hold.*

(i) *If $\alpha, \beta \in (0, \pi)$, then $T_{0,0}$ and $T_{\alpha,\beta}$ are relatively prime with respect to T_{min}.*

Moreover, for each $z \in \rho(T_{0,0}) \cap \rho(T_{\alpha,\beta})$ *the matrix*

$$K_{\alpha,\beta}(z) = \begin{pmatrix} \cot(\beta) + \widetilde{u}_1'(z,b) & -\widetilde{u}_1'(z,a) \\ \\ \widetilde{u}_2'(z,b) & -\cot(\alpha) - \widetilde{u}_2'(z,a) \end{pmatrix} \tag{3.4.8}$$

is invertible and

$$\begin{aligned}(T_{\alpha,\beta} - zI_{L_r^2((a,b))})^{-1} &= (T_{0,0} - zI_{L_r^2((a,b))})^{-1} \\ &\quad + \sum_{j,k=1}^{2} \left[K_{\alpha,\beta}(z)^{-1}\right]_{j,k} (u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))} u_k(z,\,\cdot\,). \end{aligned} \tag{3.4.9}$$

(ii) If $\beta \in (0,\pi)$*, then the maximal common part of* $T_{0,0}$ *and* $T_{0,\beta}$ *is the restriction of* T_{max} *to the set*

$$\mathcal{S}_1 = \{y \in \operatorname{dom}(T_{max}) \,|\, \widetilde{y}(a) = \widetilde{y}(b) = \widetilde{y}'(b) = 0\}. \tag{3.4.10}$$

Moreover, for each $z \in \rho(T_{0,0}) \cap \rho(T_{0,\beta})$ *the scalar*

$$K_{0,\beta}(z) = \cot(\beta) + \widetilde{u}_1'(z,b) \tag{3.4.11}$$

is nonzero and

$$\begin{aligned}&(T_{0,\beta} - zI_{L_r^2((a,b))})^{-1} \\ &\quad = (T_{0,0} - zI_{L_r^2((a,b))})^{-1} + K_{0,\beta}(z)^{-1}(u_1(\overline{z},\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))} u_1(z,\,\cdot\,).\end{aligned} \tag{3.4.12}$$

(iii) If $\alpha \in (0,\pi)$*, then the maximal common part of* $T_{0,0}$ *and* $T_{\alpha,0}$ *is the restriction of* T_{max} *to the set*

$$\mathcal{S}_2 = \{y \in \operatorname{dom}(T_{max}) \,|\, \widetilde{y}(a) = \widetilde{y}(b) = \widetilde{y}'(a) = 0\}. \tag{3.4.13}$$

Moreover, for each $z \in \rho(T_{0,0}) \cap \rho(T_{\alpha,0})$ *the scalar*

$$K_{\alpha,0}(z) = -\cot(\alpha) - \widetilde{u}_2'(z,a) \tag{3.4.14}$$

is nonzero and

$$\begin{aligned}&(T_{\alpha,0} - zI_{L_r^2((a,b))})^{-1} \\ &\quad = (T_{0,0} - zI_{L_r^2((a,b))})^{-1} + K_{\alpha,0}(z)^{-1}(u_2(\overline{z},\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))} u_2(z,\,\cdot\,).\end{aligned} \tag{3.4.15}$$

(iv) If $R_{1,2} \neq 0$, then $T_{0,0}$ and $T_{\varphi,R}$ are relatively prime with respect to T_{min}. Moreover, for each $z \in \rho(T_{0,0}) \cap \rho(T_{\varphi,R})$ the matrix

$$K_{\varphi,R}(z) = \begin{pmatrix} -\dfrac{R_{2,2}}{R_{1,2}} + \widetilde{u}_1'(z,b) & \dfrac{e^{-i\varphi}}{R_{1,2}} - \widetilde{u}_1'(z,a) \\ \dfrac{e^{i\varphi}}{R_{1,2}} + \widetilde{u}_2'(z,b) & -\dfrac{R_{1,1}}{R_{1,2}} - \widetilde{u}_2'(z,a) \end{pmatrix} \tag{3.4.16}$$

is invertible and

$$\begin{aligned} (T_{\varphi,R} - zI_{L_r^2((a,b))})^{-1} &= (T_{0,0} - zI_{L_r^2((a,b))})^{-1} \\ &\quad + \sum_{j,k=1}^{2} \left[K_{\varphi,R}(z)^{-1}\right]_{j,k} (u_j(\overline{z}, \cdot\,), \cdot\,)_{L_r^2((a,b))} u_k(z, \cdot\,). \end{aligned} \tag{3.4.17}$$

(v) If $R_{1,2} = 0$, then the maximal common part of $T_{\varphi,R}$ and $T_{0,0}$ is the restriction of T_{max} to the set

$$\mathcal{S}_{\varphi,R} = \{y \in \operatorname{dom}(T_{max}) \,|\, \widetilde{y}(a) = \widetilde{y}(b) = 0,\, \widetilde{y}'(b) = e^{i\varphi} R_{2,2} \widetilde{y}'(a)\}. \tag{3.4.18}$$

Moreover, for each $z \in \rho(T_{0,0}) \cap \rho(T_{\varphi,R})$, the scalar

$$k_{\varphi,R}(z) = -R_{2,1}R_{2,2} - e^{i\varphi} R_{2,2} \widetilde{u}_{\varphi,R}'(z,a) + \widetilde{u}_{\varphi,R}'(z,b) \tag{3.4.19}$$

is nonzero, and

$$\begin{aligned} (T_{\varphi,R} - zI_{L_r^2((a,b))})^{-1} &= (T_{0,0} - zI_{L_r^2((a,b))})^{-1} \\ &\quad + k_{\varphi,R}(z)^{-1} (u_{\varphi,R}(\overline{z}, \cdot\,), \cdot\,)_{L_r^2((a,b))} u_{\varphi,R}(z, \cdot\,), \end{aligned} \tag{3.4.20}$$

where

$$u_{\varphi,R}(\zeta, \cdot\,) = e^{-i\varphi} R_{2,2} u_2(\zeta, \cdot\,) + u_1(\zeta, \cdot\,), \quad \zeta \in \rho(T_{0,0}). \tag{3.4.21}$$

Proof. Statements *(i)*–*(v)* are direct applications of the Krein identities for singular Sturm–Liouville operators obtained in [2] which are stated in terms of boundary conditions bases and the Lagrange bracket. The conditions

$$W(\widehat{u}_a(\lambda_0, \cdot\,), u_a(\lambda_0, \cdot\,)) = W(\widehat{u}_b(\lambda_0, \cdot\,), u_b(\lambda_0, \cdot\,)) = 1 \tag{3.4.22}$$

imply that

$$\{u_c(\lambda_0, \cdot\,), \widehat{u}_c(\lambda_0, \cdot\,)\} \text{ is a boundary condition basis at } x = c \text{ for } c \in \{a, b\} \tag{3.4.23}$$

in the sense of [2, Definition 2.15] and [182, Definition 10.4.3]. The generalized boundary values take the form

$$\begin{aligned} &[g, u_a(\lambda_0, \cdot\,)](a) = \widetilde{g}(a), \quad [g, u_b(\lambda_0, \cdot\,)](b) = \widetilde{g}(b), \\ &[g, \widehat{u}_a(\lambda_0, \cdot\,)](a) = -\widetilde{g}'(a), \quad [g, \widehat{u}_b(\lambda_0, \cdot\,)](b) = -\widetilde{g}'(b), \end{aligned} \tag{3.4.24}$$

where $[\,\cdot\,,\,\cdot\,]$ denotes the Lagrange bracket (see (3.3.9)). Using the boundary condition bases in (3.4.23) and the identities in (3.4.24), statements (i)–(v) now follow from [2, Theorems 4.4, 4.5, 4.6, and 4.7] after a standard reparametrizion of the self-adjoint extensions (3.4.2) and (3.4.3) to fit the parametrization used in [2, Theorem 2.20]. $\square$

Remark 3.4.3. As an illustration of Theorem 3.4.2, we consider the Krein extension, T_{0,R_K}, under the additional assumption that $T_{min} \geqslant \varepsilon I_{L^2_r((a,b))}$ for some $\varepsilon > 0$. Then applying [68, Thm. 3.5 (ii)] and Theorem 3.4.2 (iv), one computes for the matrix K_{0,R_K} in (3.4.16),

$$K_{0,R_K}(z) = \begin{pmatrix} \widetilde{u}_1'(z,b) - \widetilde{u}_1'(0,b) & \widetilde{u}_1'(0,a) - \widetilde{u}_1'(z,a) \\ \\ \widetilde{u}_2'(z,b) - \widetilde{u}_2'(0,b) & \widetilde{u}_2'(0,a) - \widetilde{u}_2'(z,a) \end{pmatrix}, \quad z \in \rho(T_{0,0}) \cap \rho(T_{0,R_K}), \tag{3.4.25}$$

where we note that $0 \in \sigma(T_{0,R_K})$. $\diamond$

3.5 Donoghue m-functions: One Limit Circle Endpoint

In this section we construct the Donoghue m-functions in the case where τ is in the limit circle case at precisely one endpoint (which we choose to be a without loss of generality). We first focus on the Friedrichs extension of T_{min} and then use the Krein resolvent formulas from Section 3.3 to treat all remaining self-adjoint extensions of T_{min}.

Throughout this section we shall assume that Hypothesis 3.3.1 holds so that τ is in the limit circle case at a and in the limit point case at b. We begin by obtaining a general expression for the Donoghue m-function of an arbitrary self-adjoint extension

T_α of T_{min} in terms of a unit vector $\phi(i,\,\cdot\,) \in \mathcal{N}_i$. This general expression will then be made more explicit in terms of $\psi(i,\,\cdot\,)$ (cf. Hypothesis 3.3.1) in the analysis below. The Donoghue m-function for T_α is given by (see, e.g., [78, Eq. (5.5)])

$$\begin{aligned} M_{T_\alpha,\mathcal{N}_i}^{Do}(z) &= P_{\mathcal{N}_i}\big(zT_\alpha + I_{L_r^2((a,b))}\big)(T_\alpha - zI_{L_r^2((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i} \\ &= zI_{\mathcal{N}_i} + \big(z^2+1\big)P_{\mathcal{N}_i}(T_\alpha - zI_{L_r^2((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{3.5.1}$$

where $P_{\mathcal{N}_i}$ denotes the orthogonal projection onto $\mathcal{N}_i$. According to (3.5.1),

$$M_{T_\alpha,\mathcal{N}_i}^{Do}(z) \in \mathcal{B}(\mathcal{N}_i),\ \ z \in \mathbb{C}\backslash\mathbb{R},\ \text{ and } M_{T_\alpha,\mathcal{N}_i}^{Do}(\pm i) = \pm i I_{\mathcal{N}_i}. \tag{3.5.2}$$

The unit vector $\phi(i,\,\cdot\,)$ spans the one-dimensional subspace $\mathcal{N}_i$, so the orthogonal projection onto $\mathcal{N}_i$ is

$$P_{\mathcal{N}_i} = (\phi(i,\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))}\phi(i,\,\cdot\,). \tag{3.5.3}$$

Thus, the action of $M_{T_\alpha,\mathcal{N}_i}^{Do}(\,\cdot\,)$ may be computed directly in terms of $\phi(i,\,\cdot\,)$ as follows:

$$\begin{aligned} &M_{T_\alpha,\mathcal{N}_i}^{Do}(z)f \\ &\quad = \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)P_{\mathcal{N}_i}(T_\alpha - zI_{L_r^2((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}\big]f \\ &\quad = zf + \big(z^2+1\big)P_{\mathcal{N}_i}(T_\alpha - zI_{L_r^2((a,b))})^{-1}f \\ &\quad = \big(\phi(i,\,\cdot\,), \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)(T_\alpha - zI_{L_r^2((a,b))})^{-1}\big]f\big)_{L_r^2((a,b))}\phi(i,\,\cdot\,) \\ &\quad = \big(\phi(i,\,\cdot\,), \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)(T_\alpha - zI_{L_r^2((a,b))})^{-1}\big]\phi(i,\,\cdot\,)\big)_{L_r^2((a,b))} \\ &\qquad \times (\phi(i,\,\cdot\,), f)_{L_r^2((a,b))}\phi(i,\,\cdot\,) \\ &\quad = \big[z + \big(z^2+1\big)\big(\phi(i,\,\cdot\,), (T_\alpha - zI_{L_r^2((a,b))})^{-1}\phi(i,\,\cdot\,)\big)_{L_r^2((a,b))}\big] \\ &\qquad \times (\phi(i,\,\cdot\,), f)_{L_r^2((a,b))}\phi(i,\,\cdot\,), \quad f \in \mathcal{N}_i,\ z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{3.5.4}$$

where one uses $f = (\phi(i,\,\cdot\,), f)_{L_r^2((a,b))}\phi(i,\,\cdot\,)$ to obtain the fourth equality in (3.5.4). Hence,

$$\begin{aligned} M_{T_\alpha,\mathcal{N}_i}^{Do}(z) &= \big[z + \big(z^2+1\big)\big(\phi(i,\,\cdot\,), (T_\alpha - zI_{L_r^2((a,b))})^{-1}\phi(i,\,\cdot\,)\big)_{L_r^2((a,b))}\big] \\ &\qquad \times (\phi(i,\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))}\phi(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{3.5.5}$$

In order to determine $M^{Do}_{T_\alpha,\mathcal{N}_i}(\,\cdot\,)$ in terms of $\psi(i,\,\cdot\,)$, one must compute the fixed inner product in (3.5.5). That is, one must compute

$$\big(\phi(i,\,\cdot\,),(T_\alpha - zI_{L^2_r((a,b))})^{-1}\phi(i,\,\cdot\,)\big)_{L^2_r((a,b))}, \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{3.5.6}$$

In light of (3.5.2), it suffices to compute (3.5.6) under the additional assumption that $z\neq\pm i$. We will first do this for the Dirichlet-type extension T_0 (cf. (3.3.2)).

3.5.1 The Donoghue m-function $M^{Do}_{T_0,\mathcal{N}_i}(\,\cdot\,)$ for T_0

Here we shall consider the Dirichlet-type self-adjoint extension T_0 of T_{min}. Assuming Hypothesis 3.3.1 and taking

$$T_\alpha = T_0 \quad\text{and}\quad \phi(i,\,\cdot\,) := \|\psi(i,\,\cdot\,)\|^{-1}_{L^2_r((a,b))}\psi(i,\,\cdot\,), \tag{3.5.7}$$

we shall compute the inner product (3.5.6) and use (3.5.5) to obtain an explicit expression for the Donoghue m-function $M^{Do}_{T_0,\mathcal{N}_i}(\,\cdot\,)$ for T_0 in terms of $\psi(i,\,\cdot\,)$.

For the purposes of evaluating the inner product (3.5.6), we introduce the generalized Cayley transform of T_0,

$$\begin{aligned} U_{0,z,z'} &= (T_0 - z'I_{L^2_r((a,b))})(T_0 - zI_{L^2_r((a,b))})^{-1} \\ &= I_{L^2_r((a,b))} + (z-z')(T_0 - zI_{L^2_r((a,b))})^{-1}, \quad z,z'\in\rho(T_0), \end{aligned} \tag{3.5.8}$$

which forms a bijection from $\mathcal{N}_{z'}$ to $\mathcal{N}_z$. One verifies that

$$U_{0,z,z'}\psi(z',\,\cdot\,) = \psi(z,\,\cdot\,), \quad z,z'\in\rho(T_0). \tag{3.5.9}$$

In fact, for fixed $z,z'\in\rho(T_0)$, one uses the fact that $U_{0,z,z'}$ maps into $\mathcal{N}_z$ to write

$$U_{0,z,z'}\psi(z',\,\cdot\,) = c_0\psi(z,\,\cdot\,) \tag{3.5.10}$$

for some scalar $c_0\in\mathbb{C}$. The second equality in (3.5.8) then implies

$$U_{0,z,z'}\psi(z',\,\cdot\,) = \psi(z',\,\cdot\,) + (z-z')(T_0 - zI_{L^2_r((a,b))})^{-1}\psi(z',\,\cdot\,), \tag{3.5.11}$$

so that

$$[U_{0,z,z'}\psi(z',\,\cdot\,)]\widetilde{\ }(a) = \widetilde{\psi}(z',a) = 1. \tag{3.5.12}$$

Taking the generalized boundary value at a throughout (3.5.10) and using (3.5.12) yields $c_0 = 1$ in (3.5.10), and (3.5.9) follows.

Let $z \in \mathbb{C}\backslash\mathbb{R}$ with $z \neq \pm i$ be fixed. Applying (3.5.8), one computes:

$$\begin{aligned}
&\big(\phi(i,\,\cdot\,), (T_0 - zI_{L_r^2((a,b))})^{-1}\phi(i,\,\cdot\,)\big)_{L_r^2((a,b))} \\
&\quad = \frac{\big(\psi(i,\,\cdot\,), (T_0 - zI_{L_r^2((a,b))})^{-1}\psi(i,\,\cdot\,)\big)_{L_r^2((a,b))}}{\|\psi(i,\,\cdot\,)\|_{L_r^2((a,b))}^2} \\
&\quad = \frac{(\psi(i,\,\cdot\,), [U_{0,z,i} - I_{L_r^2((a,b))}]\psi(i,\,\cdot\,))_{L_r^2((a,b))}}{(z-i)\|\psi(i,\,\cdot\,)\|_{L_r^2((a,b))}^2} \\
&\quad = \frac{1}{i-z} + \frac{(\psi(i,\,\cdot\,), \psi(z,\,\cdot\,))_{L_r^2((a,b))}}{(z-i)\|\psi(i,\,\cdot\,)\|_{L_r^2((a,b))}^2}.
\end{aligned} \tag{3.5.13}$$

Furthermore, by (3.2.3) and Theorem 3.2.7 (i),

$$\begin{aligned}
&(\psi(i,\,\cdot\,), \psi(z,\,\cdot\,))_{L_r^2((a,b))} = \int_a^b r(x)dx\,\psi(-i,x)\psi(z,x) \\
&\quad = -\frac{W(\psi(-i,\,\cdot\,), \psi(z,\,\cdot\,))|_a^b}{z+i} = \frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{z+i},
\end{aligned} \tag{3.5.14}$$

where we have used that since τ is in the limit point case at b and $\psi(-i,\,\cdot\,), \psi(z,\,\cdot\,) \in \operatorname{dom}(T_{max})$, an application of Theorem 3.2.7 (i) yields

$$W(\psi(-i,\,\cdot\,), \psi(z,\,\cdot\,))(b) = 0, \tag{3.5.15}$$

and by Hypothesis 3.3.1, $\widetilde{\psi}(-i,a) = \widetilde{\psi}(z,a) = 1$, so that

$$W(\psi(-i,\,\cdot\,), \psi(z,\,\cdot\,))(a) = \widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a). \tag{3.5.16}$$

Therefore, (3.5.13)–(3.5.16) yield

$$\big(\phi(i,\,\cdot\,), (T_0 - zI_{L_r^2((a,b))})^{-1}\phi(i,\,\cdot\,)\big)_{L_r^2((a,b))} = \frac{1}{i-z} + \frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{\big(z^2+1\big)\|\psi(i,\,\cdot\,)\|_{L_r^2((a,b))}^2}. \tag{3.5.17}$$

By (3.2.3), Hypothesis 3.3.1, and the limit point assumption at b,

$$\begin{aligned}
&\|\psi(i,\,\cdot\,)\|_{L_r^2((a,b))}^2 = \int_a^b r(x)dx\,\psi(-i,x)\psi(i,x) = -\frac{W(\psi(-i,\,\cdot\,), \psi(i,\,\cdot\,))|_a^b}{2i} \\
&\quad = \frac{1}{2i}\big[\widetilde{\psi}'(i,a) - \widetilde{\psi}'(-i,a)\big] = \operatorname{Im}\big(\widetilde{\psi}'(i,a)\big).
\end{aligned} \tag{3.5.18}$$

Applying (3.5.17) in (3.5.4) and taking simplifications and (3.5.18) into account, one obtains the following fact.

Theorem 3.5.1. *Assume Hypothesis* 3.3.1. *The Donoghue m-function* $M^{Do}_{T_0,\mathcal{N}_i}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* T_0 *satisfies*

$$\begin{aligned} &M^{Do}_{T_0,\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}, \\ &M^{Do}_{T_0,\mathcal{N}_i}(z) = \left[-i + \frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{\operatorname{Im}\big(\widetilde{\psi}'(i,a)\big)} \right] I_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R},\, z \neq \pm i. \end{aligned} \tag{3.5.19}$$

3.5.2 The Donoghue m-function for Self-Adjoint Extensions Other Than T_0

The Donoghue m-function for T_0 was computed explicitly in Theorem 3.5.1. If T_α, $\alpha \in (0,\pi)$, is any other self-adjoint extension of T_{min}, then the resolvent identity in Theorem 3.3.2 may be used to obtain an explicit representation of the Donoghue m-function $M^{Do}_{T_\alpha,\mathcal{N}_i}(\,\cdot\,)$ for T_α.

Theorem 3.5.2. *Assume Hypothesis* 3.3.1 *and let* $\alpha \in (0,\pi)$. *The Donoghue m-function* $M^{Do}_{T_\alpha,\mathcal{N}_i}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* T_α *satisfies*

$$\begin{aligned} M^{Do}_{T_\alpha,\mathcal{N}_i}(\pm i) &= \pm i I_{\mathcal{N}_i}, \\ M^{Do}_{T_\alpha,\mathcal{N}_i}(z) &= M^{Do}_{T_0,\mathcal{N}_i}(z) \\ &\quad + (i-z)\frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{\cot(\alpha) + \widetilde{\psi}'(z,a)} (\psi(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\psi(i,\,\cdot\,)\Big|_{\mathcal{N}_i}, \\ &\qquad z \in \mathbb{C}\backslash\mathbb{R},\, z \neq \pm i. \end{aligned} \tag{3.5.20}$$

Proof. Let $\alpha \in (0,\pi)$ be fixed. By (3.5.2), $M^{Do}_{T_\alpha,\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}$. In order to establish (3.5.20), let $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$, be fixed. Considering (3.5.1) and invoking (3.3.5), one obtains

$$\begin{aligned} M^{Do}_{T_\alpha,\mathcal{N}_i}(z) &= M^{Do}_{T_0,\mathcal{N}_i}(z) + \big(z^2+1\big)k_\alpha(z)^{-1}(\psi(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}P_{\mathcal{N}_i}\psi(z,\,\cdot\,)\big|_{\mathcal{N}_i} \quad (3.5.21) \\ &= M^{Do}_{T_0,\mathcal{N}_i}(z) \\ &\quad + \big(z^2+1\big)k_\alpha(z)^{-1}(\psi(i,\,\cdot\,),\psi(z,\,\cdot\,))_{L^2_r((a,b))}(\psi(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\psi(i,\,\cdot\,)\big|_{\mathcal{N}_i}. \end{aligned}$$

Using (3.5.14) in (3.5.21), one obtains

$$M^{Do}_{T_\alpha,\mathcal{N}_i}(z) = M^{Do}_{T_0,\mathcal{N}_i}(z) \tag{3.5.22}$$
$$+ (z-i)\frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{k_\alpha(z)}(\psi(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\psi(i,\,\cdot\,)\bigg|_{\mathcal{N}_i}.$$

Finally, (3.5.20) follows from (3.5.22) after using the form for $k_\alpha(z)$ in (3.3.4). $\square$

3.6 Donoghue m-functions: Two Limit Circle Endpoints

The construction of Donoghue m-functions in the case where τ is in the limit circle case at a and b is the primary aim of this section. Once more we first focus on the Friedrichs extension of T_{min} and then use the Krein resolvent formulas from Section 3.4 to treat all remaining self-adjoint extensions of T_{min}.

Throughout this section, we shall assume that Hypothesis 3.4.1 holds so that τ is in the limit circle case at a and b. We begin by obtaining a general expression for the Donoghue m-function of an arbitrary self-adjoint extension $T_{A,B}$ of T_{min} in terms of an orthonormal basis for $\mathcal{N}_i$. Recall that the Donoghue m-function for $T_{A,B}$ is given by (see, e.g., [78, Eq. (5.5)])

$$\begin{aligned} M^{Do}_{T_{A,B},\mathcal{N}_i}(z) &= P_{\mathcal{N}_i}(zT_{A,B} + I_{L^2_r((a,b))})(T_{A,B} - zI_{L^2_r((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i} \qquad (3.6.1)\\ &= zI_{\mathcal{N}_i} + \big(z^2+1\big)P_{\mathcal{N}_i}(T_{A,B} - zI_{L^2_r((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}, \quad z\in\mathbb{C}\backslash\mathbb{R}, \end{aligned}$$

where $P_{\mathcal{N}_i}$ denotes the orthogonal projection onto $\mathcal{N}_i$ with $M^{Do}_{T_{A,B},\mathcal{N}_i}(z) \in \mathcal{B}(\mathcal{N}_i)$, $z\in\mathbb{C}\backslash\mathbb{R}$, and

$$M^{Do}_{T_{A,B},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}. \tag{3.6.2}$$

Let $\{v_j\}_{j=1,2}$ be an orthonormal basis for the subspace $\mathcal{N}_i$. The orthogonal projection onto $\mathcal{N}_i$ is

$$P_{\mathcal{N}_i} = \sum_{k=1}^{2}(v_k,\,\cdot\,)_{L^2_r((a,b))}v_k. \tag{3.6.3}$$

Therefore, the action of $M_{T_{A,B},\mathcal{N}_i}^{Do}(\,\cdot\,)$ may be computed directly in terms of $\{v_j\}_{j=1,2}$ as follows:

$$\begin{aligned}
M_{T_{A,B},\mathcal{N}_i}^{Do}(z)f &= \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)P_{\mathcal{N}_i}(T_{A,B} - zI_{L_r^2((a,b))})^{-1}P_{\mathcal{N}_i}\big|_{\mathcal{N}_i}\big]f \qquad (3.6.4)\\
&= zf + \big(z^2+1\big)P_{\mathcal{N}_i}(T_{A,B} - zI_{L_r^2((a,b))})^{-1}f\\
&= \sum_{j=1}^{2}\big(v_j, \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)(T_{A,B} - zI_{L_r^2((a,b))})^{-1}\big]f\big)_{L_r^2((a,b))}v_j\\
&= \sum_{j,k=1}^{2}\big(v_j, \big[zI_{\mathcal{N}_i} + \big(z^2+1\big)(T_{A,B} - zI_{L_r^2((a,b))})^{-1}\big]v_k\big)_{L_r^2((a,b))}(v_k, f)_{L_r^2((a,b))}v_j\\
&= \sum_{j,k=1}^{2}\big[z\delta_{j,k} + \big(z^2+1\big)\big(v_j, (T_{A,B} - zI_{L_r^2((a,b))})^{-1}v_k\big)_{L_r^2((a,b))}\big](v_k, f)_{L_r^2((a,b))}v_j,\\
&\qquad\qquad f \in \mathcal{N}_i,\ z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned}$$

where one uses $f = \sum_{j=1}^{2}(v_j, f)_{L_r^2((a,b))}v_j$ to obtain the fourth equality in (3.6.4). Hence,

$$\begin{aligned}
&M_{T_{A,B},\mathcal{N}_i}^{Do}(z) \qquad (3.6.5)\\
&\quad = \sum_{j,k=1}^{2}\big[z\delta_{j,k} + \big(z^2+1\big)\big(v_j, (T_{A,B} - zI_{L_r^2((a,b))})^{-1}v_k\big)_{L_r^2((a,b))}\big](v_k,\,\cdot\,)_{L_r^2((a,b))}v_j\big|_{\mathcal{N}_i},\\
&\qquad\qquad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned}$$

In order to determine $M_{T_{A,B},\mathcal{N}_i}^{Do}(\,\cdot\,)$ in terms of the orthonormal basis $\{v_j\}_{j=1,2}$, one must compute the fixed inner products in (3.6.5). That is, one must compute

$$\big(v_j, (T_{A,B} - zI_{L_r^2((a,b))})^{-1}v_k\big)_{L_r^2((a,b))}, \quad j,k \in \{1,2\},\ z \in \mathbb{C}\backslash\mathbb{R}. \qquad (3.6.6)$$

In light of (3.6.2), it suffices to compute (3.6.6) under the additional assumption that $z \neq \pm i$. We will first do this for the Dirichlet-type extension $T_{0,0}$ (cf. (3.4.4)).

3.6.1 The Donoghue m-function $M_{T_{0,0},\mathcal{N}_i}^{Do}(\,\cdot\,)$ for $T_{0,0}$

Here we shall consider the Dirichlet-type self-adjoint extension $T_{0,0}$ of T_{min}. Assuming Hypothesis 3.4.1 and taking the orthonormal basis for $\mathcal{N}_i$ obtained by applying the Gram–Schmidt process to $\{u_j(i,\,\cdot\,)\}_{j=1,2}$, we shall compute the inner products (3.6.6) and use (3.6.5) to obtain an explicit expression for the Donoghue m-function $M^{Do}_{T_{0,0},\mathcal{N}_i}(\,\cdot\,)$ for $T_{0,0}$.

In the analysis below, it will be convenient to also introduce an orthonormal basis for $\mathcal{N}_{-i}$. To set the stage for applying Gram–Schmidt to $\{u_j(\pm i,\,\cdot\,)\}_{j=1,2}$, one applies (3.2.3) and (3.4.1), to compute

$$
\begin{aligned}
&(u_j(\pm i,\,\cdot\,), u_k(\pm i,\,\cdot\,))_{L^2_r((a,b))} = \int_a^b r(x)dx\,\overline{u_j(\pm i,x)}u_k(\pm i,x)\\
&\quad = \int_a^b r(x)dx\,u_j(\mp i,x)u_k(\pm i,x) = \frac{W\big(u_j(\mp i,\,\cdot\,),u_k(\pm i,\,\cdot\,)\big)\big|_a^b}{\mp i-(\pm i)}\\
&\quad = \mp\frac{1}{2i}W\big(u_j(\mp i,\,\cdot\,),u_k(\pm i,\,\cdot\,)\big)\big|_a^b\\
&\quad = \mp\frac{1}{2i}\big\{\widetilde{u}_j(\mp i,b)\widetilde{u}_k'(\pm i,b)-\widetilde{u}_j'(\mp i,b)\widetilde{u}_k(\pm i,b)\\
&\qquad\quad -\big[\widetilde{u}_j(\mp i,a)\widetilde{u}_k'(\pm i,a)-\widetilde{u}_j'(\mp i,a)\widetilde{u}_k(\mp i,a)\big]\big\}\\
&\quad = \mp\frac{1}{2i}\big\{\widetilde{u}_k'(\pm i,b)\delta_{j,1}-\widetilde{u}_j'(\mp i,b)\delta_{k,1}\\
&\qquad\quad -\big[\widetilde{u}_k'(\pm i,a)\delta_{j,2}-\widetilde{u}_j'(\mp i,a)\delta_{k,2}\big]\big\},\quad j,k\in\{1,2\}.
\end{aligned}\tag{3.6.7}
$$

In particular, (3.6.7) implies

$$
\begin{aligned}
&(u_1(\pm i,\,\cdot\,), u_2(\pm i,\,\cdot\,))_{L^2_r((a,b))} = \mp\frac{1}{2i}\big[\widetilde{u}_2'(\pm i,b)+\widetilde{u}_1'(\mp i,a)\big]\\
&\quad = \mp\frac{1}{2i}\big[\widetilde{u}_2'(\pm i,b)-\widetilde{u}_2'(\mp i,b)\big] = \mp\frac{1}{2i}\big[\widetilde{u}_2'(\pm i,b)-\overline{\widetilde{u}_2'(\pm i,b)}\big]\\
&\quad = \mp\mathrm{Im}\big(\widetilde{u}_2'(\pm i,b)\big) = (u_2(\pm i,\,\cdot\,), u_1(\pm i,\,\cdot\,))_{L^2_r((a,b))},
\end{aligned}\tag{3.6.8}
$$

and

$$
\begin{aligned}
&\big\|u_1(\pm i,\,\cdot\,)\big\|^2_{L^2_r((a,b))} = \mp\frac{1}{2i}\big[\widetilde{u}_1'(\pm i,b)-\widetilde{u}_1'(\mp i,b)\big]\\
&\quad = \mp\frac{1}{2i}\big[\widetilde{u}_1'(\pm i,b)-\overline{\widetilde{u}_1'(\pm i,b)}\big] = \mp\mathrm{Im}\big(\widetilde{u}_1'(\pm i,b)\big),
\end{aligned}\tag{3.6.9}
$$

$$
\begin{aligned}
&\big\|u_2(\pm i,\,\cdot\,)\big\|^2_{L^2_r((a,b))} = \pm\frac{1}{2i}\big[\widetilde{u}_2'(\pm i,a)-\widetilde{u}_2'(\mp i,a)\big]\\
&\quad = \pm\frac{1}{2i}\big[\widetilde{u}_2'(\pm i,a)-\overline{\widetilde{u}_2'(\pm i,a)}\big] = \pm\mathrm{Im}\big(\widetilde{u}_2'(\pm i,a)\big).
\end{aligned}\tag{3.6.10}
$$

Applying the Gram–Schmidt process to $\{u_j(\pm i,\,\cdot\,)\}_{j=1,2}$ then yields an orthonormal basis $\{v_j(\pm i,\,\cdot\,)\}_{j=1,2}$ for $\mathcal{N}_{\pm i}$ as follows:

$$v_1(\pm i,\,\cdot\,) = c_1(\pm i)u_1(\pm i,\,\cdot\,), \tag{3.6.11}$$

$$\begin{aligned} v_2(\pm i,\,\cdot\,) &= c_2(\pm i)\left[u_2(\pm i,\,\cdot\,) - \frac{(u_1(\pm i,\,\cdot\,), u_2(\pm i,\,\cdot\,))_{L_r^2((a,b))}}{\|u_1(\pm i,\,\cdot\,)\|^2_{L_r^2((a,b))}} u_1(\pm i,\,\cdot\,)\right] \\ &= c_2(\pm i)\left[u_2(\pm i,\,\cdot\,) - \frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)} u_1(\pm i,\,\cdot\,)\right], \end{aligned} \tag{3.6.12}$$

where

$$c_1(\pm i) = \|u_1(\pm i,\,\cdot\,)\|^{-1}_{L_r^2((a,b))} = \big[\mp \operatorname{Im}\big(\widetilde{u}_1'(\pm i,b)\big)\big]^{-1/2}, \tag{3.6.13}$$

$$\begin{aligned} c_2(\pm i) &= \left\|u_2(\pm i,\,\cdot\,) - \frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)} u_1(\pm i,\,\cdot\,)\right\|^{-1}_{L_r^2((a,b))} \\ &= \left[\pm \operatorname{Im}\big(\widetilde{u}_2'(\pm i,a)\big) \pm \frac{\big[\operatorname{Im}\big(\widetilde{u}_2'(\pm i,b)\big)\big]^2}{\operatorname{Im}\big(\widetilde{u}_1'(\pm i,b)\big)}\right]^{-1/2}, \end{aligned} \tag{3.6.14}$$

and the equality $\operatorname{Im}\big(\widetilde{u}_2'(-i,b)\big)/\operatorname{Im}\big(\widetilde{u}_1'(-i,b)\big) = \operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)/\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)$ has been applied. Based on (3.4.5), one infers that

$$c_j(i) = c_j(-i), \quad j \in \{1,2\}. \tag{3.6.15}$$

In addition, by taking conjugates throughout (3.6.11)–(3.6.14) and applying (3.4.5), one obtains

$$\overline{v_j(\pm i,\,\cdot\,)} = v_j(\mp i,\,\cdot\,), \quad j \in \{1,2\}. \tag{3.6.16}$$

Taking the orthonormal basis $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ for $\mathcal{N}_i$ in (3.6.5) then yields the following expression for the Donoghue m-function $M^{Do}_{T_{0,0},\mathcal{N}_i}(\,\cdot\,)$ for $T_{0,0}$:

$$\begin{aligned} &M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \\ &\quad = \sum_{j,k=1}^{2} \Big[z\delta_{j,k} + \big(z^2+1\big)\big(v_j(i,\,\cdot\,), (T_{0,0} - zI_{L_r^2((a,b))})^{-1} v_k(i,\,\cdot\,)\big)_{L_r^2((a,b))}\Big] \\ &\qquad\qquad \times (v_k(i,\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))} v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{3.6.17}$$

In the special cases $z = \pm i$, one obtains (cf. (3.6.2))

$$M^{Do}_{T_{0,0},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}. \tag{3.6.18}$$

Thus, to obtain an explicit representation for $M^{Do}_{T_{0,0},\mathcal{N}_i}(\,\cdot\,)$, it remains to evaluate the inner products

$$\begin{aligned}\big(v_j(i,\,\cdot\,),(T_{0,0}-zI_{L^2_r((a,b))})^{-1}v_k(i,\,\cdot\,)\big)_{L^2_r((a,b))}, \quad j,k\in\{1,2\},&\\ z\in\mathbb{C}\backslash\mathbb{R},\, z\neq\pm i.&\end{aligned} \tag{3.6.19}$$

For the purposes of evaluating the inner products (3.6.19), we introduce the generalized Cayley transform of $T_{0,0}$,

$$\begin{aligned}U_{0,0,z,z'} &= (T_{0,0}-z'I_{L^2_r((a,b))})(T_{0,0}-zI_{L^2_r((a,b))})^{-1} \\ &= I_{L^2_r((a,b))}+(z-z')(T_{0,0}-zI_{L^2_r((a,b))})^{-1}, \quad z,z'\in\rho(T_{0,0}),\end{aligned} \tag{3.6.20}$$

which forms a bijection from $\mathcal{N}_{z'}$ to $\mathcal{N}_z$. One verifies that

$$U_{0,0,z,z'}u_j(z',\,\cdot\,)=u_j(z,\,\cdot\,), \quad j\in\{1,2\},\, z,z'\in\rho(T_{0,0}). \tag{3.6.21}$$

In fact, for fixed $z,z'\in\rho(T_{0,0})$, one uses the fact that $U_{0,0,z,z'}$ maps into $\mathcal{N}_z$ to write

$$U_{0,0,z,z'}u_j(z',\,\cdot\,)=\alpha_{j,1}u_1(z,\,\cdot\,)+\alpha_{j,2}u_2(z,\,\cdot\,), \quad j\in\{1,2\}, \tag{3.6.22}$$

for some scalars $\alpha_{j,k}\in\mathbb{C}$, $j,k\in\{1,2\}$. The second equality in (3.6.20) then implies

$$\begin{aligned}U_{0,0,z,z'}u_j(z',\,\cdot\,)=u_j(z',\,\cdot\,)+(z-z')(T_{0,0}-zI_{L^2_r((a,b))})^{-1}u_j(z',\,\cdot\,),&\\ j\in\{1,2\},&\end{aligned} \tag{3.6.23}$$

so that

$$[U_{0,0,z,z'}u_j(z',\,\cdot\,)]^{\widetilde{}}(x)=\widetilde{u}_j(z',x), \quad x\in\{a,b\},\, j\in\{1,2\}. \tag{3.6.24}$$

Evaluating (3.6.22) and (3.6.24) at a yields $\alpha_{1,2}=0$ and $\alpha_{2,2}=1$. Similarly, evaluating (3.6.22) and (3.6.24) at b yields $\alpha_{1,1}=1$ and $\alpha_{2,1}=0$. Hence, (3.6.21) follows.

We will now calculate the inner products (3.6.19). Let

$$z\in\mathbb{C}\backslash\mathbb{R} \text{ be fixed with } z\neq\pm i. \tag{3.6.25}$$

The system $\{v_j(z,\,\cdot\,)\}_{j=1,2}$ defined by

$$v_j(z,\,\cdot\,)=U_{0,0,z,i}v_j(i,\,\cdot\,), \quad j\in\{1,2\}, \tag{3.6.26}$$

is a basis for the subspace $\mathcal{N}_z$. Applying (3.6.11)–(3.6.12) and (3.6.21) in (3.6.26), one obtains

$$\begin{aligned} v_1(z,\,\cdot\,) &= c_1(i)u_1(z,\,\cdot\,), \\ v_2(z,\,\cdot\,) &= c_2(i)\left[u_2(z,\,\cdot\,) - \frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)}u_1(z,\,\cdot\,)\right]. \end{aligned} \tag{3.6.27}$$

The inner products (3.6.19) can be recast in terms of $\{v_j(z,\,\cdot\,)\}_{j=1,2}$ as follows:

$$\begin{aligned} &\big(v_j(i,\,\cdot\,),(T_{0,0} - zI_{L_r^2((a,b))})^{-1}v_k(i,\,\cdot\,)\big)_{L_r^2((a,b))} \\ &\quad = \frac{1}{z-i}(v_j(i,\,\cdot\,),[U_{0,0,z,i} - I_{L_r^2((a,b))}]v_k(i,\,\cdot\,))_{L_r^2((a,b))} \\ &\quad = \frac{1}{i-z}\delta_{j,k} + \frac{1}{z-i}(v_j(i,\,\cdot\,),v_k(z,\,\cdot\,))_{L_r^2((a,b))}, \quad j,k\in\{1,2\}. \end{aligned} \tag{3.6.28}$$

In turn, by (3.2.3) and (3.6.16), one obtains

$$\begin{aligned} (v_j(i,\,\cdot\,),v_k(z,\,\cdot\,))_{L_r^2((a,b))} &= \int_a^b r(x)dx\, v_j(-i,x)v_k(z,x) \\ &= -\frac{W\big(v_j(-i,\,\cdot\,),v_k(z,\,\cdot\,)\big)\big|_a^b}{z+i}, \quad j,k\in\{1,2\}. \end{aligned} \tag{3.6.29}$$

Using (3.6.29), one recasts (3.6.28) as

$$\begin{aligned} &\big(v_j(i,\,\cdot\,),(T_{0,0} - zI_{L_r^2((a,b))})^{-1}v_k(i,\,\cdot\,)\big)_{L_r^2((a,b))} \\ &\quad = \frac{1}{i-z}\delta_{j,k} - \frac{W\big(v_j(-i,\,\cdot\,),v_k(z,\,\cdot\,)\big)\big|_a^b}{1+z^2}, \quad j,k\in\{1,2\}. \end{aligned} \tag{3.6.30}$$

After substituting (3.6.30) in (3.6.17) and taking cancellations into account, one obtains

$$\begin{aligned} &M_{T_{0,0},\mathcal{N}_i}^{Do}(z) \\ &\quad = \sum_{j,k=1}^{2}\big[-i\delta_{j,k} - W\big(v_j(-i,\,\cdot\,),v_k(z,\,\cdot\,)\big)\big|_a^b\big](v_k(i,\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))}v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\, z\neq\pm i. \end{aligned} \tag{3.6.31}$$

The Wronskians

$$W_{j,k}(z) := W(v_j(-i,\,\cdot\,),v_k(z,\,\cdot\,))\big|_a^b, \quad z\in\mathbb{C}\backslash\mathbb{R},\, z\neq\pm i, \tag{3.6.32}$$

that appear in (3.6.31) can be computed by applying (3.4.1) and (3.6.27). One obtains for $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$:

$$W_{1,1}(z) = [c_1(i)]^2 \big[\widetilde{u}_1'(z,b) - \widetilde{u}_1'(-i,b)\big], \tag{3.6.33}$$

$$\begin{aligned} W_{1,2}(z) = c_1(i)c_2(i)\Bigg\{ &\frac{\mathrm{Im}\big(\widetilde{u}_2'(i,b)\big)}{\mathrm{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(-i,b) - \widetilde{u}_1'(z,b)\big] \\ &+ \widetilde{u}_2'(z,b) + \widetilde{u}_1'(-i,a)\Bigg\}, \end{aligned} \tag{3.6.34}$$

$$\begin{aligned} W_{2,1}(z) = -c_1(i)c_2(i)\Bigg\{ &\frac{\mathrm{Im}\big(\widetilde{u}_2'(i,b)\big)}{\mathrm{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(z,b) - \widetilde{u}_1'(-i,b)\big] \\ &+ \widetilde{u}_2'(-i,b) + \widetilde{u}_1'(z,a)\Bigg\}, \end{aligned} \tag{3.6.35}$$

$$\begin{aligned} W_{2,2}(z) = [c_2(i)]^2\Bigg\{ &\Bigg[\widetilde{u}_2'(-i,b) - \widetilde{u}_2'(z,b) \\ &+ \frac{\mathrm{Im}\big(\widetilde{u}_2'(i,b)\big)}{\mathrm{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(z,b) - \widetilde{u}_1'(-i,b)\big]\Bigg]\frac{\mathrm{Im}\big(\widetilde{u}_2'(i,b)\big)}{\mathrm{Im}\big(\widetilde{u}_1'(i,b)\big)} \\ &+ \widetilde{u}_2'(-i,a) - \widetilde{u}_2'(z,a) + \frac{\mathrm{Im}\big(\widetilde{u}_2'(i,b)\big)}{\mathrm{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(z,a) - \widetilde{u}_1'(-i,a)\big]\Bigg\}. \end{aligned} \tag{3.6.36}$$

The relations (3.6.18) and (3.6.31)–(3.6.36) now yield an explicit representation for the Donoghue m-function $M_{T_{0,0},\mathcal{N}_i}^{Do}(\,\cdot\,)$ for $T_{0,0}$.

Theorem 3.6.1. *Assume Hypothesis* 3.4.1 *and let* $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ *be the orthonormal basis for* $\mathcal{N}_i$ *defined in* (3.6.11)*–*(3.6.14). *The Donoghue m-function* $M_{T_{0,0},\mathcal{N}_i}^{Do}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* $T_{0,0}$ *satisfies*

$$\begin{aligned} M_{T_{0,0},\mathcal{N}_i}^{Do}(\pm i) &= \pm i I_{\mathcal{N}_i}, \\ M_{T_{0,0},\mathcal{N}_i}^{Do}(z) &= -\sum_{j,k=1}^{2}[i\delta_{j,k} + W_{j,k}(z)](v_k(i,\,\cdot\,),\,\cdot\,)_{L_r^2((a,b))}v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &= -iI_{\mathcal{N}_i} - \sum_{j,k=1}^{2} W_{j,k}(z)\big(v_k(i,\,\cdot\,),\,\cdot\,\big)_{L_r^2((a,b))}v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &\qquad\qquad z \in \mathbb{C}\backslash\mathbb{R},\ z \neq \pm i, \end{aligned} \tag{3.6.37}$$

where the matrix $\big(W_{j,k}(\,\cdot\,)\big)_{j,k=1}^2$ *is given by* (3.6.33)*–*(3.6.36).

3.6.2 The Donoghue m-function for Self-Adjoint Extensions Other Than $T_{0,0}$

The Donoghue m-function $M^{Do}_{T_{0,0},\mathcal{N}_i}(\,\cdot\,)$ for $T_{0,0}$ was computed explicitly in Theorem 3.6.1. If $T_{A,B}$ is any other self-adjoint extension of T_{min}, then the resolvent identities in Theorem 3.4.2 may be used to obtain an explicit representation of the Donoghue m-function for $T_{A,B}$.

We begin with the case when either $T_{A,B} = T_{\alpha,\beta}$ for $\alpha, \beta \in (0,\pi)$ or $T_{A,B} = T_{\varphi,R}$ for some $\varphi \in [0,\pi)$, $R \in SL(2,\mathbb{R})$, with $R_{1,2} \neq 0$. In this case, items (i) and (iv) in Theorem 3.4.2 imply

$$\begin{aligned}(T_{A,B} - zI_{L^2_r((a,b))})^{-1} &= (T_{0,0} - zI_{L^2_r((a,b))})^{-1} \\ &\quad + \sum_{j,k=1}^{2} \big[K_{A,B}(z)^{-1}\big]_{j,k} (u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} u_k(z,\,\cdot\,), \\ &\qquad z \in \rho(T_{0,0}) \cap \rho(T_{A,B}),\end{aligned} \tag{3.6.38}$$

where $K_{A,B}(\,\cdot\,) = K_{\alpha,\beta}(\,\cdot\,)$ or $K_{A,B}(\,\cdot\,) = K_{\varphi,R}(\,\cdot\,)$ (cf. (3.4.8) and (3.4.16)) according to whether $T_{A,B} = T_{\alpha,\beta}$ or $T_{A,B} = T_{\varphi,R}$, respectively. Employing (3.6.38) in (3.6.1), one obtains the following representation for the Donoghue m-function $M^{Do}_{T_{A,B},\mathcal{N}_i}(\,\cdot\,)$ of $T_{A,B}$:

$$\begin{aligned}&M^{Do}_{T_{A,B},\mathcal{N}_i}(z) \\ &\quad = zI_{\mathcal{N}_i} + (z^2+1) P_{\mathcal{N}_i} (T_{0,0} - zI_{L^2_r((a,b))})^{-1} P_{\mathcal{N}_i}\big|_{\mathcal{N}_i} \\ &\qquad + (z^2+1) \Bigg[\sum_{j,k=1}^{2} \big[K_{A,B}(z)^{-1}\big]_{j,k} (u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} P_{\mathcal{N}_i} u_k(z,\,\cdot\,) \Bigg]\Bigg|_{\mathcal{N}_i} \\ &\quad = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) + (z^2+1) \sum_{j,k=1}^{2} \big[K_{A,B}(z)^{-1}\big]_{j,k} (u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} P_{\mathcal{N}_i} u_k(z,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &\qquad z \in \mathbb{C}\backslash\mathbb{R}.\end{aligned} \tag{3.6.39}$$

In light of (3.6.2), to obtain a final expression for $M^{Do}_{T_{A,B},\mathcal{N}_i}(\,\cdot\,)$, one must compute $P_{\mathcal{N}_i} u_k(z,\,\cdot\,)$, $k \in \{1,2\}$, for $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$. Let $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$. Invoking the orthonormal basis $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ for $\mathcal{N}_i$ defined in (3.6.11)–(3.6.14), one obtains

$$P_{\mathcal{N}_i} u_k(z,\,\cdot\,) = \sum_{\ell=1}^{2} (v_\ell(i,\,\cdot\,), u_k(z,\,\cdot\,))_{L^2_r((a,b))} v_\ell(i,\,\cdot\,), \quad k \in \{1,2\}. \tag{3.6.40}$$

By (3.2.3) ,

$$\begin{aligned} \big(v_\ell(i,\,\cdot\,), u_k(z,\,\cdot\,)\big)_{L^2_r((a,b))} &= \int_a^b r(x)dx\, v_\ell(-i,x) u_k(z,x) \\ &= -\frac{W(v_\ell(-i,\,\cdot\,), u_k(z,\,\cdot\,))|_a^b}{z+i}, \quad \ell,k \in \{1,2\}. \end{aligned} \tag{3.6.41}$$

The Wronskians

$$W^{Kr}_{\ell,k}(z) := W(v_\ell(-i,\,\cdot\,), u_k(z,\,\cdot\,))|_a^b, \quad \ell,k \in \{1,2\}, \tag{3.6.42}$$

that appear in (3.6.41) can be computed by applying (3.4.1) and (3.6.11)–(3.6.12). One obtains:

$$W^{Kr}_{1,1}(z) = c_1(i)\big[\widetilde{u}_1'(z,b) - \widetilde{u}_1'(-i,b)\big], \tag{3.6.43}$$

$$W^{Kr}_{1,2}(z) = c_1(i)\big[\widetilde{u}_2'(z,b) + \widetilde{u}_1'(-i,a)\big], \tag{3.6.44}$$

$$\begin{aligned} W^{Kr}_{2,1}(z) &= \widetilde{v}_2(-i,b)\widetilde{u}_1'(z,b) - \widetilde{v}_2'(-i,b) - \widetilde{v}_2(-i,a)\widetilde{u}_1'(z,a) \\ &= -c_2(i)\bigg\{\frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(z,b) - \widetilde{u}_1'(-i,b)\big] + \widetilde{u}_2'(-i,b) + \widetilde{u}_1'(z,a)\bigg\}, \end{aligned} \tag{3.6.45}$$

$$\begin{aligned} W^{Kr}_{2,2}(z) &= \widetilde{v}_2(-i,b)\widetilde{u}_2'(z,b) - \widetilde{v}_2(-i,a)\widetilde{u}_2'(z,a) + \widetilde{v}_2'(-i,a) \\ &= -c_2(i)\bigg\{\frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_2'(z,b) + \widetilde{u}_1'(-i,a)\big] + \widetilde{u}_2'(z,a) - \widetilde{u}_2'(-i,a)\bigg\}. \end{aligned} \tag{3.6.46}$$

Therefore, (3.6.40) may be recast as

$$P_{\mathcal{N}_i} u_k(z,\,\cdot\,) = -\frac{1}{z+i}\sum_{\ell=1}^{2} W^{Kr}_{\ell,k}(z) v_\ell(i,\,\cdot\,), \quad k \in \{1,2\}. \tag{3.6.47}$$

By combining (3.6.39) and (3.6.47), one obtains

$$\begin{aligned} M^{Do}_{T_{A,B},\mathcal{N}_i}(z) &= M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \\ &\quad + (i-z)\sum_{j,k,\ell=1}^{2} \big[K_{A,B}(z)^{-1}\big]_{j,k} W^{Kr}_{\ell,k}(z)(u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i}. \end{aligned} \tag{3.6.48}$$

These considerations are summarized next.

Theorem 3.6.2. *Assume Hypothesis* 3.4.1 *and let* $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ *be the orthonormal basis for* $\mathcal{N}_i$ *defined in* (3.6.11)–(3.6.14). *The following items* (i) *and* (ii) *hold.*

(i) *If* $\alpha,\beta\in(0,\pi)$, *then the Donoghue m-function* $M^{Do}_{T_{\alpha,\beta},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{\alpha,\beta}$ *satisfies*

$$
\begin{aligned}
&M^{Do}_{T_{\alpha,\beta},\mathcal{N}_i}(\pm i)=\pm iI_{\mathcal{N}_i},\\
&\quad M^{Do}_{T_{\alpha,\beta},\mathcal{N}_i}(z)=M^{Do}_{T_{0,0},\mathcal{N}_i}(z)\\
&\qquad\qquad +(i-z)\sum_{j,k,\ell=1}^{2}\big[K_{\alpha,\beta}(z)^{-1}\big]_{j,k}W^{Kr}_{\ell,k}(z)(u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad\qquad\qquad\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}
\tag{3.6.49}
$$

where the matrices $K_{\alpha,\beta}(\,\cdot\,)$ *and* $\big(W^{Kr}_{\ell,k}(\,\cdot\,)\big)^2_{\ell,k=1}$ *are given by* (3.4.8) *and* (3.6.43)–(3.6.46), *respectively.*

(ii) *If* $\varphi\in[0,\pi)$ *and* $R\in SL(2,\mathbb{R})$ *with* $R_{1,2}\neq 0$, *then the Donoghue m-function* $M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{\varphi,R}$ *satisfies*

$$
\begin{aligned}
&M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\pm i)=\pm iI_{\mathcal{N}_i},\\
&\quad M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(z)=M^{Do}_{T_{0,0},\mathcal{N}_i}(z)\\
&\qquad\qquad +(i-z)\sum_{j,k,\ell=1}^{2}\big[K_{\varphi,R}(z)^{-1}\big]_{j,k}W^{Kr}_{\ell,k}(z)(u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad\qquad\qquad\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}
\tag{3.6.50}
$$

where the matrices $K_{\varphi,R}(\,\cdot\,)$ *and* $\big(W^{Kr}_{\ell,k}(\,\cdot\,)\big)^2_{\ell,k=1}$ *are given by* (3.4.16) *and* (3.6.43)–(3.6.46), *respectively.*

It remains to compute the Donoghue m-functions for $T_{0,\beta}$ and $T_{\alpha,0}$ with $\alpha,\beta\in(0,\pi)$ and $T_{\varphi,R}$ for $\varphi\in[0,\pi)$ and $R\in SL(2,\mathbb{R})$ with $R_{1,2}=0$.

Theorem 3.6.3. *Assume Hypothesis* 3.4.1 *and let* $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ *be the orthonormal basis for* $\mathcal{N}_i$ *defined in* (3.6.11)–(3.6.14). *The following items* $(i)-(iii)$ *hold.*

(i) *If* $\alpha\in(0,\pi)$, *then the Donoghue m-function* $M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{\alpha,0}$

satisfies

$$
\begin{aligned}
&M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \qquad\qquad (3.6.51)\\
&\qquad + \frac{z-i}{\cot(\alpha)+\widetilde{u}_2'(z,a)}(u_2(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\sum_{\ell=1}^{2} W^{Kr}_{\ell,2}(z)v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}
$$

where the scalars $\big\{W^{Kr}_{\ell,2}(\,\cdot\,)\big\}_{\ell=1,2}$ *are given by* (3.6.44) *and* (3.6.46)*.*

(ii) If $\beta\in(0,\pi)$*, then the Donoghue m-function* $M^{Do}_{T_{0,\beta},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{0,\beta}$ *satisfies*

$$
\begin{aligned}
&M^{Do}_{T_{0,\beta},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M^{Do}_{T_{0,\beta},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \qquad\qquad (3.6.52)\\
&\qquad - \frac{z-i}{\cot(\beta)+\widetilde{u}_1'(z,b)}(u_1(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\sum_{\ell=1}^{2} W^{Kr}_{\ell,1}(z)v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}
$$

where the scalars $\big\{W^{Kr}_{\ell,1}(\,\cdot\,)\big\}_{\ell=1,2}$ *are given by* (3.6.43) *and* (3.6.45)*.*

(iii) If $\varphi\in[0,\pi)$ *and* $R\in SL(2,\mathbb{R})$ *with* $R_{1,2}=0$*, then the Donoghue m-function* $M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{\varphi,R}$ *satisfies*

$$
\begin{aligned}
&M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \qquad\qquad (3.6.53)\\
&\quad - \frac{z-i}{k_{\varphi,R}(z)}(u_{\varphi,R}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\sum_{\ell=1}^{2}\big[e^{-i\varphi}R_{2,2}W^{Kr}_{\ell,2}(z)+W^{Kr}_{\ell,1}(z)\big]v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}
$$

where the scalar $k_{\varphi,R}(\,\cdot\,)$ *and the matrix* $\big(W^{Kr}_{\ell,k}(\,\cdot\,)\big)_{\ell,k=1}^2$ *are given by* (3.4.19) *and* (3.6.43)–(3.6.46)*, respectively.*

Proof. To prove item (i), let $\alpha \in (0,\pi)$. By (3.6.2), $M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}$. In order to establish (3.6.51), let $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$, be fixed. Taking $T_{A,B} = T_{\alpha,0}$ in (3.6.1) and invoking (3.4.15), one obtains

$$M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) + \big(z^2+1\big) K_{\alpha,0}(z)^{-1} (u_2(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} P_{\mathcal{N}_i} u_2(z,\,\cdot\,)\big|_{\mathcal{N}_i}. \tag{3.6.54}$$

Using (3.6.47) with $k=2$ in (3.6.54), one obtains

$$\begin{aligned} M^{Do}_{T_{\alpha,0},\mathcal{N}_i}(z) &= M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \\ &\quad + (i-z) K_{\alpha,0}(z)^{-1} (u_2(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} \sum_{\ell=1}^{2} W^{Kr}_{\ell,2}(z) v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i}. \end{aligned} \tag{3.6.55}$$

Hence, (3.6.51) follows from (3.6.55) by applying the precise form for $K_{\alpha,0}(z)$ given in (3.4.14). This completes the proof of item (i).

To prove item (ii), let $\beta \in (0,\pi)$. By (3.6.2), $M^{Do}_{T_{0,\beta},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}$. In order to establish (3.6.52), let $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$, be fixed. Taking $T_{A,B} = T_{0,\beta}$ in (3.6.1) and invoking (3.4.12), one obtains

$$M^{Do}_{T_{0,\beta},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) + \big(z^2+1\big) K_{0,\beta}(z)^{-1} (u_1(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} P_{\mathcal{N}_i} u_1(z,\,\cdot\,)\big|_{\mathcal{N}_i}. \tag{3.6.56}$$

Using (3.6.47) with $k=1$ in (3.6.56), one obtains

$$\begin{aligned} M^{Do}_{T_{0,\beta},\mathcal{N}_i}(z) &= M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \\ &\quad + (i-z) K_{0,\beta}(z)^{-1} (u_1(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))} \sum_{\ell=1}^{2} W^{Kr}_{\ell,1}(z) v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i}. \end{aligned} \tag{3.6.57}$$

Hence, (3.6.52) follows from (3.6.57) by applying the precise form for $K_{0,\beta}(z)$ given in (3.4.11). This completes the proof of item (ii).

To prove item (iii), let $\varphi \in [0,\pi)$ and $R \in SL(2,\mathbb{R})$ with $R_{1,2} = 0$. By (3.6.2), $M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}$. In order to establish (3.6.53), let $z \in \mathbb{C}\backslash\mathbb{R}$, $z \neq \pm i$, be fixed. Taking $T_{A,B} = T_{\varphi,R}$ in (3.6.1) and invoking (3.4.20), one obtains

$$M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \tag{3.6.58}$$

$$+\big(z^2+1\big)k_{\varphi,R}(z)^{-1}(u_{\varphi,R}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}P_{\mathcal{N}_i}u_{\varphi,R}(z,\,\cdot\,)\big|_{\mathcal{N}_i}.$$

By (3.6.41) and (3.6.42),

$$\begin{aligned}P_{\mathcal{N}_i}u_{\varphi,R}(z,\,\cdot\,) &= \sum_{\ell=1}^{2}\big(v_\ell(i,\,\cdot\,),e^{-i\varphi}R_{2,2}u_2(z,\,\cdot\,)+u_1(z,\,\cdot\,)\big)_{L^2_r((a,b))}v_\ell(i,\,\cdot\,)\\ &= -\frac{1}{z+i}\sum_{\ell=1}^{2}\big[e^{-i\varphi}R_{2,2}W^{Kr}_{\ell,2}(z)+W^{Kr}_{\ell,1}(z)\big]v_\ell(i,\,\cdot\,).\end{aligned} \tag{3.6.59}$$

Finally, (3.6.53) follows by combining (3.6.58) and (3.6.59). □

3.7 A Generalized Bessel-Type Operator Example

As an illustration of these results, we consider the following explicitly solvable generalized Bessel-type equation following the analysis in [79] (see also [68]). Let $a=0$, $b\in(0,\infty)\cup\{\infty\}$, and consider

$$\begin{gathered}p(x)=x^{\nu},\quad r(x)=x^{\delta},\quad q(x)=\frac{(2+\delta-\nu)^2\gamma^2-(1-\nu)^2}{4}x^{\nu-2},\\ \delta>-1,\ \nu<1,\ \gamma\geqslant 0,\ x\in(0,b).\end{gathered} \tag{3.7.1}$$

Then

$$\begin{gathered}\tau_{\delta,\nu,\gamma}=x^{-\delta}\left[-\frac{d}{dx}x^{\nu}\frac{d}{dx}+\frac{(2+\delta-\nu)^2\gamma^2-(1-\nu)^2}{4}x^{\nu-2}\right],\\ \delta>-1,\ \nu<1,\ \gamma\geqslant 0,\ x\in(0,b),\end{gathered} \tag{3.7.2}$$

is singular at the endpoint $x=0$ (since the potential, q is not integrable near $x=0$), regular at $x=b$ when $b\in(0,\infty)$, and in the limit point case at $x=b$ when $b=\infty$. Furthermore, $\tau_{\delta,\nu,\gamma}$ is in the limit circle case at $x=0$ if $0\leqslant\gamma<1$ and in the limit point case at $x=0$ when $\gamma\geqslant 1$.

Solutions to $\tau_{\delta,\nu,\gamma}u=zu$ are given by (cf. [109], [110, No. 2.162, p. 440])

$$y_{1,\delta,\nu,\gamma}(z,x)=x^{(1-\nu)/2}J_{\gamma}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big),\quad \gamma\geqslant 0, \tag{3.7.3}$$

$$y_{2,\delta,\nu,\gamma}(z,x)=\begin{cases}x^{(1-\nu)/2}J_{-\gamma}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma\notin\mathbb{N}_0,\\ x^{(1-\nu)/2}Y_{\gamma}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma\in\mathbb{N}_0,\end{cases}\quad \gamma\geqslant 0, \tag{3.7.4}$$

where $J_\mu(\,\cdot\,), Y_\mu(\,\cdot\,)$ are the standard Bessel functions of order $\mu \in \mathbb{R}$ (cf. [1, Ch. 9]). In the following we assume that

$$\gamma \in [0,1) \tag{3.7.5}$$

to ensure the limit circle case at $x = 0$. In this case it suffices to focus on the generalized boundary values at the singular endpoint $x = 0$ following [75]. For this purpose we introduce principal and nonprincipal solutions $u_{0,\delta,\nu,\gamma}(0,\,\cdot\,)$ and $\widehat{u}_{0,\delta,\nu,\gamma}(0,\,\cdot\,)$ of $\tau_{\delta,\nu,\gamma} u = 0$ at $x = 0$ by

$$\begin{aligned} &u_{0,\delta,\nu,\gamma}(0,x) = (1-\nu)^{-1} x^{[1-\nu+(2+\delta-\nu)\gamma]/2}, \quad \gamma \in [0,1), \\ &\widehat{u}_{0,\delta,\nu,\gamma}(0,x) = \begin{cases} (1-\nu)[(2+\delta-\nu)\gamma]^{-1} x^{[1-\nu-(2+\delta-\nu)\gamma]/2}, & \gamma \in (0,1), \\ (1-\nu) x^{(1-\nu)/2} \ln(1/x), & \gamma = 0, \end{cases} \\ &\qquad\qquad \delta > -1,\ \nu < 1,\ x \in (0,1). \end{aligned} \tag{3.7.6}$$

Remark 3.7.1. Since the singularity of q at $x = 0$ renders $\tau_{\delta,\nu,\gamma}$ singular at $x = 0$ (unless, of course, $\gamma = (1-\nu)/(2+\delta-\nu)$, in which case $\tau_{\delta,\nu,(1-\nu)/(2+\delta-\nu)}$ is regular at $x = 0$), there is a certain freedom in the choice of the multiplicative constant in the principal solution $u_{0,\delta,\nu,\gamma}$ of $\tau_{\delta,\nu,\gamma} u = 0$ at $x = 0$. Our choice of $(1-\nu)^{-1}$ in (3.7.6) reflects continuity in the parameters when comparing to boundary conditions in the regular case (cf. [75, Remark 3.12 (ii)]), that is, in the case $\delta > -1$, $\nu < 1$, and $\gamma = (1-\nu)/(2+\delta-\nu)$ treated in [60]. $\diamond$

The generalized boundary values for $g \in \operatorname{dom}(T_{max,\delta,\nu,\gamma})$ are then of the form

$$\begin{aligned} \widetilde{g}(0) &= -W(u_{0,\delta,\nu,\gamma}(0,\,\cdot\,), g)(0) \\ &= \begin{cases} \lim_{x\downarrow 0} g(x) \big/ \big[(1-\nu)[(2+\delta-\nu)\gamma]^{-1} x^{[1-\nu-(2+\delta-\nu)\gamma]/2}\big], & \gamma \in (0,1), \\ \lim_{x\downarrow 0} g(x) \big/ \big[(1-\nu) x^{(1-\nu)/2} \ln(1/x)\big], & \gamma = 0, \end{cases} \end{aligned} \tag{3.7.7}$$

$$\widetilde{g}'(0) = W(\widehat{u}_{0,\delta,\nu,\gamma}(0,\,\cdot\,), g)(0) \tag{3.7.8}$$

$$= \begin{cases} \lim_{x\downarrow 0} \big[g(x) - \widetilde{g}(0)(1-\nu)[(2+\delta-\nu)\gamma]^{-1} x^{[1-\nu-(2+\delta-\nu)\gamma]/2}\big] \\ \qquad \big/\big[(1-\nu)^{-1} x^{[1-\nu+(2+\delta-\nu)\gamma]/2}\big], & \gamma \in (0,1), \\ \lim_{x\downarrow 0} \big[g(x) - \widetilde{g}(0)(1-\nu) x^{(1-\nu)/2} \ln(1/x)\big] \\ \qquad \big/\big[(1-\nu)^{-1} x^{(1-\nu)/2}\big], & \gamma = 0. \end{cases}$$

Next, introducing the standard normalized (at $x = 0$) fundamental system of solutions $\phi_{\delta,\nu,\gamma}(z,\,\cdot\,,0), \theta_{\delta,\nu,\gamma}(z,\,\cdot\,,0)$ of $\tau_{\delta,\nu,\gamma} u = zu$, $z \in \mathbb{C}$, that is real-valued for $z \in \mathbb{R}$ and entire with respect to $z \in \mathbb{C}$ by

$$\begin{aligned} &\widetilde{\phi}_{\delta,\nu,\gamma}(z,0,0) = 0, \quad \widetilde{\phi}'_{\delta,\nu,\gamma}(z,0,0) = 1, \\ &\widetilde{\theta}_{\delta,\nu,\gamma}(z,0,0) = 1, \quad \widetilde{\theta}'_{\delta,\nu,\gamma}(z,0,0) = 0, \quad z \in \mathbb{C}, \end{aligned} \tag{3.7.9}$$

one obtains explicitly,

$$\begin{aligned} \phi_{\delta,\nu,\gamma}(z,x,0) &= (1-\nu)^{-1}(2+\delta-\nu)^{\gamma}\Gamma(1+\gamma) z^{-\gamma/2} y_{1,\delta,\nu,\gamma}(z,x), \\ &\qquad \delta > -1,\ \nu < 1,\ \gamma \in [0,1),\ z \in \mathbb{C},\ x \in (0,b), \end{aligned} \tag{3.7.10}$$

$$\begin{aligned} \theta_{\delta,\nu,\gamma}(z,x,0) &= \begin{cases} (1-\nu)(2+\delta-\nu)^{-\gamma-1}\gamma^{-1}\Gamma(1-\gamma) z^{\gamma/2} y_{2,\delta,\nu,\gamma}(z,x), & \gamma \in (0,1), \\ (1-\nu)(2+\delta-\nu)^{-1}[-\pi y_{2,\delta,\nu,0}(z,x) \\ \quad +(\ln(z) - 2\ln(2+\delta-\nu) + 2\gamma_E) y_{1,\delta,\nu,0}(z,x)], & \gamma = 0, \end{cases} \\ &\qquad \delta > -1,\ \nu < 1,\ z \in \mathbb{C},\ x \in (0,b), \end{aligned} \tag{3.7.11}$$

$$W(\theta_{\delta,\nu,\gamma}(z,\,\cdot\,,0), \phi_{\delta,\nu,\gamma}(z,\,\cdot\,,0)) = 1, \quad z \in \mathbb{C}, \tag{3.7.12}$$

where $\Gamma(\,\cdot\,)$ denotes the Gamma function, and $\gamma_E = 0.57721\dots$ represents Euler's constant.

We now turn to the cases of computing Donoghue m-functions for the generalized Bessel operator in general on the infinite interval and for the Krein–von Neumann extension on the finite interval.

Example 3.7.2 (Infinite Interval). *Let $b = \infty$. We begin by finding $\psi_{0,\delta,\nu,\gamma}(z,\,\cdot\,)$ described in Hypothesis* 3.3.1 *for this example.*

Since $\tau_{\delta,\nu,\gamma}$ is in the limit point case at ∞ (actually, it is in the strong limit point case at infinity since q is bounded on any interval of the form $[R,\infty)$, $R>0$, and the strong limit point property of $\tau_{\delta,\nu,\gamma=(1-\nu)/(2+\delta-\nu)}$ has been shown in [60]*), to find the Weyl–Titchmarsh solution and m-function corresponding to the Friedrichs (resp., Dirichlet) boundary condition at $x=0$, one considers the requirement*

$$\psi_{0,\delta,\nu,\gamma}(z,\,\cdot\,) = \theta_{\delta,\nu,\gamma}(z,\,\cdot\,,0) + m_{0,\delta,\nu,\gamma}(z)\phi_{\delta,\nu,\gamma}(z,\,\cdot\,,0) \in L^2((0,\infty);x^\delta dx), \quad z\in\mathbb{C}\backslash[0,\infty). \tag{3.7.13}$$

This implies

$$\psi_{0,\delta,\nu,\gamma}(z,x) = \begin{cases} i(1-\nu)(2+\delta-\nu)^{-\gamma-1}\gamma^{-1}\Gamma(1-\gamma)\sin(\pi\gamma)z^{\gamma/2} \\ \quad\times x^{(1-\nu)/2}H^{(1)}_{\gamma}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma\in(0,1), \\ i\pi(1-\nu)/(2+\delta-\nu)x^{(1-\nu)/2} \\ \quad\times H^{(1)}_0\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma=0, \end{cases}$$
$$\delta>-1,\ \nu<1,\ z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty), \tag{3.7.14}$$

$$m_{0,\delta,\nu,\gamma}(z) = \begin{cases} -e^{-i\pi\gamma}(1-\nu)^2(2+\delta-\nu)^{-2\gamma-1}\gamma^{-1} \\ \quad\times[\Gamma(1-\gamma)/\Gamma(1+\gamma)]z^{\gamma}, & \gamma\in(0,1), \\ (1-\nu)^2/(2+\delta-\nu) \\ \quad\times[i\pi-\ln(z)+2\ln(2+\delta-\nu)-2\gamma_E], & \gamma=0, \end{cases} \tag{3.7.15}$$
$$\delta>-1,\ \nu<1,\ z\in\mathbb{C}\backslash[0,\infty),$$

where $H^{(1)}_{\mu}(\,\cdot\,)$ is the Hankel function of the first kind and of order $\mu\in\mathbb{R}$ (cf. [1, Ch. 9]*). In particular, it is immediate from* (3.7.13) *and* (3.7.9) *that $\widetilde{\psi}_{0,\delta,\nu,\gamma}(z,0)=1$. We mention that the results* (3.7.14) *and* (3.7.15) *coincide with the ones obtained in* [75] *when $\delta=\nu=0$ and* [60] *when $\gamma=(1-\nu)/(2+\delta-\nu)$.*

Substituting the explicit form of $\psi_{0,\delta,\nu,\gamma}(z,\,\cdot\,)$ given in (3.7.14) *into Theorems* 3.5.1 *and* 3.5.2 *yields the Friedrichs extension Donoghue m-function, $M^{Do}_{T_{0,\delta,\nu,\gamma},\mathcal{N}_i}(z)$,* *and the Donoghue m-function for all other self-adjoint extensions,* $M^{Do}_{T_{\alpha,\delta,\nu,\gamma},\mathcal{N}_i}(z)$*,* $\alpha \in (0,\pi)$*, respectively. In particular, since* $\widetilde{\psi}'_{0,\delta,\nu,\gamma}(z,0) = m_{0,\delta,\nu,\gamma}(z)$ *one finds from Theorem* 3.5.1 *and* (3.7.15)*,*

$$\begin{aligned}
M^{Do}_{T_{0,\delta,\nu,\gamma},\mathcal{N}_i}(z) &= \bigg[-i + \frac{m_{0,\delta,\nu,\gamma}(z) - m_{0,\delta,\nu,\gamma}(-i)}{\operatorname{Im}(m_{0,\delta,\nu,\gamma}(i))}\bigg] I_{\mathcal{N}_i} \\
&= \begin{cases} \big\{-i - [\sin(\pi\gamma/2)]^{-1} e^{-i\pi\gamma}\big(z^\gamma - e^{3i\pi/2}\big)\big\} I_{\mathcal{N}_i}, & \gamma \in (0,1), \\ \{-i + (2/\pi)[(3i\pi/2) - \ln(z)]\} I_{\mathcal{N}_i}, & \gamma = 0, \end{cases} \\
&\qquad \delta > -1,\ \nu < 1,\ z \in \mathbb{C}\backslash[0,\infty),
\end{aligned} \tag{3.7.16}$$

where the branch of the logarithm is chosen so that $\ln(-i) = 3i\pi/2$*. Thus, by Theorem* 3.5.2 *with* $\alpha \in (0,\pi)$*,*

$$\begin{aligned}
M^{Do}_{T_{\alpha,\delta,\nu,\gamma},\mathcal{N}_i}(z) &= M^{Do}_{T_{0,\delta,\nu,\gamma},\mathcal{N}_i}(z) + (i - z)\frac{m_{0,\delta,\nu,\gamma}(z) - m_{0,\delta,\nu,\gamma}(-i)}{\cot(\alpha) + m_{0,\delta,\nu,\gamma}(z)} \\
&\quad \times (\psi_{0,\delta,\nu,\gamma}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2_r((a,b))}\psi_{0,\delta,\nu,\gamma}(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\
&\qquad \delta > -1,\ \nu < 1,\ \gamma \in [0,1),\ z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{3.7.17}$$

Example 3.7.3 (Finite Interval). *Let* $b \in (0,\infty)$*. It is well known that* $T_{min,\delta,\nu,\gamma} \geqslant \varepsilon I_{L^2_r((a,b))}$ *for some* $\varepsilon > 0$ (*see, e.g., the simpler case* $\delta = \nu = 0$ *treated in* [80, Thm. 5.1])*. Thus, the Krein–von Neumann extension* $T_{0,R_K,\delta,\nu,\gamma}$ *of* $T_{min,\delta,\nu,\gamma}$ *is of the form* (*see* [68, Example 4.1])

$$T_{0,R_K,\delta,\nu,\gamma} f = \tau_{\delta,\nu,\gamma} f, \tag{3.7.18}$$

$$f \in \operatorname{dom}(T_{0,R_K,\delta,\nu,\gamma}) = \left\{ g \in \operatorname{dom}(T_{max,\delta,\nu,\gamma}) \,\middle|\, \begin{pmatrix} g(b) \\ g^{[1]}(b) \end{pmatrix} = R_{K,\delta,\nu,\gamma} \begin{pmatrix} \widetilde{g}(0) \\ \widetilde{g}'(0) \end{pmatrix} \right\},$$

where

$$R_{K,\delta,\nu,\gamma} = \begin{cases} b^{[\nu-1-(2+\delta-\nu)\gamma]/2} \\ \quad \times \begin{pmatrix} \dfrac{1-\nu}{(2+\delta-\nu)\gamma} b^{1-\nu} & \dfrac{1}{1-\nu} b^{1-\nu+(2+\delta-\nu)\gamma} \\ \dfrac{(1-\nu)^2}{2(2+\delta-\nu)\gamma} - \dfrac{1-\nu}{2} & \left[\dfrac{1}{2} + \dfrac{(2+\delta-\nu)\gamma}{2(1-\nu)}\right] b^{(2+\delta-\nu)\gamma} \end{pmatrix}, \\ \hfill \gamma \in (0,1), \\ \begin{pmatrix} (1-\nu)\ln(1/b) b^{(1-\nu)/2} & \dfrac{1}{1-\nu} b^{(1-\nu)/2} \\ \dfrac{(1-\nu)^2 \ln(1/b) - 2(1-\nu)}{2} b^{(\nu-1)/2} & \dfrac{1}{2} b^{(\nu-1)/2} \end{pmatrix}, \quad \gamma = 0, \end{cases}$$

$$\delta > -1, \ \nu < 1. \tag{3.7.19}$$

One now explicitly finds the solutions in (3.4.1) *for this example by choosing*

$$\begin{aligned} &u_{1,\delta,\nu,\gamma}(z,x) = \phi_{\delta,\nu,\gamma}(z,x,0)/\phi_{\delta,\nu,\gamma}(z,b,0), \\ &u_{2,\delta,\nu,\gamma}(z,x) = \theta_{\delta,\nu,\gamma}(z,x,0) - [\theta_{\delta,\nu,\gamma}(z,b,0)/\phi_{\delta,\nu,\gamma}(z,b,0)]\phi_{\delta,\nu,\gamma}(z,x,0), \\ &\qquad \delta > -1, \ \nu < 1, \ \gamma \in [0,1), \ x \in (0,b), \end{aligned} \tag{3.7.20}$$

from which substituting (3.7.20) *into* (3.6.27) *yields the expressions for* $v_{j,\delta,\nu,\gamma}(z,\,\cdot\,)$, $j = 1,2$. *Finally, substituting the expressions for* $u_{j,\delta,\nu,\gamma}(z,\,\cdot\,)$, $v_{j,\delta,\nu,\gamma}(z,\,\cdot\,)$, $j = 1,2$, *and the explicit form of* $K_{0,R_K,\delta,\nu,\gamma}(z)$ *given in* (3.4.25) (*utilizing* (3.7.6)) *into Theorems* 3.6.1 *and* 3.6.2 *yields the Friedrichs extension Donoghue m-function,* $M^{Do}_{T_{0,0,\delta,\nu,\gamma},\mathcal{N}_i}(z)$, *and the Krein extension Donoghue m-function,* $M^{Do}_{T_{0,R_K,\delta,\nu,\gamma},\mathcal{N}_i}(z)$, *respectively.*

CHAPTER FOUR

The Jacobi Operator and its Donoghue m-functions

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4.1 Introduction

This chapter should be regarded as a sequel to the recent [76] (the content of the previous chapter) in which the Donoghue m-function was derived for singular Sturm–Liouville operators. To illustrate the theory, we now apply it to a representative example, the Jacobi differential operator associated with $L^2\big((-1,1);(1-x)^\alpha(1+x)^\beta dx\big)$-realizations of the the differential expression,

$$\begin{aligned}\tau_{\alpha,\beta} = -(1-x)^{-\alpha}(1+x)^{-\beta}(d/dx)\big((1-x)^{\alpha+1}(1+x)^{\beta+1}\big)(d/dx),&\\ x\in(-1,1),\ \alpha,\beta\in\mathbb{R},&\end{aligned} \tag{4.1.1}$$

whenever at least one endpoint, $x=\pm1$, is in the limit circle case (see, e.g. [1, Ch. 22], [14], [21], [58, Sect. 23], [103, Ch. 4], [121, Sects. VII.6.1, XIV.2], [152, Ch. 18], [173, Ch. IV]). In particular, this provides a full treatment of m-functions corresponding to coupled boundary conditions whenever both endpoints are in the limit circle case, a new result.

Turning to the content of each section, we recall the Donoghue m-functions in the two limit circle and one limit circle endpoint cases in Sections 4.2 and 4.3, respectively. The Jacobi operator and its Donoghue m-functions are the topic of Section 4.4, with Sections 4.5–4.7 providing a detailed treatment of solutions of the Jacobi differential equation and the associated hypergeometric differential equations.

4.2 Donoghue m-functions: Two Limit Circle Endpoints

The Donoghue m-functions in the case where τ is in the limit circle case at a and b is the primary topic of this section following [76, Sect. 6].

Hypothesis 4.2.1. *In addition to Hypothesis* 3.2.1 *assume that τ is in the limit circle case at a and b. Moreover, for $z \in \rho(T_{0,0})$, let $\{u_j(z, \cdot)\}_{j=1,2}$ denote solutions to $\tau u = zu$ which satisfy the boundary conditions*

$$\begin{aligned} &\widetilde{u}_1(z,a) = 0, \quad \widetilde{u}_1(z,b) = 1, \\ &\widetilde{u}_2(z,a) = 1, \quad \widetilde{u}_2(z,b) = 0. \end{aligned} \tag{4.2.1}$$

Assume Hypotheses 4.2.1. By Theorem 3.2.8 or Theorem 3.2.15, the following statements (i)–(iii) hold.

(i) If $\gamma, \delta \in [0, \pi)$, then the operator $T_{\gamma,\delta}$ defined by

$$\begin{aligned} &T_{\gamma,\delta} f = T_{max} f, \\ &f \in \operatorname{dom}(T_{\gamma,\delta}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{matrix} \cos(\gamma)\widetilde{g}(a) + \sin(\gamma)\widetilde{g}'(a) = 0, \\ \cos(\delta)\widetilde{g}(b) + \sin(\delta)\widetilde{g}'(b) = 0 \end{matrix} \right\}, \end{aligned} \tag{4.2.2}$$

is a self-adjoint extension of T_{min}.

(ii) If $\varphi \in [0, \pi)$ and $R \in \mathrm{SL}(2, \mathbb{R})$, then the operator $T_{\varphi,R}$ defined by

$$\begin{aligned} &T_{\varphi,R} f = T_{max} f, \\ &f \in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{max}) \,\middle|\, \begin{pmatrix} \widetilde{g}(b) \\ \widetilde{g}'(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} \widetilde{g}(a) \\ \widetilde{g}'(a) \end{pmatrix} \right\}, \end{aligned} \tag{4.2.3}$$

is a self-adjoint extension of T_{min}.

(iii) If T is a self-adjoint extension of T_{min}, then either $T = T_{\gamma,\delta}$ for some $\gamma, \delta \in [0, \pi)$, or $T = T_{\varphi,R}$ for some $\varphi \in [0, \pi)$ and some $R \in \mathrm{SL}(2, \mathbb{R})$.

Notational Convention. *To describe all possible self-adjoint boundary conditions associated with self-adjoint extensions of T_{min} effectively, we will frequently employ* *the notation $T_{A,B}$, $M_{A,B}^{Do}(\,\cdot\,)$, etc., where A, B represents γ, δ in the case of separated boundary conditions and φ, R in the context of coupled boundary conditions.*

Choosing $\gamma = \delta = 0$ in (4.2.2) yields the self-adjoint extension with Dirichlet-type boundary conditions at a and b, equivalently, the Friedrichs extension T_F of T_{min}:

$$\operatorname{dom}(T_{0,0}) = \operatorname{dom}(T_F) = \{g \in \operatorname{dom}(T_{max}) \,|\, \widetilde{g}(a) = \widetilde{g}(b) = 0\}. \tag{4.2.4}$$

Since the coefficients of the Sturm–Liouville differential expression are real, the following conjugation property holds:

$$\overline{u_j(z,\,\cdot\,)} = u_j(\overline{z},\,\cdot\,), \quad z \in \rho(T_{0,0}),\, j \in \{1,2\}. \tag{4.2.5}$$

Applying (4.2.1), one computes

$$\begin{aligned} &W(u_1(z,\,\cdot\,), u_2(z,\,\cdot\,)(a) = -\widetilde{u}_1'(z,a), \\ &W(u_1(z,\,\cdot\,), u_2(z,\,\cdot\,)(b) = \widetilde{u}_2'(z,b), \quad z \in \rho(T_{0,0}). \end{aligned} \tag{4.2.6}$$

In particular, since the Wronskian of two solutions is constant,

$$\widetilde{u}_2'(z,b) = -\widetilde{u}_1'(z,a), \quad z \in \rho(T_{0,0}). \tag{4.2.7}$$

We begin by recalling the orthonormal basis for $\mathcal{N}_{\pm i}$ given by $\{v_j(\pm i,\,\cdot\,)\}_{j=1,2}$,

$$v_1(\pm i,\,\cdot\,) = c_1(\pm i) u_1(\pm i,\,\cdot\,), \tag{4.2.8}$$

$$\begin{aligned} v_2(\pm i,\,\cdot\,) &= c_2(\pm i)\left[u_2(\pm i,\,\cdot\,) - \frac{(u_1(\pm i,\,\cdot\,), u_2(\pm i,\,\cdot\,))_{L^2((a,b);rdx)}}{\|u_1(\pm i,\,\cdot\,)\|^2_{L^2((a,b);rdx)}} u_1(\pm i,\,\cdot\,)\right] \\ &= c_2(\pm i)\left[u_2(\pm i,\,\cdot\,) - \frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)} u_1(\pm i,\,\cdot\,)\right], \end{aligned} \tag{4.2.9}$$

with

$$c_1(\pm i) = \|u_1(\pm i,\,\cdot\,)\|^{-1}_{L^2((a,b);rdx)} = \big[\mp \operatorname{Im}\big(\widetilde{u}_1'(\pm i,b)\big)\big]^{-1/2}, \tag{4.2.10}$$

$$\begin{aligned} c_2(\pm i) &= \left\| u_2(\pm i,\,\cdot\,) - \frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)} u_1(\pm i,\,\cdot\,)\right\|^{-1}_{L^2((a,b);rdx)} \\ &= \left[\pm \operatorname{Im}\big(\widetilde{u}_2'(\pm i,a)\big) \pm \frac{\big[\operatorname{Im}\big(\widetilde{u}_2'(\pm i,b)\big)\big]^2}{\operatorname{Im}\big(\widetilde{u}_1'(\pm i,b)\big)}\right]^{-1/2}. \end{aligned} \tag{4.2.11}$$

The Donoghue m-function $M^{Do}_{T_{A,B},\mathcal{N}_i}(\,\cdot\,)$ with $T_{A,B}$ any self-adjoint extension of T_{min} is provided next (cf. Theorems 6.1–6.3 in [76]).

Theorem 4.2.2. *Assume Hypothesis* 4.2.1 *and let* $\{v_j(i,\,\cdot\,)\}_{j=1,2}$ *be the orthonormal basis for* $\mathcal{N}_i$ *defined in* (4.2.8)–(4.2.11). *The Donoghue m-function* $M^{Do}_{T_{0,0},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{0,0}$ *satisfies*

$$\begin{aligned}
&M^{Do}_{T_{0,0},\mathcal{N}_i}(\pm i)=\pm iI_{\mathcal{N}_i},\\
&M^{Do}_{T_{0,0},\mathcal{N}_i}(z)=-\sum_{j,k=1}^{2}[i\delta_{j,k}+W_{j,k}(z)](v_k(i,\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)}v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \qquad (4.2.12)\\
&\qquad\qquad =-iI_{\mathcal{N}_i}-\sum_{j,k=1}^{2}W_{j,k}(z)\big(v_k(i,\,\cdot\,),\,\cdot\,\big)_{L^2((a,b);rdx)}v_j(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq\pm i,
\end{aligned}$$

where the matrix $\big(W_{j,k}(\,\cdot\,)\big)_{j,k=1}^2$, $z\in\mathbb{C}\backslash\mathbb{R}$, $z\neq\pm i$, *is given by*

$$W_{1,1}(z)=[c_1(i)]^2\big[\widetilde u_1'(z,b)-\widetilde u_1'(-i,b)\big], \qquad (4.2.13)$$

$$\begin{aligned}
W_{1,2}(z)=c_1(i)c_2(i)\Bigg\{&\frac{\operatorname{Im}\big(\widetilde u_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde u_1'(i,b)\big)}\big[\widetilde u_1'(-i,b)-\widetilde u_1'(z,b)\big] \qquad (4.2.14)\\
&+\widetilde u_2'(z,b)+\widetilde u_1'(-i,a)\Bigg\},
\end{aligned}$$

$$\begin{aligned}
W_{2,1}(z)=-c_1(i)c_2(i)\Bigg\{&\frac{\operatorname{Im}\big(\widetilde u_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde u_1'(i,b)\big)}\big[\widetilde u_1'(z,b)-\widetilde u_1'(-i,b)\big] \qquad (4.2.15)\\
&+\widetilde u_2'(-i,b)+\widetilde u_1'(z,a)\Bigg\},
\end{aligned}$$

$$\begin{aligned}
W_{2,2}(z)=[c_2(i)]^2\Bigg\{&\Bigg[\widetilde u_2'(-i,b)-\widetilde u_2'(z,b) \qquad (4.2.16)\\
&+\frac{\operatorname{Im}\big(\widetilde u_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde u_1'(i,b)\big)}\big[\widetilde u_1'(z,b)-\widetilde u_1'(-i,b)\big]\Bigg]\frac{\operatorname{Im}\big(\widetilde u_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde u_1'(i,b)\big)}\\
&+\widetilde u_2'(-i,a)-\widetilde u_2'(z,a)+\frac{\operatorname{Im}\big(\widetilde u_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde u_1'(i,b)\big)}\big[\widetilde u_1'(z,a)-\widetilde u_1'(-i,a)\big]\Bigg\}.
\end{aligned}$$

Furthermore, the following items (*i*)*–*(*v*) *hold.*

(*i*) *If* $\gamma,\delta\in(0,\pi)$, *then the Donoghue m-function* $M^{Do}_{T_{\gamma,\delta},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for*

$T_{\gamma,\delta}$ *satisfies*

$$\begin{aligned}
&M^{Do}_{T_{\gamma,\delta},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M^{Do}_{T_{\gamma,\delta},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \qquad (4.2.17)\\
&\quad + (i-z)\sum_{j,k,\ell=1}^{2}\big[K_{\gamma,\delta}(z)^{-1}\big]_{j,k} W^{Kr}_{\ell,k}(z)(u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)} v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq \pm i,
\end{aligned}$$

where the invertible matrix $K_{\gamma,\delta}(\,\cdot\,)$ *and* $\big(W^{Kr}_{\ell,k}(\,\cdot\,)\big)_{\ell,k=1}^{2}$ *are given by*

$$K_{\gamma,\delta}(z) = \begin{pmatrix} \cot(\delta)+\widetilde{u}_1'(z,b) & -\widetilde{u}_1'(z,a) \\ \widetilde{u}_2'(z,b) & -\cot(\gamma)-\widetilde{u}_2'(z,a)\end{pmatrix}, \qquad (4.2.18)$$

$$W^{Kr}_{1,1}(z) = c_1(i)\big[\widetilde{u}_1'(z,b)-\widetilde{u}_1'(-i,b)\big], \qquad (4.2.19)$$

$$W^{Kr}_{1,2}(z) = c_1(i)\big[\widetilde{u}_2'(z,b)+\widetilde{u}_1'(-i,a)\big], \qquad (4.2.20)$$

$$\begin{aligned}
W^{Kr}_{2,1}(z) &= \widetilde{v}_2(-i,b)\widetilde{u}_1'(z,b)-\widetilde{v}_2'(-i,b)-\widetilde{v}_2(-i,a)\widetilde{u}_1'(z,a) \qquad (4.2.21)\\
&= -c_2(i)\bigg\{\frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_1'(z,b)-\widetilde{u}_1'(-i,b)\big]+\widetilde{u}_2'(-i,b)+\widetilde{u}_1'(z,a)\bigg\},
\end{aligned}$$

$$\begin{aligned}
W^{Kr}_{2,2}(z) &= \widetilde{v}_2(-i,b)\widetilde{u}_2'(z,b)-\widetilde{v}_2(-i,a)\widetilde{u}_2'(z,a)+\widetilde{v}_2'(-i,a) \qquad (4.2.22)\\
&= -c_2(i)\bigg\{\frac{\operatorname{Im}\big(\widetilde{u}_2'(i,b)\big)}{\operatorname{Im}\big(\widetilde{u}_1'(i,b)\big)}\big[\widetilde{u}_2'(z,b)+\widetilde{u}_1'(-i,a)\big]+\widetilde{u}_2'(z,a)-\widetilde{u}_2'(-i,a)\bigg\}.
\end{aligned}$$

(ii) If $\varphi\in[0,\pi)$ *and* $R\in \mathrm{SL}(2,\mathbb{R})$ *with* $R_{1,2}\neq 0$*, then the Donoghue m-function* $M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\,\cdot\,):\mathbb{C}\backslash\mathbb{R}\to\mathcal{B}(\mathcal{N}_i)$ *for* $T_{\varphi,R}$ *satisfies*

$$\begin{aligned}
&M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M^{Do}_{T_{\varphi,R},\mathcal{N}_i}(z) = M^{Do}_{T_{0,0},\mathcal{N}_i}(z) \qquad (4.2.23)\\
&\quad + (i-z)\sum_{j,k,\ell=1}^{2}\big[K_{\varphi,R}(z)^{-1}\big]_{j,k} W^{Kr}_{\ell,k}(z)(u_j(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)} v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z\in\mathbb{C}\backslash\mathbb{R},\ z\neq \pm i,
\end{aligned}$$

where $\big(W_{\ell,k}^{Kr}(\,\cdot\,)\big)_{\ell,k=1}^{2}$ *is once again given in* (4.2.19)–(4.2.22) *and the invertible matrix* $K_{\varphi,R}(\,\cdot\,)$ *is given by*

$$K_{\varphi,R}(z) = \begin{pmatrix} -\dfrac{R_{2,2}}{R_{1,2}} + \widetilde{u}_1'(z,b) & \dfrac{e^{-i\varphi}}{R_{1,2}} - \widetilde{u}_1'(z,a) \\ \dfrac{e^{i\varphi}}{R_{1,2}} + \widetilde{u}_2'(z,b) & -\dfrac{R_{1,1}}{R_{1,2}} - \widetilde{u}_2'(z,a) \end{pmatrix}. \tag{4.2.24}$$

(iii) If $\gamma \in (0,\pi)$, *then the Donoghue m-function* $M_{T_{\gamma,0},\mathcal{N}_i}^{Do}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* $T_{\gamma,0}$ *satisfies*

$$\begin{aligned} &M_{T_{\gamma,0},\mathcal{N}_i}^{Do}(\pm i) = \pm i I_{\mathcal{N}_i}, \\ &M_{T_{\gamma,0},\mathcal{N}_i}^{Do}(z) = M_{T_{0,0},\mathcal{N}_i}^{Do}(z) \\ &\qquad + \frac{z-i}{\cot(\gamma) + \widetilde{u}_2'(z,a)} (u_2(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)} \sum_{\ell=1}^{2} W_{\ell,2}^{Kr}(z) v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &\qquad\qquad z \in \mathbb{C}\backslash\mathbb{R},\ z \neq \pm i, \end{aligned} \tag{4.2.25}$$

where $\cot(\gamma) + \widetilde{u}_2'(z,a) \neq 0$ *and the scalars* $\big\{W_{\ell,2}^{Kr}(\,\cdot\,)\big\}_{\ell=1,2}$ *are given by* (4.2.20) *and* (4.2.22).

(iv) If $\delta \in (0,\pi)$, *then the Donoghue m-function* $M_{T_{0,\delta},\mathcal{N}_i}^{Do}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* $T_{0,\delta}$ *satisfies*

$$\begin{aligned} &M_{T_{0,\delta},\mathcal{N}_i}^{Do}(\pm i) = \pm i I_{\mathcal{N}_i}, \\ &M_{T_{0,\delta},\mathcal{N}_i}^{Do}(z) = M_{T_{0,0},\mathcal{N}_i}^{Do}(z) \\ &\qquad - \frac{z-i}{\cot(\delta) + \widetilde{u}_1'(z,b)} (u_1(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)} \sum_{\ell=1}^{2} W_{\ell,1}^{Kr}(z) v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \\ &\qquad\qquad z \in \mathbb{C}\backslash\mathbb{R},\ z \neq \pm i, \end{aligned} \tag{4.2.26}$$

where $\cot(\delta) + \widetilde{u}_1'(z,b) \neq 0$ *and the scalars* $\big\{W_{\ell,1}^{Kr}(\,\cdot\,)\big\}_{\ell=1,2}$ *are given by* (4.2.19) *and* (4.2.21).

(v) If $\varphi \in [0,\pi)$ *and* $R \in \mathrm{SL}(2,\mathbb{R})$ *with* $R_{1,2} = 0$, *then the Donoghue m-function*

$M_{T_{\varphi,R},\mathcal{N}_i}^{Do}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* $T_{\varphi,R}$ *satisfies*

$$
\begin{aligned}
&M_{T_{\varphi,R},\mathcal{N}_i}^{Do}(\pm i) = \pm i I_{\mathcal{N}_i},\\
&M_{T_{\varphi,R},\mathcal{N}_i}^{Do}(z) = M_{T_{0,0},\mathcal{N}_i}^{Do}(z) \qquad\qquad (4.2.27)\\
&\quad - \frac{z-i}{k_{\varphi,R}(z)}(u_{\varphi,R}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)} \sum_{\ell=1}^{2} \big[e^{-i\varphi} R_{2,2} W_{\ell,2}^{Kr}(z) + W_{\ell,1}^{Kr}(z)\big] v_\ell(i,\,\cdot\,)\big|_{\mathcal{N}_i},\\
&\qquad\qquad z \in \mathbb{C}\backslash\mathbb{R},\ z \neq \pm i,
\end{aligned}
$$

where the matrix $\big(W_{\ell,k}^{Kr}(\,\cdot\,)\big)_{\ell,k=1}^2$ *is once again given in* (4.2.19)–(4.2.22) *and the nonzero scalar* $k_{\varphi,R}(\,\cdot\,)$ *is given by*

$$k_{\varphi,R}(z) = -R_{2,1}R_{2,2} - e^{i\varphi} R_{2,2}\widetilde{u}'_{\varphi,R}(z,a) + \widetilde{u}'_{\varphi,R}(z,b), \qquad (4.2.28)$$

where

$$u_{\varphi,R}(\zeta,\,\cdot\,) = e^{-i\varphi} R_{2,2} u_2(\zeta,\,\cdot\,) + u_1(\zeta,\,\cdot\,), \quad \zeta \in \rho(T_{0,0}). \qquad (4.2.29)$$

Remark 4.2.3. For the Krein extension, T_{0,R_K}, under the additional assumption that $T_{min} \geqslant \varepsilon I_{L^2((a,b);rdx)}$ for some $\varepsilon > 0$, applying [68, Theorem 3.5 (ii)], one computes for the matrix K_{0,R_K},

$$K_{0,R_K}(z) = \begin{pmatrix} \widetilde{u}_1'(z,b) - \widetilde{u}_1'(0,b) & \widetilde{u}_1'(0,a) - \widetilde{u}_1'(z,a) \\ \\ \widetilde{u}_2'(z,b) - \widetilde{u}_2'(0,b) & \widetilde{u}_2'(0,a) - \widetilde{u}_2'(z,a) \end{pmatrix}, \quad z \in \rho(T_{0,0}) \cap \rho(T_{0,R_K}); \qquad (4.2.30)$$

in this case one has $0 \in \sigma(T_{0,R_K})$. $\diamond$

4.3 Donoghue m-functions: One Limit Circle Endpoint

In this section we recall the Donoghue m-functions in the case where τ is in the limit circle case at precisely one endpoint (which we choose to be a without loss of generality) following [76, Sect. 5].

Hypothesis 4.3.1. *In addition to Hypothesis* 3.2.1 *assume that* τ *is in the limit circle case at* a *and in the limit point case at* b. *Moreover, for* $z \in \rho(T_0)$, *let* $\psi(z,\,\cdot\,)$

denote the unique solution to $(\tau - z)y = 0$ *that satisfies* $\psi(z, \cdot\,) \in L^2((a,b); rdx)$ *and* $\widetilde{\psi}(z,a) = 1$.

Assume Hypothesis 4.3.1. By Theorem 3.2.8 or Theorem 3.2.15, the following statements (i) and (ii) hold.

(i) If $\gamma \in [0, \pi)$, then the operator T_γ defined by

$$\begin{aligned} &T_\gamma f = T_{max} f, \\ &f \in \operatorname{dom}(T_\gamma) = \{g \in \operatorname{dom}(T_{max}) \,|\, \cos(\gamma)\widetilde{g}(a) + \sin(\gamma)\widetilde{g}'(a) = 0\}, \end{aligned} \tag{4.3.1}$$

is a self-adjoint extension of T_{min}.

(ii) If T is a self-adjoint extension of T_{min}, then $T = T_\gamma$ for some $\gamma \in [0, \pi)$.

Statements analogous to (i) and (ii) hold if τ is in the limit point case at a and in the limit circle case at b; for brevity we omit the details.

Choosing $\gamma = 0$ in (4.3.1) yields the self-adjoint extension T_0 with a Dirichlet-type boundary condition at a:

$$\operatorname{dom}(T_0) = \{g \in \operatorname{dom}(T_{max}) \,|\, \widetilde{g}(a) = 0\}. \tag{4.3.2}$$

Since the coefficients p, q, and r are real-valued, the solution $\psi(z, \cdot\,)$ has the following conjugation property:

$$\overline{\psi(z, \cdot\,)} = \psi(\overline{z}, \cdot\,), \quad z \in \rho(T_0). \tag{4.3.3}$$

We now turn to the Donoghue m-function $M^{Do}_{T_\gamma, \mathcal{N}_i}(\,\cdot\,)$ with T_γ any self-adjoint extension of T_{min} (cf. Theorems 5.1 and 5.2 in [76]).

Theorem 4.3.2. *Assume Hypothesis* 4.3.1 *and let* $\gamma \in [0, \pi)$. *The Donoghue m-function* $M^{Do}_{T_\gamma, \mathcal{N}_i}(\,\cdot\,) : \mathbb{C}\backslash\mathbb{R} \to \mathcal{B}(\mathcal{N}_i)$ *for* T_γ *satisfies*

$$\begin{aligned} &M^{Do}_{T_\gamma, \mathcal{N}_i}(\pm i) = \pm i I_{\mathcal{N}_i}, \quad \gamma \in [0, \pi), \\ &M^{Do}_{T_0, \mathcal{N}_i}(z) = \left[-i + \frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{\operatorname{Im}\big(\widetilde{\psi}'(i,a)\big)} \right] I_{\mathcal{N}_i}, \quad z \in \mathbb{C}\backslash\mathbb{R},\, z \neq \pm i, \\ &M^{Do}_{T_\gamma, \mathcal{N}_i}(z) = M^{Do}_{T_0, \mathcal{N}_i}(z) \end{aligned} \tag{4.3.4}$$

$$+ (i-z)\frac{\widetilde{\psi}'(z,a) - \widetilde{\psi}'(-i,a)}{\cot(\gamma) + \widetilde{\psi}'(z,a)}(\psi(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)}\psi(i,\,\cdot\,)\bigg|_{\mathcal{N}_i},$$
$$\gamma \in (0,\pi),\ z \in \mathbb{C}\backslash\mathbb{R},\ z \neq \pm i.$$

4.4 The Jacobi Operator and its Donoghue m-functions

We now turn to the principal topic of this chapter, the Jacobi differential expression

$$\begin{aligned} \tau_{\alpha,\beta} = -(1-x)^{-\alpha}(1+x)^{-\beta}(d/dx)\big((1-x)^{\alpha+1}(1+x)^{\beta+1}\big)(d/dx),& \\ x \in (-1,1),\ \alpha,\beta \in \mathbb{R},& \end{aligned} \tag{4.4.1}$$

that is, in connection with Section 3.2 one now has

$$\begin{aligned} &a=-1, \quad b=1, \\ &p(x) = p_{\alpha,\beta}(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}, \quad q(x) = q_{\alpha,\beta}(x) = 0, \\ &r(x) = r_{\alpha,\beta}(x) = (1-x)^{\alpha}(1+x)^{\beta}, \quad x \in (-1,1), \quad \alpha,\beta \in \mathbb{R} \end{aligned} \tag{4.4.2}$$

(see, e.g. [1, Ch. 22], [14], [21], [58, Sect. 23], [103, Ch. 4], [121, Sects. VII.6.1, XIV.2], [152, Ch. 18], [173, Ch. IV]).

L^2-realizations of $\tau_{\alpha,\beta}$ are thus most naturally associated with the Hilbert space $L^2((-1,1); r_{\alpha,\beta}dx)$. However, occasionally the weight function is absorbed into the Hilbert space leading to an equivalent differential expression in the Hilbert space $L^2((-1,1); dx)$ (cf. [51, p. 1510–1520], [58, Sect. 37], [89]). For more recent developments see, for instance, [59], [66], [67], [120], [125].

To decide the limit point/limit circle classification of $\tau_{\alpha,\beta}$ at the interval endpoints ± 1, it suffices to note that if y_1 is a given solution of $\tau y = 0$, then a 2nd linearly independent solution y_2 of $\tau y = 0$ is obtained via the standard formula

$$y_2(x) = y_1(x)\int_c^x dx'\, p(x')^{-1} y_1(x')^{-2}, \quad c,x \in (a,b). \tag{4.4.3}$$

Returning to the concrete Jacobi case at hand, one can choose

$$y_1(x) = 1, \quad x \in (-1,1),$$

$$y_2(x) = \int_0^x dx' \,(1-x')^{-1-\alpha}(1+x')^{-1-\beta}, \quad x \in (-1,1), \tag{4.4.4}$$
$$= \begin{cases} 2^{-1-\alpha}\beta^{-1}(1+x)^{-\beta}[1+O(1+x)] + O(1), & \alpha \in \mathbb{R},\ \beta \in \mathbb{R}\backslash\{0\},\ \text{as } x \downarrow -1, \\ -2^{-1-\alpha}\ln(1+x) + O(1), & \alpha \in \mathbb{R},\ \beta = 0,\ \text{as } x \downarrow -1, \\ 2^{-1-\beta}\alpha^{-1}(1-x)^{-\alpha}[1+O(1-x)] + O(1), & \alpha \in \mathbb{R}\backslash\{0\},\ \beta \in \mathbb{R},\ \text{as } x \uparrow +1, \\ -2^{-1-\beta}\ln(1-x) + O(1), & \alpha = 0,\ \beta \in \mathbb{R},\ \text{as } x \uparrow +1. \end{cases}$$

Thus, one has the classification,

$$\tau_{\alpha,\beta} \text{ is } \begin{cases} \text{regular at } -1 \text{ if and only if } \alpha \in \mathbb{R},\ \beta \in (-1,0), \\ \text{in the limit circle case and singular at } -1 \text{ if and only if} \\ \quad \alpha \in \mathbb{R},\ \beta \in [0,1), \\ \text{in the limit point case at } -1 \text{ if and only if } \alpha \in \mathbb{R},\ \beta \in \mathbb{R}\backslash(-1,1), \\ \text{regular at } +1 \text{ if and only if } \alpha \in (-1,0),\ \beta \in \mathbb{R}, \\ \text{in the limit circle case and singular at } +1 \text{ if and only if} \\ \quad \alpha \in [0,1),\ \beta \in \mathbb{R}, \\ \text{in the limit point case at } +1 \text{ if and only if } \alpha \in \mathbb{R}\backslash(-1,1),\ \beta \in \mathbb{R}. \end{cases} \tag{4.4.5}$$

The maximal and preminimal operators, $T_{max,\alpha,\beta}$ and $T_{min,0,\alpha,\beta}$, associated to $\tau_{\alpha,\beta}$ in $L^2((-1,1);r_{\alpha,\beta}dx)$ are then given by

$$\begin{aligned} &T_{max,\alpha,\beta}f = \tau_{\alpha,\beta}f, \\ &f \in \operatorname{dom}(T_{max,\alpha,\beta}) = \big\{g \in L^2((-1,1);r_{\alpha,\beta}dx) \,\big|\, g, g^{[1]} \in AC_{loc}((-1,1)); \\ &\qquad\qquad\qquad\qquad\qquad \tau_{\alpha,\beta}g \in L^2((-1,1);r_{\alpha,\beta}dx)\big\}, \end{aligned} \tag{4.4.6}$$

and

$$\begin{aligned} &T_{min,0,\alpha,\beta}f = \tau_{\alpha,\beta}f, \\ &f \in \operatorname{dom}(T_{min,0,\alpha,\beta}) = \big\{g \in L^2((-1,1);r_{\alpha,\beta}dx) \,\big|\, g, g^{[1]} \in AC_{loc}((-1,1)); \end{aligned} \tag{4.4.7}$$

$$\operatorname{supp}(g) \subset (-1,1) \text{ is compact; } \tau_{\alpha,\beta} g \in L^2((-1,1); r_{\alpha,\beta} dx)\big\}.$$

The fact (4.4.4) naturally leads to principal and nonprincipal solutions $u_{\pm 1,\alpha,\beta}(0,x)$ and $\widehat{u}_{\pm 1,\alpha,\beta}(0,x)$ of $\tau_{\alpha,\beta} y = 0$ near ± 1 as follows:

$$\begin{aligned}
u_{-1,\alpha,\beta}(0,x) &= \begin{cases} -2^{-\alpha-1}\beta^{-1}(1+x)^{-\beta}[1+O(1+x)], & \beta \in (-\infty,0), \\ 1, & \beta \in [0,\infty), \end{cases} \\
\widehat{u}_{-1,\alpha,\beta}(0,x) &= \begin{cases} 1, & \beta \in (-\infty,0), \\ -2^{-\alpha-1}\ln((1+x)/2), & \beta = 0, \\ 2^{-\alpha-1}\beta^{-1}(1+x)^{-\beta}[1+O(1+x)], & \beta \in (0,\infty), \end{cases} \qquad \alpha \in \mathbb{R},
\end{aligned} \tag{4.4.8}$$

and

$$\begin{aligned}
u_{+1,\alpha,\beta}(0,x) &= \begin{cases} 2^{-\beta-1}\alpha^{-1}(1-x)^{-\alpha}[1+O(1-x)], & \alpha \in (-\infty,0), \\ 1, & \alpha \in [0,\infty), \end{cases} \\
\widehat{u}_{+1,\alpha,\beta}(0,x) &= \begin{cases} 1, & \alpha \in (-\infty,0), \\ 2^{-\beta-1}\ln((1-x)/2), & \alpha = 0, \\ -2^{-\beta-1}\alpha^{-1}(1-x)^{-\alpha}[1+O(1-x)], & \alpha \in (0,\infty), \end{cases} \qquad \beta \in \mathbb{R}.
\end{aligned} \tag{4.4.9}$$

Combining the fact (4.4.5) with Theorem 3.2.5, $T_{min,0,\alpha,\beta}$ is essentially self-adjoint in $L^2((-1,1); r_{\alpha,\beta} dx)$ if and only if $\alpha, \beta \in \mathbb{R}\backslash(-1,1)$. Thus, boundary values for $T_{max,\alpha,\beta}$ at -1 exist if and only if $\alpha \in \mathbb{R}$, $\beta \in (-1,1)$, and similarly, boundary values for $T_{max,\alpha,\beta}$ at $+1$ exist if and only if $\alpha \in (-1,1)$, $\beta \in \mathbb{R}$.

Employing the principal and nonprincipal solutions (4.4.8), (4.4.9) at ± 1, generalized boundary values for $g \in \operatorname{dom}(T_{max,\alpha,\beta})$ are of the form

$$
\begin{aligned}
&\widetilde{g}(-1) = \begin{cases} g(-1), & \beta \in (-1,0), \\ -2^{\alpha+1} \lim_{x\downarrow -1} g(x)/\ln((1+x)/2), & \beta = 0, \\ \beta 2^{\alpha+1} \lim_{x\downarrow -1} (1+x)^{\beta} g(x), & \beta \in (0,1), \end{cases} \\
&\widetilde{g}'(-1) = \begin{cases} g^{[1]}(-1), & \beta \in (-1,0), \\ \lim_{x\downarrow -1} \big[g(x) + \widetilde{g}(-1) 2^{-\alpha-1} \ln((1+x)/2)\big], & \beta = 0, \\ \lim_{x\downarrow -1} \big[g(x) - \widetilde{g}(-1) 2^{-\alpha-1} \beta^{-1} (1+x)^{-\beta}\big], & \beta \in (0,1), \end{cases}
\end{aligned} \quad \alpha \in \mathbb{R},
\tag{4.4.10}
$$

$$
\begin{aligned}
&\widetilde{g}(1) = \begin{cases} g(1), & \alpha \in (-1,0), \\ 2^{\beta+1} \lim_{x\uparrow 1} g(x)/\ln((1-x)/2), & \alpha = 0, \\ -\alpha 2^{\beta+1} \lim_{x\uparrow 1} (1-x)^{\alpha} g(x), & \alpha \in (0,1), \end{cases} \\
&\widetilde{g}'(1) = \begin{cases} g^{[1]}(1), & \alpha \in (-1,0), \\ \lim_{x\uparrow 1} \big[g(x) - \widetilde{g}(1) 2^{-\beta-1} \ln((1-x)/2)\big], & \alpha = 0, \\ \lim_{x\uparrow 1} \big[g(x) + \widetilde{g}(1) 2^{-\beta-1} \alpha^{-1} (1-x)^{-\alpha}\big], & \alpha \in (0,1), \end{cases}
\end{aligned} \quad \beta \in \mathbb{R}.
\tag{4.4.11}
$$

As a result, the minimal operator T_{min} associated to $\tau_{\alpha,\beta}$, that is, $T_{min} = \overline{T_{min,0}}$, is thus given by

$$
\begin{aligned}
&T_{min,\alpha,\beta} f = \tau_{\alpha,\beta} f, \\
&f \in \operatorname{dom}(T_{min,\alpha,\beta}) = \big\{ g \in L^2((-1,1); r_{\alpha,\beta}dx) \,\big|\, g, g^{[1]} \in AC_{loc}((-1,1)); \\
&\qquad \widetilde{g}(-1) = \widetilde{g}'(-1) = \widetilde{g}(1) = \widetilde{g}'(1) = 0; \ \tau_{\alpha,\beta} g \in L^2((-1,1); r_{\alpha,\beta}dx) \big\}.
\end{aligned}
\tag{4.4.12}
$$

For a detailed treatment of solutions of the Jacobi differential equation and the associated hypergeometric differential equations we refer to Sections 4.5–4.7.

Remark 4.4.1. We now mention a few special cases of interest. The Legendre equation ($\alpha = \beta = 0$) has frequently been discussed in the literature, see, for instance, [75] and the extensive list of references cited therein. The Gegenbauer, or ultraspherical, equation (see, e.g., [1, Ch. 22], [152, Ch. 18], [173, Ch. IV]) can be realized by choosing the parameters $\alpha = \beta = \mu - 1/2$, noting at the endpoints $x = \pm 1$, τ_μ is regular for $\mu \in (-1/2, 1/2)$, in the limit circle case and singular for $\mu \in [1/2, 3/2)$, and in the limit point case for $\mu \in \mathbb{R}\backslash(-1/2, 3/2)$. The Chebyshev equations of the first and second kinds are two more important special cases, with the first kind realized by choosing $\mu = 0$ in the Gegenbauer equation, or $\alpha = \beta = -1/2$ in the Jacobi equation (see, e.g., [1, Ch. 22], [152, Ch. 18], [173, Ch. IV]), whereas the second kind is realized by choosing $\mu = 1$ in the Gegenbauer equation, or $\alpha = \beta = 1/2$ in the Jacobi equation (see, e.g., [1, Ch. 22], [152, Ch. 18], [173, Ch. IV]). $\diamond$

We now determine the solutions $\phi_{0,\alpha,\beta}(z, \cdot\,)$ and $\theta_{0,\alpha,\beta}(z, \cdot\,)$ of $\tau_{\alpha,\beta} u = zu$, $z \in \mathbb{C}$, that are subject to the conditions

$$\begin{aligned} &\widetilde{\phi}_{0,\alpha,\beta}(z,-1) = 0, \quad \widetilde{\phi}'_{0,\alpha,\beta}(z,-1) = 1, \\ &\widetilde{\theta}_{0,\alpha,\beta}(z,-1) = 1, \quad \widetilde{\theta}'_{0,\alpha,\beta}(z,-1) = 0. \end{aligned} \tag{4.4.13}$$

In particular, one obtains from (4.7.1),

$$\begin{aligned} &\phi_{0,\alpha,\beta}(z,x) = \begin{cases} -2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x), & \beta \in (-1,0), \\ y_{1,\alpha,\beta,-1}(z,x), & \beta \in [0,1), \end{cases} \\ &\theta_{0,\alpha,\beta}(z,x) = \begin{cases} y_{1,\alpha,\beta,-1}(z,x), & \beta \in (-1,0), \\ -2^{-\alpha-1} y_{2,\alpha,0,-1}(z,x), & \beta = 0, \\ 2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x), & \beta \in (0,1), \end{cases} \\ &\qquad\qquad \alpha \in \mathbb{R},\ z \in \mathbb{C},\ x \in (-1,1). \end{aligned} \tag{4.4.14}$$

4.4.1 The Regular and Limit Circle Case $\alpha, \beta \in (-1, 1)$

In this section we compute the Donoghue m-function when the Jacobi problem considered is either in the regular or limit circle case at ± 1.

Using (4.4.13), the solutions in (4.2.1) for this example are given by

$$\begin{aligned}
u_{1,\alpha,\beta}(z,x) &= \phi_{0,\alpha,\beta}(z,x)/\widetilde{\phi}_{0,\alpha,\beta}(z,1) \\
&= \begin{cases} y_{2,\alpha,\beta,-1}(z,x)/\widetilde{y}_{2,\alpha,\beta,-1}(z,1), & \beta \in (-1,0), \\ y_{1,\alpha,\beta,-1}(z,x)/\widetilde{y}_{1,\alpha,\beta,-1}(z,1), & \beta \in [0,1), \end{cases} \\
u_{2,\alpha,\beta}(z,x) &= \theta_{0,\alpha,\beta}(z,x) - [\widetilde{\theta}_{0,\alpha,\beta}(z,1)/\widetilde{\phi}_{0,\alpha,\beta}(z,1)]\phi_{0,\alpha,\beta}(z,x) \\
&= \begin{cases} y_{1,\alpha,\beta,-1}(z,x) - [\widetilde{y}_{1,\alpha,\beta,-1}(z,1)/\widetilde{y}_{2,\alpha,\beta,-1}(z,1)]y_{2,\alpha,\beta,-1}(z,x), \\ \hfill \beta \in (-1,0), \\ -2^{-\alpha-1}\{y_{2,\alpha,0,-1}(z,x) - [\widetilde{y}_{2,\alpha,0,-1}(z,1)/\widetilde{y}_{1,\alpha,0,-1}(z,1)]y_{1,\alpha,0,-1}(z,x)\}, \\ \hfill \beta = 0, \\ 2^{-\alpha-1}\beta^{-1}\{y_{2,\alpha,\beta,-1}(z,x) - [\widetilde{y}_{2,\alpha,\beta,-1}(z,1)/\widetilde{y}_{1,\alpha,\beta,-1}(z,1)]y_{1,\alpha,\beta,-1}(z,x)\}, \\ \hfill \beta \in (0,1), \end{cases} \\
&\qquad \alpha \in (-1,1),\ z \in \mathbb{C},\ x \in (-1,1),
\end{aligned} \tag{4.4.15}$$

where the generalized boundary values are given in (4.7.2)–(4.7.4). Hence substituting (4.4.15) into (4.2.8)–(4.2.11) and applying Theorem 4.2.2 yields the (Nevanlinna–Herglotz) Donoghue m-function $M^{Do}_{T_{A,B,\alpha,\beta},\mathcal{N}_i}(\,\cdot\,)$ for any self-adjoint extension $T_{A,B,\alpha,\beta}$ of T_{min} with $\alpha, \beta \in (-1,1)$.

As an example of coupled boundary conditions, we consider the Krein–von Neumann extension following Example 4.3 found in [68]. For $\alpha, \beta \in (-1,1)$, the following five cases are associated with a strictly positive minimal operator $T_{min,\alpha,\beta}$ and we now provide the corresponding choices of $R_{K,\alpha,\beta}$ for the Krein–von Neumann extension $T_{0,R_K,\alpha,\beta}$ of $T_{min,\alpha,\beta}$:

$$T_{0,R_K,\alpha,\beta} f = \tau_{\alpha,\beta} f, \tag{4.4.16}$$

$$f \in \operatorname{dom}(T_{0,R_K,\alpha,\beta}) = \left\{ g \in \operatorname{dom}(T_{max,\alpha,\beta}) \,\middle|\, \begin{pmatrix} \widetilde{g}(1) \\ \widetilde{g}'(1) \end{pmatrix} = R_{K,\alpha,\beta} \begin{pmatrix} \widetilde{g}(-1) \\ \widetilde{g}'(-1) \end{pmatrix} \right\},$$

$$R_{K,\alpha,\beta} = \begin{cases} \begin{pmatrix} 1 & 2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} \\ 0 & 1 \end{pmatrix}, & \alpha,\beta \in (-1,0), \\ \begin{pmatrix} -2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} & 1 \\ -1 & 0 \end{pmatrix}, & \alpha \in (-1,0),\ \beta \in (0,1), \\ \begin{pmatrix} 0 & -1 \\ 1 & 2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} \end{pmatrix}, & \alpha \in (0,1),\ \beta \in (-1,0), \\ \begin{pmatrix} 0 & -1 \\ 1 & -2^{-\beta-1}[\gamma_E + \psi(-\beta)] \end{pmatrix}, & \alpha = 0,\ \beta \in (-1,0) \\ \begin{pmatrix} 2^{-\alpha-1}[\gamma_E + \psi(-\alpha)] & 1 \\ -1 & 0 \end{pmatrix}, & \alpha \in (-1,0),\ \beta = 0, \end{cases} \tag{4.4.17}$$

where we interpret $1/\Gamma(0) = 0$, $\psi(\,\cdot\,) = \Gamma'(\,\cdot\,)/\Gamma(\,\cdot\,)$ denotes the Digamma function, and $\gamma_E = -\psi(1) = 0.57721\ldots$ represents Euler's constant. Obviously, $\det(R_{K,\alpha,\beta}) = 1$ in all five cases. Furthermore, as $R_{1,2} \neq 0$ for each case, Theorem 4.2.2 *(ii)* applies and one obtains the Donoghue m-function $M^{Do}_{T_{0,R_K,\alpha,\beta},\mathcal{N}_i}(\,\cdot\,)$ for the Krein–von Neumann extension $T_{0,R_K,\alpha,\beta}$ by utilizing (4.4.15) and (4.4.17) as well as the explicit form of $K_{0,R_K}(\,\cdot\,)$ in (4.2.30). We note once again that $M^{Do}_{T_{0,R_K,\alpha,\beta},\mathcal{N}_i}(\,\cdot\,)$ is a Nevanlinna–Herglotz function.

In the remaining four cases not covered by (4.4.17), given by all combinations of $\alpha = 0,\ \beta = 0,\ \alpha \in (0,1)$, and $\beta \in (0,1)$, one observes that [68, Theorem 3.5] is not applicable as the underlying minimal operator, $T_{min,\alpha,\beta}$, is nonnegative but not strictly positive. In particular, the Jacobi polynomials satisfy Friedrichs boundary conditions for $\alpha, \beta \in [0,1)$, hence $0 \in \sigma(T_{F,\alpha,\beta})$, $\alpha, \beta \in [0,1)$ and $T_{min,\alpha,\beta} \geqslant 0$ is nonnegative, but not strictly positive when $\alpha, \beta \in [0,1)$.

4.4.2 Precisely One Interval Endpoint in the Limit Point Case

In this section we determine the Donoghue m-function in all situations where precisely one interval endpoint is in the limit point case. We will focus on the case when $\alpha \in (-\infty,-1]$ or $\alpha \in [1,\infty)$, so that the right endpoint $x=1$ represents the limit point case. The converse situation can be obtained by reflection with respect to the origin (i.e., considering the transform $(-1,1) \ni x \mapsto -x \in (-1,1)$).

We recall from [75, Sect. 6] that the Weyl–Titchmarsh–Kodaira solution and m-function corresponding to the Friedrichs (resp., Dirichlet) boundary condition at $x=-1$ is determined via the requirement

$$\begin{aligned}
&\psi_{0,\alpha,\beta}(z,\,\cdot\,) = \theta_{0,\alpha,\beta}(z,\,\cdot\,) + m_{0,\alpha,\beta}(z)\phi_{0,\alpha,\beta}(z,\,\cdot\,) \in L^2((c,1); r_{\alpha,\beta}dx), \\
&\quad z \in \mathbb{C}\backslash\sigma(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1] \cup [1,\infty),\ \beta \in (-1,1),\ c \in (-1,1).
\end{aligned} \tag{4.4.18}$$

In particular, since $\widetilde{\psi}'_{0,\alpha,\beta}(z,-1) = m_{0,\alpha,\beta}(z)$ one finds from Theorem 4.3.2,

$$\begin{aligned}
M_{T_{0,\alpha,\beta},\mathcal{N}_i}^{Do}(z) &= \left[-i + \frac{m_{0,\alpha,\beta}(z) - m_{0,\alpha,\beta}(-i)}{\operatorname{Im}(m_{0,\alpha,\beta}(i))} \right] I_{\mathcal{N}_i}, \\
M_{T_{\gamma,\alpha,\beta},\mathcal{N}_i}^{Do}(z) &= M_{T_{0,\alpha,\beta},\mathcal{N}_i}^{Do}(z) + (i-z)\frac{m_{0,\alpha,\beta}(z) - m_{0,\alpha,\beta}(-i)}{\cot(\gamma) + m_{0,\alpha,\beta}(z)} \\
&\qquad \times (\psi_{0,\alpha,\beta}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)}\psi_{0,\alpha,\beta}(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \quad \gamma \in (0,\pi), \\
&\qquad\qquad \alpha \in (-\infty,-1] \cup [1,\infty),\ \beta \in (-1,1),\ z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned} \tag{4.4.19}$$

where $\psi_{0,\alpha,\beta}(z,\,\cdot\,)$ and $m_{0,\alpha,\beta}(z,\,\cdot\,)$ are given by the following:

(I) The Case $\boldsymbol{\alpha \in [1,\infty)}$ and $\boldsymbol{\beta \in (-1,0)}$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= y_{1,\alpha,\beta,-1}(z,x) - 2^{-\alpha-1}\beta^{-1}y_{2,\alpha,\beta,-1}(z,x)m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= 2^{1+\alpha+\beta}\beta\frac{\Gamma(1+\beta)}{\Gamma(1-\beta)} \\
&\quad \times \frac{\Gamma([1+\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\alpha+\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha+\beta-\sigma_{\alpha,\beta}(z)]/2)}, \\
&\qquad\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in [1,\infty),\ \beta \in (-1,0), \\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\beta)(n+1+\alpha)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta \in (-1,0),
\end{aligned} \tag{4.4.20}$$

with

$$\sigma_{\alpha,\beta}(z) = \big[(1+\alpha+\beta)^2 + 4z\big]^{1/2}. \tag{4.4.21}$$

(II) The Case $\boldsymbol{\alpha \in [1,\infty)}$ and $\boldsymbol{\beta = 0}$:

$$\begin{aligned}
\psi_{0,\alpha,0}(z,x) &= -2^{-\alpha-1}y_{2,\alpha,0,-1}(z,x) + y_{1,\alpha,0,-1}(z,x)m_{0,\alpha,0}(z), \\
m_{0,\alpha,0}(z) &= -2^{-\alpha-1}\{2\gamma_E + \psi([1+\alpha+\sigma_{\alpha,0}(z)]/2) + \psi([1+\alpha-\sigma_{\alpha,0}(z)]/2)\}, \\
&\qquad\qquad z \in \rho(T_{F,\alpha,0}),\ \alpha \in [1,\infty),\ \beta = 0, \\
\sigma(T_{F,\alpha,0}) &= \{n(n+1+\alpha)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta = 0.
\end{aligned} \tag{4.4.22}$$

(III) The Case $\boldsymbol{\alpha \in [1,\infty)}$ and $\boldsymbol{\beta \in (0,1)}$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= 2^{-\alpha-1}\beta^{-1}y_{2,\alpha,\beta,-1}(z,x) + y_{1,\alpha,\beta,-1}(z,x)m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= \beta^{-1}2^{-1-\alpha-\beta}\frac{-\Gamma(1-\beta)}{\Gamma(1+\beta)} \\
&\quad \times \frac{\Gamma([1+\alpha+\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha+\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma((1+\alpha-\beta-\sigma_{\alpha,\beta}(z))/2)}, \\
&\qquad\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in [1,\infty),\ \beta \in (0,1), \\
\sigma(T_{F,\alpha,\beta}) &= \{n(n+1+\alpha+\beta)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta \in (0,1).
\end{aligned} \tag{4.4.23}$$

(IV) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta \in (-1, 0)}$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= y_{1,\alpha,\beta,-1}(z,x) - 2^{-\alpha-1}\beta^{-1}y_{2,\alpha,\beta,-1}(z,x)m_{0,\alpha,\beta}(z),\\
m_{0,\alpha\,\beta}(z) &= 2^{1+\alpha+\beta}\beta\frac{\Gamma(1+\beta)}{\Gamma(1-\beta)}\\
&\quad\times\frac{\Gamma([1-\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1-\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\beta-\alpha+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\beta-\alpha-\sigma_{\alpha,\beta}(z)]/2)}, \qquad (4.4.24)\\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1],\ \beta \in (-1,0),\\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\alpha-\beta)(n+1)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta \in (-1,0).
\end{aligned}$$

(V) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta = 0}$:

$$\begin{aligned}
\psi_{0,\alpha,0}(z,x) &= -2^{-\alpha-1}y_{2,\alpha,0,-1}(z,x) + y_{1,\alpha,0,-1}(z,x)m_{0,\alpha,0}(z),\\
m_{0,\alpha,0}(z) &= -2^{-\alpha-1}\{2\gamma_E + \psi([1-\alpha+\sigma_{\alpha,0}(z)]/2) + \psi([1-\alpha-\sigma_{\alpha,0}(z)]/2)\},\\
&\qquad z \in \rho(T_{F,\alpha,0}),\ \alpha \in (-\infty,-1],\ \beta = 0,\\
\sigma(T_{F,\alpha,0}) &= \{(n-\alpha)(n+1)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta = 0. \qquad (4.4.25)
\end{aligned}$$

(VI) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta \in (0, 1)}$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= 2^{-\alpha-1}\beta^{-1}y_{2,\alpha,\beta,-1}(z,x) + y_{1,\alpha,\beta,-1}(z,x)m_{0,\alpha,\beta}(z),\\
m_{0,\alpha\,\beta}(z) &= -\beta^{-1}2^{-1-\alpha-\beta}\frac{\Gamma(1-\beta)}{\Gamma(1+\beta)}\\
&\quad\times\frac{\Gamma([1+\beta-\alpha+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\beta-\alpha-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1-\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1-\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}, \qquad (4.4.26)\\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1],\ \beta \in (0,1),\\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\alpha)(n+1+\beta)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta \in (0,1).
\end{aligned}$$

4.5 The Hypergeometric and Jacobi Differential Equations

In this section we provide the connection between the hypergeometric differential equation (cf. [1, Sect. 15.5])

$$\xi(1-\xi)\ddot{w}(\xi) + [c-(a+b+1)\xi]\dot{w}(\xi) - abw(\xi) = 0, \quad \xi \in (0,1), \qquad (4.5.1)$$

(where $\bullet = d/d\xi$) and the Jacobi differential equation

$$\tau_{\alpha,\beta} y(z,x) = -(1-x^2)y''(z,x) + [\alpha - \beta + (\alpha+\beta+2)x]y'(z,x) = zy(z,x), \\ \alpha,\beta \in \mathbb{R},\ x \in (-1,1), \tag{4.5.2}$$

(where $' = d/dx$). Making the substitution $\xi = (1+x)/2$ in (4.5.2) yields

$$\xi(1-\xi)\ddot{y}(z,\xi) + [\beta + 1 - (\alpha+\beta+2)\xi]\dot{y}(z,\xi) + zy(z,\xi) = 0, \\ \alpha,\beta \in \mathbb{R},\ \xi \in (0,1), \tag{4.5.3}$$

which is equal to (4.5.1) once one identifies,

$$a = [1+\alpha+\beta+\sigma_{\alpha,\beta}(z)]/2, \quad b = [1+\alpha+\beta-\sigma_{\alpha,\beta}(z)]/2, \quad c = 1+\beta, \\ \sigma_{\alpha,\beta}(z) = \big[(1+\alpha+\beta)^2 + 4z\big]^{1/2}. \tag{4.5.4}$$

At the endpoint $x = -1$ of the Jacobi equation the substitution used to arrive at (4.5.3) yields $\xi = 0$, hence we next consider solutions of (4.5.1) near $\xi = 0$ (cf. [1, Eqs. 15.5.3, 15.5.4]) (analogous solutions near $\xi = 1$ are found in (4.5.13))

$$w_{1,0}(\xi) = F(a,b;c;\xi) = \sum_{n\in\mathbb{N}_0} \frac{(a)_n(b)_n}{(c)_n}\frac{\xi^n}{n!}, \quad a,b \in \mathbb{C},\ c \in \mathbb{C}\backslash(-\mathbb{N}_0), \\ w_{2,0}(\xi) = \xi^{1-c}F(a-c+1, b-c+1; 2-c; \xi), \quad a,b \in \mathbb{C},\ (c-1) \in \mathbb{C}\backslash\mathbb{N}, \\ \xi \in (0,1). \tag{4.5.5}$$

Here $F(\,\cdot\,,\,\cdot\,;\,\cdot\,;\,\cdot\,)$ (frequently written as ${}_2F_1(\,\cdot\,,\,\cdot\,;\,\cdot\,;\,\cdot\,)$) denotes the hypergeometric function (see, e.g., [1, Ch. 15]), $\psi(\,\cdot\,) = \Gamma'(\,\cdot\,)/\Gamma(\,\cdot\,)$ the Digamma function, $\gamma_E = -\psi(1) = 0.57721\ldots$ represents Euler's constant, and

$$(\zeta)_0 = 1, \quad (\zeta)_n = \Gamma(\zeta+n)/\Gamma(\zeta),\ n \in \mathbb{N}, \quad \zeta \in \mathbb{C}\backslash(-\mathbb{N}_0), \tag{4.5.6}$$

abbreviates Pochhammer's symbol (see, e.g., [1, Ch. 6]).

In addition,

$$w_{1,0} \text{ and } w_{2,0} \text{ are linearly independent if } c \in \mathbb{C}\backslash\mathbb{Z}, \tag{4.5.7}$$

which can be seen by noticing the different behaviors of $w_{1,0}(\xi)$, $w_{2,0}(\xi)$ around $\xi = 0$. One notes that only the case $c = 1 + \beta \in (0,2)$ is needed. Thus, for $c = 1$ we will use instead

$$
\begin{aligned}
&w_{1,0}(\xi) = F(a,b;1;\xi), \quad a,b \in \mathbb{C}, \\
&w_{2,0}^{\ln}(\xi) = F(a,b;1;\xi)\ \ln(\xi) + \sum_{n\in\mathbb{N}} \frac{(a)_n(b)_n}{(n!)^2}\xi^n \\
&\quad \times [\psi(a+n) - \psi(a) + \psi(b+n) - \psi(b) - 2\psi(n+1) - 2\gamma_E], \quad a,b \in \mathbb{C}\backslash(-\mathbb{N}_0), \\
&\qquad \xi \in (0,1),
\end{aligned} \tag{4.5.8}
$$

where the superscipt "ln" indicates the presence of a logarithmic term (familiar from Frobenius theory).

Using (4.5.4) in formulas (4.5.5) and (4.5.8), one obtains for the solutions of the Jacobi differential equation $\tau_{\alpha,\beta} y(z,\,\cdot\,) = zy(z,\,\cdot\,)$ (cf. (4.5.2)) near $x=-1$,

$$
y_{1,\alpha,\beta,-1}(z,x) = F(a_{\alpha,\beta,\sigma_{\alpha,\beta}(z)}, a_{\alpha,\beta,-\sigma_{\alpha,\beta}(z)}; 1+\beta; (1+x)/2), \quad \beta \in \mathbb{R}\backslash(-\mathbb{N}), \tag{4.5.9}
$$

$$
y_{2,\alpha,\beta,-1}(z,x) = (1+x)^{-\beta} F(a_{\alpha,-\beta,\sigma_{\alpha,\beta}(z)}, a_{\alpha,-\beta,-\sigma_{\alpha,\beta}(z)}; 1-\beta; (1+x)/2), \quad \beta \in \mathbb{R}\backslash\mathbb{N}_0, \tag{4.5.10}
$$

$$
\begin{aligned}
y_{2,\alpha,0,-1}(z,x) &= F(a_{\alpha,0,\sigma_{\alpha,0}(z)}, a_{\alpha,0,-\sigma_{\alpha,0}(z)}; 1; (1+x)/2)\ \ln((1+x)/2) \\
&\quad + \sum_{n\in\mathbb{N}} \frac{(a_{\alpha,0,\sigma_{\alpha,0}(z)})_n (a_{\alpha,0,-\sigma_{\alpha,0}(z)})_n}{2^n (n!)^2} (1+x)^n \\
&\quad \times [\psi(a_{\alpha,0,\sigma_{\alpha,0}(z)}+n) - \psi(a_{\alpha,0,\sigma_{\alpha,0}(z)}) + \psi(a_{\alpha,0,-\sigma_{\alpha,0}(z)}+n) \\
&\quad - \psi(a_{\alpha,0,-\sigma_{\alpha,0}(z)}) - 2\psi(n+1) - 2\gamma_E], \quad \beta = 0, \\
&\qquad \alpha \in \mathbb{R},\ z \in \mathbb{C},\ x \in (-1,1),
\end{aligned} \tag{4.5.11}
$$

where we abbreviated

$$
a_{\mu,\nu,\pm\sigma} = [1+\mu+\nu\pm\sigma]/2, \quad \mu,\nu,\sigma \in \mathbb{C}. \tag{4.5.12}
$$

Again one observes that for $z \in \mathbb{C}$, $y_{1,\alpha,\beta,-1}(z,\,\cdot\,)$ and $y_{2,\alpha,\beta,-1}(z,\,\cdot\,)$ are linearly independent for $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}\backslash\mathbb{Z}$. Similarly, for $z \in \mathbb{C}$, $y_{1,\alpha,0,-1}(z,\,\cdot\,)$ and $y_{2,\alpha,0,-1}(z,\,\cdot\,)$ are linearly independent for $\alpha \in \mathbb{R}$.

In precisely the same manner additional solutions of (4.5.1) are given by

$$
\begin{aligned}
&w_{1,1}(\xi) = F(a,b;a+b-c+1;1-\xi), \quad a,b \in \mathbb{C},\ c-a-b \in \mathbb{C}\backslash\mathbb{N}, \\
&w_{2,1}(\xi) = (1-\xi)^{c-a-b} F(c-a,c-b;c-a-b+1;1-\xi), \\
&\qquad\qquad a,b \in \mathbb{C},\ a+b-c \in \mathbb{C}\backslash\mathbb{N},
\end{aligned}
\tag{4.5.13}
$$

and for $a+b-c=0$,

$$
\begin{aligned}
&w_{1,1}(\xi) = F(a,b;1;1-\xi), \quad a,b \in \mathbb{C}, \\
&w_{2,1}^{\ln}(\xi) = F(a,b;1;1-\xi)\ln(1-\xi) + \sum_{n\in\mathbb{N}} \frac{(a)_n (b)_n}{(n!)^2}(1-\xi)^n \\
&\qquad \times [\psi(a+n) - \psi(a) + \psi(b+n) - \psi(b) - 2\psi(n+1) - 2\gamma_E], \\
&\qquad\qquad a,b \in \mathbb{C},\ \xi \in (0,1),
\end{aligned}
\tag{4.5.14}
$$

which are obtained from (4.5.5) and (4.5.8) by the change of variables

$$
(a,\, b,\, c,\, \xi) \to (a,\, b,\, a+b-c+1,\, 1-\xi). \tag{4.5.15}
$$

Together with the identification $x = (1+\xi)/2$ and (4.5.4) one obtains the following solutions of $\tau_{\alpha,\beta} y(z,\,\cdot\,) = zy(z,\,\cdot\,)$ near $x=+1$,

$$
\begin{aligned}
&y_{1,\alpha,\beta,+1}(z,x) = F(a_{\alpha,\beta,\sigma_{\alpha,\beta}(z)}, a_{\alpha,\beta,-\sigma_{\alpha,\beta}(z)}; 1+\alpha; (1-x)/2), \\
&\qquad\qquad \alpha \in \mathbb{R}\backslash(-\mathbb{N}),
\end{aligned}
\tag{4.5.16}
$$

$$
\begin{aligned}
&y_{2,\alpha,\beta,+1}(z,x) = (1-x)^{-\alpha} F(a_{-\alpha,\beta,\sigma_{\alpha,\beta}(z)}, a_{-\alpha,\beta,-\sigma_{\alpha,\beta}(z)}; 1-\alpha; (1-x)/2) \\
&\qquad\qquad \alpha \in \mathbb{R}\backslash\mathbb{N},
\end{aligned}
\tag{4.5.17}
$$

$$
\begin{aligned}
&y_{2,0,\beta,+1}(z,x) = F(a_{0,\beta,\sigma_{0,\beta}(z)}, a_{0,\beta,-\sigma_{0,\beta}(z)}; 1; (1-x)/2)\ \ln((1-x)/2) \\
&\quad + \sum_{n\in\mathbb{N}} \frac{(a_{0,\beta,\sigma_{0,\beta}(z)})_n (a_{0,\beta,-\sigma_{0,\beta}(z)})_n}{2^n (n!)^2}(1-x)^n \\
&\quad \times [\psi(a_{0,\beta,\sigma_{0,\beta}(z)}+n) - \psi(a_{0,\beta,\sigma_{0,\beta}(z)}) + \psi(a_{0,\beta,-\sigma_{0,\beta}(z)}+n) \\
&\quad - \psi(a_{0,\beta,-\sigma_{0,\beta}(z)}) - 2\psi(n+1) - 2\gamma_E], \quad \alpha = 0, \\
&\qquad\qquad \beta \in \mathbb{R},\ z \in \mathbb{C},\ x \in (-1,1).
\end{aligned}
\tag{4.5.18}
$$

Again, for $z \in \mathbb{C}$, $y_{1,\alpha,\beta,+1}(z,\,\cdot\,)$ and $y_{2,\alpha,\beta,+1}(z,\,\cdot\,)$ are linearly independent for $\alpha \in \mathbb{R}\backslash\mathbb{Z}$, $\beta \in \mathbb{R}$. Similarly, for $z \in \mathbb{C}$, $y_{1,0,\beta,+1}(z,\,\cdot\,)$ and $y_{2,0,\beta,+1}(z,\,\cdot\,)$ are linearly independent for $\beta \in \mathbb{R}$.

In the limit point case at $x = 1$, where $\alpha \in (-\infty,-1] \cup [1,\infty)$, one only needs the principal solutions, which are $y_{1,\alpha,\beta,+1}(z,\,\cdot\,)$ for $\alpha \geqslant 1$ and $y_{2,\alpha,\beta,+1}(z,\,\cdot\,)$ for $\alpha \leqslant -1$. Thus, one concludes from (4.5.16) and (4.5.17) that these case are already covered, and one does not have to define an additional solution for $\alpha \in \mathbb{Z}\backslash\{0\}$.

Since $(a_{\alpha,\beta,\sigma_{\alpha,\beta}(z)})_n(a_{\alpha,\beta,-\sigma_{\alpha,\beta}(z)})_n$, $n \in \mathbb{N}_0$, depends polynomially on $z \in \mathbb{C}$, one infers that

$$\text{for fixed } x \in (0,1),\ y_{j,\alpha,\beta,\pm1}(z,x),\ j = 1,2, \text{ are entire with respect to } z \in \mathbb{C}. \tag{4.5.19}$$

Moreover $y_{j,\alpha,\beta,\pm1}(z,x)$ satisfy the relations (cf. (4.5.28))

$$y_{1,\alpha,\beta,-1}(z,x) = (1+x)^{-\beta} y_{2,\alpha,-\beta,-1}(z + (1+\alpha)\beta, x), \quad \alpha \in \mathbb{R},\ \beta \in \mathbb{R}\backslash\{0\}, \tag{4.5.20}$$

$$y_{2,\alpha,\beta,-1}(z,x) = (1+x)^{-\beta} y_{1,\alpha,-\beta,-1}(z + (1+\alpha)\beta, x), \quad \alpha \in \mathbb{R},\ \beta \in \mathbb{R}\backslash\{0\}, \tag{4.5.21}$$

$$y_{1,\alpha,\beta,+1}(z,x) = (1-x)^{-\alpha} y_{2,-\alpha,\beta,+1}(z + (1+\beta)\alpha, x), \quad \alpha \in \mathbb{R}\backslash\{0\},\ \beta \in \mathbb{R}, \tag{4.5.22}$$

$$y_{2,\alpha,\beta,+1}(z,x) = (1-x)^{-\alpha} y_{1,-\alpha,\beta,+1}(z + (1+\beta)\alpha, x), \quad \alpha \in \mathbb{R}\backslash\{0\},\ \beta \in \mathbb{R}, \tag{4.5.23}$$

where we used the fact

$$\sigma_{\alpha,\beta}(z) = \begin{cases} \sigma_{\alpha,-\beta}(z + (1+\alpha)\beta), \\ \sigma_{-\alpha,\beta}(z + (1+\beta)\alpha), \\ \sigma_{-\alpha,-\beta}(z + \alpha + \beta). \end{cases} \tag{4.5.24}$$

Remark 4.5.1. We conclude this section by briefly discussing Jacobi polynomials and quasi-rational eigenfunctions. The nth Jacobi polynomial is defined as (see [151, Eq. 18.5.7])

$$\begin{aligned} P_n^{\alpha,\beta}(x) := \frac{(\alpha+1)_n}{n!} F(-n, n+\alpha+\beta+1; \alpha+1; (1-x)/2), \\ n \in \mathbb{N}_0,\ -\alpha \notin \mathbb{N},\ (-n-\alpha-\beta-1) \notin \mathbb{N}, \end{aligned} \tag{4.5.25}$$

and can be defined by continuity for all parameters $\alpha, \beta \in \mathbb{R}$. Note that $P_n^{\alpha,\beta}(x)$ is a polynomial of degree at most n, and has strictly smaller degree if and only if $-n-\alpha-\beta \in \{1, \dots, n\}$ (cf. [173, p. 64]). It satisfies the equation

$$\tau_{\alpha,\beta} P_n^{\alpha,\beta}(x) = \lambda_n^{\alpha,\beta} P_n^{\alpha,\beta}(x), \tag{4.5.26}$$

with

$$\lambda_n^{\alpha,\beta} := n(n+1+\alpha+\beta). \tag{4.5.27}$$

In particular, one can verify that the Jacobi polynomials are solutions of the Jacobi differential equation (4.5.2) with Neumann boundary conditions at $x = +1$ (resp. $x = -1$) if $\alpha \in (-1, 0)$ (resp. $\beta \in (-1, 0)$) and Friedrichs boundary conditions if $\alpha \geqslant 0$ (resp. $\beta \geqslant 0$).

More generally, all quasi-rational solutions, meaning the logarithmic derivative being rational, can be derived from the the Jacobi polynomials together with

$$\begin{aligned} &(1+x)^{-\beta} \circ \tau_{\alpha,-\beta} \circ (1+x)^{\beta} = \tau_{\alpha,\beta} + (1+\alpha)\beta, \\ &(1-x)^{-\alpha} \circ \tau_{-\alpha,\beta} \circ (1-x)^{\alpha} = \tau_{\alpha,\beta} + (1+\beta)\alpha, \\ &(1-x)^{-\alpha}(1+x)^{-\beta} \circ \tau_{-\alpha,-\beta} \circ (1-x)^{\alpha}(1+x)^{\beta} = \tau_{\alpha,\beta} + \alpha + \beta, \end{aligned} \tag{4.5.28}$$

where $(1+x)^{\pm\beta}$ and $(1-x)^{\pm\alpha}$ are regarded as formal multiplication operators. This is summarized in Table 4.1, which is taken from [22]. Here $(1-x)^{-\alpha} P_n^{-\alpha,\beta}(x)$ satisfy at $x = +1$ the Friedrichs boundary condition for $\alpha \leqslant 0$ and Neumann for $\alpha \in (0, 1)$, while at $x = -1$ they satisfy the Friedrichs for $\beta \geqslant 0$ and Neumann for $\beta \in (-1, 0)$. For $(1+x)^{-\beta} P_n^{\alpha,-\beta}(x)$ the roles of α and β interchange compared to the last case,

Table 4.1. Formal quasi-rational eigensolutions of $\tau_{\alpha,\beta}$

Eigenfunctions	Eigenvalues
$P_n^{\alpha,\beta}(x)$	$n(n+1+\alpha+\beta)$
$(1-x)^{-\alpha}P_n^{-\alpha,\beta}(x)$	$n(n+1-\alpha+\beta)-\alpha(1+\beta)$
$(1+x)^{-\beta}P_n^{\alpha,-\beta}(x)$	$n(n+1+\alpha-\beta)-\beta(1+\alpha)$
$(1-x)^{-\alpha}(1+x)^{-\beta}P_n^{-\alpha,-\beta}(x)$	$n(n+1-\alpha-\beta)-(\alpha+\beta)$

meaning Friedrichs at $x=+1$ for $\alpha \geqslant 0$, Neumann for $\alpha \in (-1,0)$, and at $x=-1$, Friedrichs for $\beta \leqslant 0$, Neumann for $\beta \in (0,1)$. Finally $(1-x)^{-\alpha}(1+x)^{-\beta}P_n^{-\alpha,-\beta}(x)$ satisfy at $x=+1$ (resp. $x=-1$) the Friedrichs boundary condition for $\alpha \leqslant 0$ (resp. $\beta \leqslant 0$) and Neumann for $\alpha \in (0,1)$ (resp. $\beta \in (0,1)$). $\diamond$

4.6 Connection Formulas

In this section we provide the connection formulas utilized to find the solution behaviors in Section 4.7. We express them using $w_{1,0}(\xi)$ and $w_{2,0}(\xi)$ $\big(w_{2,0}^{\ln}(\xi)\big)$ and their analogs $w_{1,1}(\xi)$ and $w_{2,1}(\xi)$ $\big(w_{2,1}^{\ln}(\xi)\big)$ at the endpoint $\xi=1$.

We recall the relations (4.5.4) connecting the parameters a,b,c and α,β.

(**I**) *The case $\alpha \in \mathbb{R}\backslash\mathbb{Z}$, $\beta \in (-1,1)\backslash\{0\}$, that is, $c \in (0,2)\backslash\{1\}$, $a+b-c \in \mathbb{R}\backslash\mathbb{Z}$:*

The two connection formulas are given by (cf. [152, Eq. 15.10.21–22])

$$w_{1,0}(\xi) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}w_{1,1}(\xi) + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}w_{2,1}(\xi), \tag{4.6.1}$$

$$w_{2,0}(\xi) = \frac{\Gamma(2-c)\Gamma(c-a-b)}{\Gamma(1-a)\Gamma(1-b)}w_{1,1}(\xi) + \frac{\Gamma(2-c)\Gamma(a+b-c)}{\Gamma(a-c+1)\Gamma(b-c+1)}w_{2,1}(\xi). \tag{4.6.2}$$

One notes that poles occur on the right-hand side of (4.6.1), (4.6.2) whenever $(a+b-c) \in \mathbb{Z}$. Using (4.5.15) one can also express $w_{1,1}(\xi)$ or $w_{2,1}(\xi)$ as a linear combination of $w_{1,0}(\xi)$ and $w_{2,0}(\xi)$:

$$w_{1,1}(\xi) = \frac{\Gamma(a+b-c+1)\Gamma(1-c)}{\Gamma(a-c+1)\Gamma(b-c+1)}w_{1,0}(\xi) + \frac{\Gamma(a+b-c+1)\Gamma(c-1)}{\Gamma(a)\Gamma(b)}w_{2,0}(\xi), \tag{4.6.3}$$

$$w_{2,1}(\xi) = \frac{\Gamma(1+c-a-b)\Gamma(1-c)}{\Gamma(1-a)\Gamma(1-b)} w_{1,0}(\xi) + \frac{\Gamma(1+c-a-b)\Gamma(c-1)}{\Gamma(c-a)\Gamma(c-b)} w_{2,0}(\xi), \tag{4.6.4}$$

though, in the following we shall only write down one pair of connection formulas for brevity.

(**II**) *The case $\alpha = 0$, $\beta \in \mathbb{R}\backslash\mathbb{Z}$, that is, $c \in \mathbb{R}\backslash\mathbb{Z}$, $a + b = c$:*

The solution $w_{1,0}(\xi) = F(a, b; a+b; \xi)$ can be expanded at $\xi = 1$ (cf. [1, Eq. 15.3.10]):

$$\begin{aligned} F(a, b; a+b; \xi) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \sum_{n\in\mathbb{N}_0} \frac{(a)_n(b)_n}{(n!)^2} &[2\psi(n+1) - \psi(a+n) - \psi(b+n) \\ &- \ln(1-\xi)](1-\xi)^n. \end{aligned} \tag{4.6.5}$$

Meanwhile, two linearly independent solutions at $\xi = 1$ are taken from (4.5.14). The connection formula for $w_{1,1}(\xi)$ is given by (4.6.3) with $a + b = c$. To obtain a second connection formula one compares the expansion of $w_{2,1}^{\ln}(\xi)$ at $\xi = 1$ with the expansion of $F(a, b; a + b; \xi)$ at $\xi = 1$, using (4.6.5), and then obtains

$$\begin{aligned} w_{2,1}^{\ln}(\xi) = &- [\psi(1-a) + \psi(1-b) + 2\gamma_E] \frac{\Gamma(1-a-b)}{\Gamma(1-a)\Gamma(1-b)} w_{1,0}(\xi) \\ &- [\psi(a) + \psi(b) + 2\gamma_E] \frac{\Gamma(a+b-1)}{\Gamma(a)\Gamma(b)} w_{2,0}(\xi). \end{aligned} \tag{4.6.6}$$

(**III**) *The case $\alpha \in \mathbb{R}\backslash\mathbb{Z}$, $\beta = 0$, that is, $c = 1$, $a + b \in \mathbb{R}\backslash\mathbb{Z}$:*

This case is analogous to the previous case, with the roles of α and β interchanged. Concretely, this means that the connection formulas (4.6.5) and (4.6.6) must be changed through the renaming (4.5.15) with $c \to a + b - c + 1 = a + b$, as $c = 1$. As c does not appear in (4.6.5) and (4.6.6) (it was eliminated via $c = a + b$), one can adopt the aforementioned formulas directly, only changing the second index in the w's

$$w_{1,0}(\xi) = \frac{\Gamma(1-a-b)}{\Gamma(1-a)\Gamma(1-b)} w_{1,1}(\xi) + \frac{\Gamma(a+b-1)}{\Gamma(a)\Gamma(b)} w_{2,1}(\xi), \tag{4.6.7}$$

$$w_{2,0}^{\ln}(\xi) = -[\psi(1-a) + \psi(1-b) + 2\gamma_E] \frac{\Gamma(1-a-b)}{\Gamma(1-a)\Gamma(1-b)} w_{1,1}(\xi)$$

$$- [\psi(a) + \psi(b) + 2\gamma_E]\frac{\Gamma(a+b-1)}{\Gamma(a)\Gamma(b)} w_{2,1}(\xi). \tag{4.6.8}$$

(**IV**) *The case $\alpha = \beta = 0$, that is, $a + b = c = 1$:*

For $\alpha = 0$ and $\beta = 0$ the Jacobi differential expression (4.4.1) becomes the Legendre differential expression. Since this case was treated in detail in [75], we shall only present the connection formulas for completeness.

The special solutions $w_{1,i}(\xi)$ and $w_{2,i}^{\ln}(\xi)$ for $i = 1, 2$ are given by (4.5.8) and (4.5.14), respectively. Note that the following relations hold

$$w_{1,1}(\xi) = w_{1,0}(1-\xi), \qquad w_{2,1}^{\ln}(\xi) = w_{2,0}^{\ln}(1-\xi). \tag{4.6.9}$$

Using [1, Eq. 15.3.10] together with $w_{1,0}(\xi) = F(a, b; a + b; \xi)$ and Euler's famous reflection formula, $\Gamma(z)\Gamma(1 - z) = \pi \csc(\pi z)$ (cf. [1, Eq. 6.1.17]), one obtains

$$w_{1,0}(\xi) = -\pi^{-1}\sin(\pi a)\big([\psi(a) + \psi(b) + 2\gamma_E] w_{1,1}(\xi) + w_{2,1}^{\ln}(\xi)\big). \tag{4.6.10}$$

The two relations (4.6.9) immediately imply

$$w_{1,1}(\xi) = -\pi^{-1}\sin(\pi a)\big([\psi(a) + \psi(b) + 2\gamma_E] w_{1,0}(\xi) + w_{2,0}^{\ln}(\xi)\big), \tag{4.6.11}$$

$$\begin{aligned} w_{2,1}^{\ln}(\xi) = \pi^{-1}\sin(\pi a)\big[&\big([\psi(a) + \psi(b) + 2\gamma_E]^2 - \pi^2[\sin(\pi a)]^{-2}\big) w_{1,0}(\xi) \\ &+ [\psi(a) + \psi(b) + 2\gamma_E] w_{2,0}^{\ln}(\xi)\big]. \end{aligned} \tag{4.6.12}$$

4.7 Behavior of $y_{j,\alpha,\beta,\mp 1}(z,x)$, $j=1,2$, near $x=\pm 1$

In this section we focus on the generalized boundary values for the solutions $y_{j,\alpha,\beta,-1}(z,x),\ j=1,2$ at $x=\mp 1$. One obtains for $z\in\mathbb{C}$,

$$
\left.\begin{aligned}
&\widetilde{y}_{1,\alpha,\beta,-1}(z,-1)=\begin{cases}1, & \beta\in(-1,0),\\ 0, & \beta=0,\\ 0, & \beta\in(0,1),\end{cases}\\
&\widetilde{y}'_{1,\alpha,\beta,-1}(z,-1)=\begin{cases}0, & \beta\in(-1,0),\\ 1, & \beta=0,\\ 1, & \beta\in(0,1),\end{cases}\\
&\widetilde{y}_{2,\alpha,\beta,-1}(z,-1)=\begin{cases}0, & \beta\in(-1,0),\\ -2^{\alpha+1}, & \beta=0,\\ \beta 2^{\alpha+1}, & \beta\in(0,1),\end{cases}\\
&\widetilde{y}'_{2,\alpha,\beta,-1}(z,-1)=\begin{cases}-\beta 2^{\alpha+1}, & \beta\in(-1,0),\\ 0, & \beta=0,\\ 0, & \beta\in(0,1),\end{cases}
\end{aligned}\right\}\quad \alpha\in\mathbb{R}, \tag{4.7.1}
$$

and employing connection formulas for the endpoint $x=+1$,

$$
\widetilde{y}_{1,\alpha,\beta,-1}(z,1)=\begin{cases}\dfrac{\Gamma(1+\beta)\Gamma(-\alpha)}{\Gamma(a_{-\alpha,\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{-\alpha,\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha\in(-1,0),\\[2ex] \dfrac{-2^{1+\alpha+\beta}\Gamma(1+\alpha)\Gamma(1+\beta)}{\Gamma(a_{\alpha,\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{\alpha,\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha\in[0,1),\end{cases}
$$

$$\widetilde{y}'_{1,\alpha,\beta,-1}(z,1) = \begin{cases} \dfrac{2^{1+\alpha+\beta}\Gamma(1+\alpha)\Gamma(1+\beta)}{\Gamma(a_{\alpha,\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{\alpha,\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in (-1,0), \\ \dfrac{-\Gamma(1+\beta)}{\Gamma(a_{0,\beta,\sigma_{0,\beta}(z)})\Gamma(a_{0,\beta,-\sigma_{0,\beta}(z)})}[2\gamma_E & \\ \quad +\psi(a_{0,\beta,\sigma_{0,\beta}(z)}) + \psi(a_{0,\beta,-\sigma_{0,\beta}(z)})], & \alpha = 0, \\ \dfrac{\Gamma(1+\beta)\Gamma(-\alpha)}{\Gamma(a_{-\alpha,\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{-\alpha,\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in (0,1), \end{cases}$$

$$\beta \in (-1,1), \tag{4.7.2}$$

$$\widetilde{y}_{2,\alpha,\beta,-1}(z,1) = \begin{cases} \dfrac{2^{-\beta}\Gamma(1-\beta)\Gamma(-\alpha)}{\Gamma(a_{-\alpha,-\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{-\alpha,-\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in (-1,0), \\ \dfrac{-2^{\alpha+1}\Gamma(1+\alpha)\Gamma(1-\beta)}{\Gamma(a_{\alpha,-\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{\alpha,-\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in [0,1), \end{cases}$$

$$\widetilde{y}'_{2,\alpha,\beta,-1}(z,1) = \begin{cases} \dfrac{2^{\alpha+1}\Gamma(1+\alpha)\Gamma(1-\beta)}{\Gamma(a_{\alpha,-\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{\alpha,-\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in (-1,0), \\ \dfrac{-2^{-\beta}\Gamma(1-\beta)}{\Gamma(a_{0,-\beta,\sigma_{0,\beta}(z)})\Gamma(a_{0,-\beta,-\sigma_{0,\beta}(z)})}[2\gamma_E & \\ \quad +\psi(a_{0,-\beta,\sigma_{0,\beta}(z)}) + \psi(a_{0,-\beta,-\sigma_{0,\beta}(z)})], & \alpha = 0, \\ \dfrac{2^{-\beta}\Gamma(1-\beta)\Gamma(-\alpha)}{\Gamma(a_{-\alpha,-\beta,\sigma_{\alpha,\beta}(z)})\Gamma(a_{-\alpha,-\beta,-\sigma_{\alpha,\beta}(z)})}, & \alpha \in (0,1), \end{cases}$$

$$\beta \in (-1,1)\backslash\{0\}, \tag{4.7.3}$$

$$\widetilde{y}_{2,\alpha,0,-1}(z,1) = \begin{cases} \dfrac{-[2\gamma_E + \psi(a_{-\alpha,0,\sigma_{\alpha,0}(z)}) + \psi(a_{-\alpha,0,-\sigma_{\alpha,0}(z)})]\Gamma(-\alpha)}{\Gamma(a_{-\alpha,0,\sigma_{\alpha,0}(z)})\Gamma(a_{-\alpha,0,-\sigma_{\alpha,0}(z)})}, \\ \qquad \alpha \in (-1,0), \\ \dfrac{[2\gamma_E + \psi(a_{\alpha,0,\sigma_{\alpha,0}(z)}) + \psi(a_{\alpha,0,-\sigma_{\alpha,0}(z)})]\Gamma(1+\alpha)}{2^{-\alpha-1}\Gamma(a_{\alpha,0,\sigma_{\alpha,0}(z)})\Gamma(a_{\alpha,0,-\sigma_{\alpha,0}(z)})}, \\ \qquad \alpha \in [0,1), \end{cases}$$

$$\widetilde{y}'_{2,\alpha,0,-1}(z,1) = \begin{cases} \dfrac{[2\gamma_E + \psi(a_{\alpha,0,\sigma_{\alpha,0}(z)}) + \psi(a_{\alpha,0,-\sigma_{\alpha,0}(z)})]\Gamma(1+\alpha)}{-2^{-\alpha-1}\Gamma(a_{\alpha,0,\sigma_{\alpha,0}(z)})\Gamma(a_{\alpha,0,-\sigma_{\alpha,0}(z)})}, \\ \qquad\qquad\qquad\qquad\qquad\qquad \alpha \in (-1,0), \\ -\Gamma((1+\sigma_{0,0}(z))/2)\Gamma((1-\sigma_{0,0}(z))/2) \\ +\dfrac{[2\gamma_E + \psi((1+\sigma_{0,0}(z))/2) + \psi((1-\sigma_{0,0}(z))/2)]^2}{\Gamma((1+\sigma_{0,0}(z))/2)\Gamma((1-\sigma_{0,0}(z))/2)}, \quad \alpha = 0, \\ \dfrac{-[2\gamma_E + \psi(a_{-\alpha,0,\sigma_{\alpha,0}(z)}) + \psi(a_{-\alpha,0,-\sigma_{\alpha,0}(z)})]\Gamma(-\alpha)}{\Gamma(a_{-\alpha,0,\sigma_{\alpha,0}(z)})\Gamma(a_{-\alpha,0,-\sigma_{\alpha,0}(z)})}, \\ \qquad\qquad\qquad\qquad\qquad\qquad \alpha \in (0,1), \end{cases}$$

$$\beta = 0. \tag{4.7.4}$$

CHAPTER FIVE

Conclusion

In Chapter Two, we employed a recently developed unified approach to the computation of Fredholm determinants, traces of resolvents, and ζ-functions to compute positive integer values of spectral ζ-functions associated with regular Sturm–Liouville operators. We proved the following result relating these values and the characteristic function $F_{A,B}(\,\cdot\,)$:

Theorem 2.4.1. *Assume Hypothesis* 2.2.1*, denote by $T_{A,B}$ the self-adjoint extension of T_{min} with either separated or coupled boundary conditions as described in Theorem* 2.2.2*, and let $m_0 = 0, 1, 2,$ denote the multiplicity of zero as an eigenvalue of $T_{A,B}$* (*with $m_0 = 0$ denoting zero is not an eigenvalue*)*. Suppose that $F_{A,B}(z)$ given in* (2.2.39) *has the series expansion,*

$$F_{A,B}(z) = \sum_{j=0}^{\infty} a_j z^j, \quad 0 \leqslant |z| \text{ sufficiently small.} \tag{5.0.1}$$

Then,

$$\zeta(n; T_{A,B}) = -\mathrm{Res}\left[z^{-n} \frac{d}{dz} \ln(F_{A,B}(z));\ z = 0\right] = -n\, b_n, \quad n \in \mathbb{N}, \tag{5.0.2}$$

where

$$\begin{aligned} &b_1 = a_{1+m_0}/a_{m_0}, \\ &b_j = [a_{j+m_0}/a_{m_0}] - \sum_{\ell=1}^{j-1} [\ell/j][a_{j-\ell+m_0}/a_{m_0}] b_\ell, \quad j \in \mathbb{N},\ j \geqslant 2. \end{aligned} \tag{5.0.3}$$

In particular, if zero is not an eigenvalue of $T_{A,B}$, then

$$\mathrm{tr}_{L^2_r((a,b))}\big(T_{A,B}^{-1}\big) = \zeta(1; T_{A,B}) = -a_1/a_0. \tag{5.0.4}$$

This result along with the series expansions proven in Section 2.3.1 using Volterra integral equations allows for an efficient computation of positive integer values of spectral ζ-functions as illustrated in Section 2.4.2. In particular, when considering general self-adjoint boundary conditions we proved

$$\zeta(n;T_{\alpha,\beta}) = -\mathrm{Res}\left[z^{-n}\frac{d}{dz}\ln(F_{\alpha,\beta}(z));\ z=0\right] = -n\,b_n, \quad n\in\mathbb{N}, \tag{5.0.5}$$

where for separated boundary conditions,

$$b_1 = \frac{\cos(\alpha)\big[\cos(\beta)\phi_{1+m_0}(b)-\sin(\beta)\phi^{[1]}_{1+m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{1+m_0}(b)-\sin(\beta)\theta^{[1]}_{1+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b)-\sin(\beta)\phi^{[1]}_{m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b)-\sin(\beta)\theta^{[1]}_{m_0}(b)\big]},$$

$$\begin{aligned} b_j = {} & \frac{\cos(\alpha)\big[\cos(\beta)\phi_{j+m_0}(b)-\sin(\beta)\phi^{[1]}_{j+m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{j+m_0}(b)-\sin(\beta)\theta^{[1]}_{j+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b)-\sin(\beta)\phi^{[1]}_{m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b)-\sin(\beta)\theta^{[1]}_{m_0}(b)\big]} \\ & -\sum_{\ell=1}^{j-1}\left(\frac{\ell}{j}\right)\frac{\cos(\alpha)\big[\cos(\beta)\phi_{j-\ell+m_0}(b)-\sin(\beta)\phi^{[1]}_{j-\ell+m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{j-\ell+m_0}(b)-\sin(\beta)\theta^{[1]}_{j-\ell+m_0}(b)\big]}{\cos(\alpha)\big[\cos(\beta)\phi_{m_0}(b)-\sin(\beta)\phi^{[1]}_{m_0}(b)\big]-\sin(\alpha)\big[\cos(\beta)\theta_{m_0}(b)-\sin(\beta)\theta^{[1]}_{m_0}(b)\big]}b_\ell, \\ & j\in\mathbb{N},\ j\geqslant 2, \end{aligned} \tag{5.0.6}$$

while for coupled boundary conditions with $m_0 = 0$,

$$\begin{aligned} b_1 &= \frac{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b)-R_{22}\theta_1(b)+R_{21}\phi_1(b)-R_{11}\phi_1^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b)-R_{22}\theta_0(b)+R_{21}\phi_0(b)-R_{11}\phi_0^{[1]}(b)\big)+e^{2i\varphi}+1}, \\ b_j &= \frac{e^{i\varphi}\big(R_{12}\theta_j^{[1]}(b)-R_{22}\theta_j(b)+R_{21}\phi_j(b)-R_{11}\phi_j^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b)-R_{22}\theta_0(b)+R_{21}\phi_0(b)-R_{11}\phi_0^{[1]}(b)\big)+e^{2i\varphi}+1} \\ &\quad -\sum_{\ell=1}^{j-1}\frac{\ell}{j}\frac{e^{i\varphi}\big(R_{12}\theta_{j-\ell}^{[1]}(b)-R_{22}\theta_{j-\ell}(b)+R_{21}\phi_{j-\ell}(b)-R_{11}\phi_{j-\ell}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_0^{[1]}(b)-R_{22}\theta_0(b)+R_{21}\phi_0(b)-R_{11}\phi_0^{[1]}(b)\big)+e^{2i\varphi}+1}b_\ell, \\ &\quad j\in\mathbb{N},\ j\geqslant 2, \end{aligned} \tag{5.0.7}$$

and for $m_0 = 1$,

$$\begin{aligned} b_1 &= \frac{e^{i\varphi}\big(R_{12}\theta_2^{[1]}(b)-R_{22}\theta_2(b)+R_{21}\phi_2(b)-R_{11}\phi_2^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b)-R_{22}\theta_1(b)+R_{21}\phi_1(b)-R_{11}\phi_1^{[1]}(b)\big)}, \\ b_j &= \frac{e^{i\varphi}\big(R_{12}\theta_{j+1}^{[1]}(b)-R_{22}\theta_{j+1}(b)+R_{21}\phi_{j+1}(b)-R_{11}\phi_{j+1}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b)-R_{22}\theta_1(b)+R_{21}\phi_1(b)-R_{11}\phi_1^{[1]}(b)\big)} \\ &\quad -\sum_{\ell=1}^{j-1}\frac{\ell}{j}\frac{e^{i\varphi}\big(R_{12}\theta_{j-\ell+1}^{[1]}(b)-R_{22}\theta_{j-\ell+1}(b)+R_{21}\phi_{j-\ell+1}(b)-R_{11}\phi_{j-\ell+1}^{[1]}(b)\big)}{e^{i\varphi}\big(R_{12}\theta_1^{[1]}(b)-R_{22}\theta_1(b)+R_{21}\phi_1(b)-R_{11}\phi_1^{[1]}(b)\big)}b_\ell, \\ &\quad j\in\mathbb{N},\ j\geqslant 2. \end{aligned} \tag{5.0.8}$$

For the case $m_0 = 2$, we need only consider the Krein-von Neumann extension of T_{min} defined by

$$\varphi = 0, \quad R_K = \begin{pmatrix} \theta(0,b,a) & \phi(0,b,a) \\ \theta^{[1]}(0,b,a) & \phi^{[1]}(0,b,a) \end{pmatrix}, \tag{5.0.9}$$

where

$$b_1 = \frac{\phi_0(b)\theta_3^{[1]}(b) - \phi_0^{[1]}(b)\theta_3(b) + \theta_0^{[1]}(b)\phi_3(b) - \theta_0(b)\phi_3^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)},$$

$$\begin{aligned} b_j = {} & \frac{\phi_0(b)\theta_{j+2}^{[1]}(b) - \phi_0^{[1]}(b)\theta_{j+2}(b) + \theta_0^{[1]}(b)\phi_{j+2}(b) - \theta_0(b)\phi_{j+2}^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)} \\ & - \sum_{\ell=1}^{j-1} \frac{\ell}{j} \, \frac{\phi_0(b)\theta_{j-\ell+2}^{[1]}(b) - \phi_0^{[1]}(b)\theta_{j-\ell+2}(b) + \theta_0^{[1]}(b)\phi_{j-\ell+2}(b) - \theta_0(b)\phi_{j-\ell+2}^{[1]}(b)}{\phi_0(b)\theta_2^{[1]}(b) - \phi_0^{[1]}(b)\theta_2(b) + \theta_0^{[1]}(b)\phi_2(b) - \theta_0(b)\phi_2^{[1]}(b)} b_\ell, \\ & j \in \mathbb{N},\ j \geqslant 2. \end{aligned} \tag{5.0.10}$$

Furthermore, assuming Hypothesis 2.3.1, we computed the asymptotic expansion in the spectral parameter of the characteristic function where more assumptions are needed on the transformed potential depending on the number of terms included. We then used this expansion to obtain the remarkably simple formula

$$\zeta'(0; T_{A,B}) = i\pi n - \ln(2c|\mathcal{F}_{m_0}/\Gamma_{k_0}|), \tag{5.0.11}$$

where n is the number of strictly negative eigenvalues of $T_{A,B}$. This allows one to efficiently compute the associated ζ-regularized functional determinant for this restricted class of regular Sturm–Liouville operators. Finally, we applied these results to regular Schrödinger operators with zero, piecewise constant, and a linear potential on a compact interval.

In Chapter Three, we systematically constructed the Donoghue m-functions (resp., 2×2 matrices) associated to the singular Sturm–Liouville operator in all cases where at least at one interval endpoint a or b is in the limit circle case. For brevity, we do not list the full form of the Donoghue m-functions here but instead recall that they are summarized succinctly in Sections 4.2 and 4.3 for two limit circle endpoints and one limit circle endpoint, respectively. As an application of these results, we considered the generalized Bessel operator.

Let $a = 0$, $b \in (0, \infty) \cup \{\infty\}$, and consider

$$\begin{aligned} p(x) = x^{\nu}, \quad r(x) = x^{\delta}, \quad q(x) = \frac{(2+\delta-\nu)^2\gamma^2 - (1-\nu)^2}{4} x^{\nu-2}, \\ \delta > -1,\ \nu < 1,\ \gamma \geqslant 0,\ x \in (0,b), \end{aligned} \tag{5.0.12}$$

so that

$$\begin{aligned} \tau_{\delta,\nu,\gamma} = x^{-\delta}\left[-\frac{d}{dx}x^{\nu}\frac{d}{dx} + \frac{(2+\delta-\nu)^2\gamma^2 - (1-\nu)^2}{4}x^{\nu-2}\right], \\ \delta > -1,\ \nu < 1,\ \gamma \geqslant 0,\ x \in (0,b), \end{aligned} \tag{5.0.13}$$

which is singular at the endpoint $x = 0$ (since the potential, q is not integrable near $x = 0$), regular at $x = b$ when $b \in (0, \infty)$, and in the limit point case at $x = b$ when $b = \infty$. Furthermore, $\tau_{\delta,\nu,\gamma}$ is in the limit circle case at $x = 0$ if $0 \leqslant \gamma < 1$ and in the limit point case at $x = 0$ when $\gamma \geqslant 1$. In the infinite interval case, we proved in Example 3.7.2 that

$$\begin{aligned} M^{Do}_{T_{0,\delta,\nu,\gamma},\mathcal{N}_i}(z) &= \left[-i + \frac{m_{0,\delta,\nu,\gamma}(z) - m_{0,\delta,\nu,\gamma}(-i)}{\operatorname{Im}(m_{0,\delta,\nu,\gamma}(i))}\right] I_{\mathcal{N}_i} \\ &= \begin{cases} \big\{-i - [\sin(\pi\gamma/2)]^{-1} e^{-i\pi\gamma}\big(z^{\gamma} - e^{3i\pi/2}\big)\big\} I_{\mathcal{N}_i}, & \gamma \in (0,1), \\ \{-i + (2/\pi)[(3i\pi/2) - \ln(z)]\} I_{\mathcal{N}_i}, & \gamma = 0, \end{cases} \\ &\qquad \delta > -1,\ \nu < 1,\ z \in \mathbb{C}\backslash[0,\infty), \end{aligned} \tag{5.0.14}$$

and for $\alpha \in (0, \pi)$,

$$\begin{aligned} M^{Do}_{T_{\alpha,\delta,\nu,\gamma},\mathcal{N}_i}(z) = M^{Do}_{T_{0,\delta,\nu,\gamma},\mathcal{N}_i}(z) + (i - z)\frac{m_{0,\delta,\nu,\gamma}(z) - m_{0,\delta,\nu,\gamma}(-i)}{\cot(\alpha) + m_{0,\delta,\nu,\gamma}(z)} \\ \times \left(\psi_{0,\delta,\nu,\gamma}(\overline{z}, \cdot\,), \cdot\,\right)_{L^2_r((a,b))} \psi_{0,\delta,\nu,\gamma}(i, \cdot\,)\big|_{\mathcal{N}_i}, \\ \delta > -1,\ \nu < 1,\ \gamma \in [0,1),\ z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{5.0.15}$$

with

$$\psi_{0,\delta,\nu,\gamma}(z,x) = \begin{cases} i(1-\nu)(2+\delta-\nu)^{-\gamma-1}\gamma^{-1}\Gamma(1-\gamma)\sin(\pi\gamma)z^{\gamma/2} \\ \quad \times x^{(1-\nu)/2}H_{\gamma}^{(1)}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma\in(0,1), \\ i\pi(1-\nu)/(2+\delta-\nu)x^{(1-\nu)/2} \\ \quad \times H_0^{(1)}\big(2z^{1/2}x^{(2+\delta-\nu)/2}/(2+\delta-\nu)\big), & \gamma=0, \end{cases}$$

$$\delta>-1,\ \nu<1,\ z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty), \qquad (5.0.16)$$

$$m_{0,\delta,\nu,\gamma}(z) = \begin{cases} -e^{-i\pi\gamma}(1-\nu)^2(2+\delta-\nu)^{-2\gamma-1}\gamma^{-1} \\ \quad \times[\Gamma(1-\gamma)/\Gamma(1+\gamma)]z^{\gamma}, & \gamma\in(0,1), \\ (1-\nu)^2/(2+\delta-\nu) \\ \quad \times[i\pi-\ln(z)+2\ln(2+\delta-\nu)-2\gamma_E], & \gamma=0, \end{cases} \qquad (5.0.17)$$

$$\delta>-1,\ \nu<1,\ z\in\mathbb{C}\backslash[0,\infty),$$

where $H_{\mu}^{(1)}(\,\cdot\,)$ is the Hankel function of the first kind and of order $\mu\in\mathbb{R}$ (cf. [1, Ch. 9]). Moreover, we considered the finite interval Krein–von Neumann extension in Example 3.7.3, with our results summarized there.

Lastly, we investigated the Jacobi differential expression in Chapter Four which is given by

$$\begin{aligned} \tau_{\alpha,\beta} = -(1-x)^{-\alpha}(1+x)^{-\beta}(d/dx)\big((1-x)^{\alpha+1}(1+x)^{\beta+1}\big)(d/dx), \\ x\in(-1,1),\ \alpha,\beta\in\mathbb{R}. \end{aligned} \qquad (5.0.18)$$

We fully explored the limit point/limit circle classification in order to construct the associated Donoghue m-function, providing a detailed treatment of solutions of the Jacobi differential equation and the associated hypergeometric differential equations in Sections 4.5–4.7. We then employed the results from Chapter Three in order to construct the Donoghue m-function associated with the Jacobi differential operator.

As an example of coupled boundary conditions, we once again considered the Krein–von Neumann extension in Section 4.4.1. In particular, for $\alpha, \beta \in (-1,1)$, the following five cases are associated with a strictly positive minimal operator $T_{min,\alpha,\beta}$ and provided the corresponding choices of $R_{K,\alpha,\beta}$ for the Krein–von Neumann extension $T_{0,R_K,\alpha,\beta}$ of $T_{min,\alpha,\beta}$:

$$T_{0,R_K,\alpha,\beta} f = \tau_{\alpha,\beta} f, \tag{5.0.19}$$

$$f \in \operatorname{dom}(T_{0,R_K,\alpha,\beta}) = \left\{ g \in \operatorname{dom}(T_{max,\alpha,\beta}) \,\middle|\, \begin{pmatrix} \widetilde{g}(1) \\ \widetilde{g}'(1) \end{pmatrix} = R_{K,\alpha,\beta} \begin{pmatrix} \widetilde{g}(-1) \\ \widetilde{g}'(-1) \end{pmatrix} \right\},$$

$$R_{K,\alpha,\beta} = \begin{cases} \begin{pmatrix} 1 & 2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} \\ 0 & 1 \end{pmatrix}, & \alpha, \beta \in (-1,0), \\ \begin{pmatrix} -2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} & 1 \\ -1 & 0 \end{pmatrix}, & \alpha \in (-1,0),\ \beta \in (0,1), \\ \begin{pmatrix} 0 & -1 \\ 1 & 2^{-\alpha-\beta-1}\dfrac{\Gamma(-\alpha)\Gamma(-\beta)}{\Gamma(-\alpha-\beta)} \end{pmatrix}, & \alpha \in (0,1),\ \beta \in (-1,0), \\ \begin{pmatrix} 0 & -1 \\ 1 & -2^{-\beta-1}[\gamma_E + \psi(-\beta)] \end{pmatrix}, & \alpha = 0,\ \beta \in (-1,0) \\ \begin{pmatrix} 2^{-\alpha-1}[\gamma_E + \psi(-\alpha)] & 1 \\ -1 & 0 \end{pmatrix}, & \alpha \in (-1,0),\ \beta = 0, \end{cases} \tag{5.0.20}$$

where we interpret $1/\Gamma(0) = 0$, $\psi(\,\cdot\,) = \Gamma'(\,\cdot\,)/\Gamma(\,\cdot\,)$ denotes the Digamma function, and $\gamma_E = -\psi(1) = 0.57721\ldots$ represents Euler's constant. Obviously, $\det(R_{K,\alpha,\beta}) = 1$ in all five cases. Furthermore, as $R_{1,2} \neq 0$ for each case, Theorem 4.2.2 (ii) applies and one obtains the Donoghue m-function $M^{Do}_{T_{0,R_K,\alpha,\beta},\mathcal{N}_i}(\,\cdot\,)$ for the Krein–von Neumann extension $T_{0,R_K,\alpha,\beta}$ by utilizing (4.4.15) and (4.4.17) as well as the explicit form of $K_{0,R_K}(\,\cdot\,)$ in (4.2.30). Once again, $M^{Do}_{T_{0,R_K,\alpha,\beta},\mathcal{N}_i}(\,\cdot\,)$ is a Nevanlinna–

Herglotz function. In the remaining four cases not covered by (4.4.17), given by all combinations of $\alpha = 0,\ \beta = 0,\ \alpha \in (0,1)$, and $\beta \in (0,1)$, one observes that [68, Theorem 3.5] is not applicable as the underlying minimal operator, $T_{min,\alpha,\beta}$, is nonnegative but not strictly positive.

Our final result was the construction of the Donoghue m-function where precisely one interval endpoint is in the limit point case. We focused on the case when $\alpha \in (-\infty,-1]$ or $\alpha \in [1,\infty)$, so that the right endpoint $x = 1$ represents the limit point case. The converse situation can be obtained by reflection with respect to the origin (i.e., considering the transform $(-1,1) \ni x \mapsto -x \in (-1,1)$). Recall that the Weyl–Titchmarsh–Kodaira solution and m-function corresponding to the Friedrichs (resp., Dirichlet) boundary condition at $x = -1$ is determined via the requirement

$$\begin{aligned}
&\psi_{0,\alpha,\beta}(z,\,\cdot\,) = \theta_{0,\alpha,\beta}(z,\,\cdot\,) + m_{0,\alpha,\beta}(z)\phi_{0,\alpha,\beta}(z,\,\cdot\,) \in L^2((c,1); r_{\alpha,\beta}dx),\\
&z \in \mathbb{C}\backslash\sigma(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1] \cup [1,\infty),\ \beta \in (-1,1),\ c \in (-1,1).
\end{aligned} \tag{5.0.21}$$

Since $\widetilde{\psi}'_{0,\alpha,\beta}(z,-1) = m_{0,\alpha,\beta}(z)$, we showed using Theorem 4.3.2,

$$\begin{aligned}
M^{Do}_{T_{0,\alpha,\beta},\mathcal{N}_i}(z) &= \left[-i + \frac{m_{0,\alpha,\beta}(z) - m_{0,\alpha,\beta}(-i)}{\operatorname{Im}(m_{0,\alpha,\beta}(i))} \right] I_{\mathcal{N}_i},\\
M^{Do}_{T_{\gamma,\alpha,\beta},\mathcal{N}_i}(z) &= M^{Do}_{T_{0,\alpha,\beta},\mathcal{N}_i}(z) + (i-z)\frac{m_{0,\alpha,\beta}(z) - m_{0,\alpha,\beta}(-i)}{\cot(\gamma) + m_{0,\alpha,\beta}(z)}\\
&\qquad \times (\psi_{0,\alpha,\beta}(\overline{z},\,\cdot\,),\,\cdot\,)_{L^2((a,b);rdx)}\psi_{0,\alpha,\beta}(i,\,\cdot\,)\big|_{\mathcal{N}_i}, \quad \gamma \in (0,\pi),\\
&\qquad \alpha \in (-\infty,-1] \cup [1,\infty),\ \beta \in (-1,1),\ z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned} \tag{5.0.22}$$

where $\psi_{0,\alpha,\beta}(z,\,\cdot\,)$ and $m_{0,\alpha,\beta}(z,\,\cdot\,)$ are given by the following:

(I) The Case $\alpha \in [1,\infty)$ and $\beta \in (-1,0)$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= y_{1,\alpha,\beta,-1}(z,x) - 2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x) m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= 2^{1+\alpha+\beta}\beta \frac{\Gamma(1+\beta)}{\Gamma(1-\beta)} \\
&\quad \times \frac{\Gamma([1+\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\alpha+\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha+\beta-\sigma_{\alpha,\beta}(z)]/2)}, \\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in [1,\infty),\ \beta \in (-1,0), \\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\beta)(n+1+\alpha)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta \in (-1,0),
\end{aligned} \tag{5.0.23}$$

with

$$\sigma_{\alpha,\beta}(z) = \big[(1+\alpha+\beta)^2 + 4z\big]^{1/2}. \tag{5.0.24}$$

(II) The Case $\alpha \in [1,\infty)$ and $\beta = 0$:

$$\begin{aligned}
\psi_{0,\alpha,0}(z,x) &= -2^{-\alpha-1} y_{2,\alpha,0,-1}(z,x) + y_{1,\alpha,0,-1}(z,x) m_{0,\alpha,0}(z), \\
m_{0,\alpha,0}(z) &= -2^{-\alpha-1}\{2\gamma_E + \psi([1+\alpha+\sigma_{\alpha,0}(z)]/2) + \psi([1+\alpha-\sigma_{\alpha,0}(z)]/2)\}, \\
&\qquad z \in \rho(T_{F,\alpha,0}),\ \alpha \in [1,\infty),\ \beta = 0, \\
\sigma(T_{F,\alpha,0}) &= \{n(n+1+\alpha)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta = 0.
\end{aligned} \tag{5.0.25}$$

(III) The Case $\alpha \in [1,\infty)$ and $\beta \in (0,1)$:

$$\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= 2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x) + y_{1,\alpha,\beta,-1}(z,x) m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= \beta^{-1} 2^{-1-\alpha-\beta} \frac{-\Gamma(1-\beta)}{\Gamma(1+\beta)} \\
&\quad \times \frac{\Gamma([1+\alpha+\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\alpha+\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma((1+\alpha-\beta-\sigma_{\alpha,\beta}(z))/2)}, \\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in [1,\infty),\ \beta \in (0,1), \\
\sigma(T_{F,\alpha,\beta}) &= \{n(n+1+\alpha+\beta)\}_{n\in\mathbb{N}_0}, \quad \alpha \in [1,\infty),\ \beta \in (0,1).
\end{aligned} \tag{5.0.26}$$

(IV) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta \in (-1, 0)}$:

$$
\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= y_{1,\alpha,\beta,-1}(z,x) - 2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x) m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= 2^{1+\alpha+\beta}\beta \frac{\Gamma(1+\beta)}{\Gamma(1-\beta)} \\
&\quad \times \frac{\Gamma([1-\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1-\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1+\beta-\alpha+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\beta-\alpha-\sigma_{\alpha,\beta}(z)]/2)}, \\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1],\ \beta \in (-1,0), \\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\alpha-\beta)(n+1)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta \in (-1,0).
\end{aligned}
\tag{5.0.27}
$$

(V) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta = 0}$:

$$
\begin{aligned}
\psi_{0,\alpha,0}(z,x) &= -2^{-\alpha-1} y_{2,\alpha,0,-1}(z,x) + y_{1,\alpha,0,-1}(z,x) m_{0,\alpha,0}(z), \\
m_{0,\alpha,0}(z) &= -2^{-\alpha-1}\{2\gamma_E + \psi([1-\alpha+\sigma_{\alpha,0}(z)]/2) + \psi([1-\alpha-\sigma_{\alpha,0}(z)]/2)\}, \\
&\qquad z \in \rho(T_{F,\alpha,0}),\ \alpha \in (-\infty,-1],\ \beta = 0, \\
\sigma(T_{F,\alpha,0}) &= \{(n-\alpha)(n+1)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta = 0.
\end{aligned}
\tag{5.0.28}
$$

(VI) The Case $\boldsymbol{\alpha \in (-\infty, -1]}$ and $\boldsymbol{\beta \in (0, 1)}$:

$$
\begin{aligned}
\psi_{0,\alpha,\beta}(z,x) &= 2^{-\alpha-1}\beta^{-1} y_{2,\alpha,\beta,-1}(z,x) + y_{1,\alpha,\beta,-1}(z,x) m_{0,\alpha,\beta}(z), \\
m_{0,\alpha\,\beta}(z) &= -\beta^{-1} 2^{-1-\alpha-\beta} \frac{\Gamma(1-\beta)}{\Gamma(1+\beta)} \\
&\quad \times \frac{\Gamma([1+\beta-\alpha+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1+\beta-\alpha-\sigma_{\alpha,\beta}(z)]/2)}{\Gamma([1-\alpha-\beta+\sigma_{\alpha,\beta}(z)]/2)\Gamma([1-\alpha-\beta-\sigma_{\alpha,\beta}(z)]/2)}, \\
&\qquad z \in \rho(T_{F,\alpha,\beta}),\ \alpha \in (-\infty,-1],\ \beta \in (0,1), \\
\sigma(T_{F,\alpha,\beta}) &= \{(n-\alpha)(n+1+\beta)\}_{n\in\mathbb{N}_0}, \quad \alpha \in (-\infty,-1],\ \beta \in (0,1).
\end{aligned}
\tag{5.0.29}
$$

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