Estimating spectral density functions for Sturm-Liouville problems with two singular endpoints

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Keywords: Sturm-Liouville problem; spectral density function; spectral function; initial value problem; Regular Singular Point; Frobenius power series solution; Whittaker functions; Asymptotic expansions; piecewise trigonometric - hyperbolic splines

Abstract

In this paper we consider the Sturm-Liouville equation $-y'' + qy = \lambda y$ on the half line $(0, \infty)$ under the assumptions that $x = 0$ is a regular singular point and nonoscillatory for all real $\lambda$, and that either (i) $q$ is $L_1$ near $x = \infty$, or (ii) $q'$ is $L_1$ near $\infty$ with $q(x) \to 0$ as $x \to \infty$, so that there is absolutely continuous spectrum in $(0, \infty)$. Characterizations of the spectral density function for this doubly singular problem, similar to those obtained in [12] and [13] (when the left endpoint is regular) are established; corresponding approximants from the two algorithms in [12] and [13] are then utilized, along with Frobenius recurrence relations and piecewise trigonometric - hyperbolic splines, to generate numerical approximations to the spectral density function associated with the doubly singular problem on $(0, \infty)$. In the case of the radial part of the separated hydrogen atom problem, the new algorithms are capable of achieving near machine precision accuracy over the range of $\lambda$ from 0.1 to 10000, accuracies which could not be achieved using the SLEDGE software package.

This research partially supported by National Science Foundation Grant DMS-0109022 to Florida Institute of Technology, and by Engineering and Physical Sciences Research Council Grant S63403/01 to University of Hull.
1 Introduction

In this paper we consider the Sturm-Liouville equation,

\[-y'' + q(x)y = \lambda y,\]  \hspace{1cm} (1.1)

on \((0, \infty)\), with two singular endpoints on the half line \((0, \infty)\) under the same assumptions as in \([10, 13]\) under which \(x = 0\) is a regular singular point of type \(\text{LC/N}\) or \(\text{LP/N}\) (limit circle or limit point and nonoscillatory at \(x = 0\) for all real \(\lambda\)) and \(x = \infty\) is of type \(\text{LP/O-N}\) with cutoff \(\Lambda = 0\) (limit point and nonoscillatory at \(x = \infty\) for \(\lambda \in (-\infty, 0)\) and oscillatory for \(\lambda \in (0, \infty)\)); see \([15, \text{p. 114}]\) for these definitions of endpoint classifications developed in connection with the SLEDGE software package. Under these assumptions, the spectrum is simple and the eigenfunction expansion associated with equation (1.1) has the general form

\[f(x) = \int_{-\infty}^{\infty} T(\lambda) \cdot \phi(x, \lambda) d\rho(\lambda)
= \sum_{\lambda_n \leq 0} \left[ \int_0^{\infty} \frac{f(t) \phi(t, \lambda_n) dt}{\|\phi(t, \lambda_n)\|^2} \right] \phi(x, \lambda_n) + \int_{0}^{\infty} T(\lambda) \cdot \phi(x, \lambda) d\rho(\lambda) \]  \hspace{1cm} (1.2)

where

\[T(\lambda) := \lim_{b \to \infty} \int_0^{b} f(x) \phi(x, \lambda) dx,\]  \hspace{1cm} (1.3)

and the solution \(\phi(\cdot, \lambda)\) is a suitably normalized Frobenius solution near the regular singular point \(x = 0\).

If we make, in addition to the above assumptions, the more stringent assumptions posed in \([12]\) (see Assumption 3 below), then there is absolutely continuous (a.c.) spectrum in \((0, \infty)\), and the spectral function \(\rho(\lambda)\) in (1.2) is absolutely continuous on all closed intervals in \((0, \infty)\).

The purpose of this paper is (i) to extend the analysis in \([12, 13]\) under suitable assumptions on \(q(x)\) to show that the spectral density function associated with (1.2) over the a.c. range \((0, \infty)\), that is,

\[f(\lambda) = \rho'(\lambda), \quad \rho(\lambda) = \int_{0}^{\lambda} f(\mu) \, d\mu \]  \hspace{1cm} (1.4)

can be represented for all \(\lambda \in (0, \infty)\) as (see Theorem 3 below)

\[f(\lambda) = \frac{1}{\pi [P(\cdot, \lambda)\phi(\cdot, \lambda)^2 + Q(\cdot, \lambda)\phi(\cdot, \lambda)\phi'(\cdot, \lambda) + R(\cdot, \lambda)\phi'(\cdot, \lambda)^2]}. \]  \hspace{1cm} (1.5)

where \((P(\cdot, \lambda), Q(\cdot, \lambda), R(\cdot, \lambda))^T\) is the unique solution of the initial value problem at \(x = \infty:\)

\[
\frac{dU}{dx} = \begin{bmatrix} P \\ Q \\ R \end{bmatrix}
= \begin{bmatrix} 0 & \lambda - q & 0 \\ -2 & 0 & 2(\lambda - q) \\ 0 & -1 & 0 \end{bmatrix}
\cdot
\begin{bmatrix} P \\ Q \\ R \end{bmatrix}.
\]  \hspace{1cm} (1.6)

\[
\lim_{x \to \infty}
\begin{pmatrix} P(x, \lambda) \\ Q(x, \lambda) \\ R(x, \lambda) \end{pmatrix}
= \begin{pmatrix} \sqrt{\lambda} \\ 0 \\ 0 \end{pmatrix}, \quad \lambda \in (0, \infty), \]  \hspace{1cm} (1.7)

and (ii) to extend the numerical algorithms from \([12, 13]\) for the computation of the spectral density.
function $f(\lambda)$. We illustrate the new numerical algorithms on several examples, including the radial part of the separated hydrogen atom. For the first objective (i) we make use of the fact that $f(\lambda)$ is characterized as the boundary value of a suitable Titchmarsh-Weyl m-function by the Titchmarsh-Kodaira formula, which was recently established for such doubly singular problems in [16, 14] (see Theorem 2 below). For the second objective (ii) we make use of exact Frobenius power series to estimate the solution $\phi(x, \lambda)$ and its derivative near $x = 0$, and then apply initial conditions at a suitable point $x_0(\lambda) > 0$ using values of $\phi(x_0(\lambda), \lambda)$ and $\phi'(x_0(\lambda), \lambda)$ which can generally be computed to machine precision, so that numerical algorithms from [12, 13] with the left endpoint regular can be adapted to approximate the right hand side of (1.5); this is done by shooting with piecewise trigonometric / hyperbolic splines to compute the solution $\phi$ of (1.1) and the solution $(P, Q, R)^T$ of (1.6) at a suitable ‘matching’ point $x \in (x_0(\lambda), \infty)$.

The organization of topics needed in this paper to accomplish the above two objectives is as follows:

In section 2 we give the main assumptions near $x = 0$ from [10, 14], and the general forms of two linearly independent Frobenius power series solutions in all the cases we consider in this paper. In section 3 we list (without proof) the elementary results which relate and interconnect solutions of the Sturm-Liouville equation (1.1) with solutions of Appell’s first order system (1.6); none of these elementary results require any special assumptions on the potential $q$. In section 4 we add the main assumptions from [12] under which the initial value problem (1.6)-(1.7) has a unique solution in $(0, \infty)$, and reformulate in terms of solutions of Appell’s system (1.6) results obtained by D.B. Pearson and his student Al-Naggar in [11, 2]. This yields the spectral density function characterization (1.5) in the relatively simple case of a regular left endpoint. In contrast to [11, 2] we do not focus the analysis on the third order ordinary differential equation (see (1.13) below) which is satisfied by the third component, $R(x, \lambda)$, of (1.6), but make use instead of many of the elegant formulas from section 2. In section 5 we generalize the methods of [11, 2] to the doubly singular problem on $(0, \infty)$, when the m-function is defined relative to the suitably normalized Frobenius fundamental system as in [10, 14]. This yields Theorem 3 below (a new result) in which the new Titchmarsh-Kodaira formula (see Theorem 2 below) for the (single) spectral density function associated with the doubly singular problem gets converted to the form (1.5). In section 6 we list four test examples of equations on $(0, \infty)$ from [13, 14] for which explicit closed form formulas for the spectral density function were obtained. In section 7 we describe how the two different types of numerical algorithms from [12] and [13] (for cases involving a regular left endpoint) can be adapted, using appropriate heuristics, to yield new algorithms for computing the spectral density function when both endpoints are singular, which is done by utilizing the characterization (1.5) in an appropriate way. In section 8 we give numerical output showing that the new algorithms for doubly singular problems can achieve very high accuracy on the four test examples in section 6; we also give numerical output demonstrating convergence of our numerical approximations for a potential on $(0, \infty)$ from quantum chemistry where the potential has an infinite series representation satisfying all our assumptions. In section 9 we make use of our new code, AutoB, for the spectral density computation in order to generate, by quadratures, approximations to the spectral functions for the four examples in section 6, and give comparisons on timing and accuracy with the corresponding SLEDGE runs. Our main conclusion is that the new algorithms for doubly singular problems are very much superior to the older algorithms for doubly singular problems which were implemented in the SLEDGE software package.

Remark. In our previous papers [12, 13] the system (1.6) was referred to as the “PQR equations” (our notation); however, the analysis leading to them (particularly the motivating property (3.14) ) was discovered by M. Appell [6] in 1880. Accordingly, we will henceforth refer to this first order system as the Appell equations.

2 Suitably Normalized Frobenius Solutions

In this section we repeat the basic definitions and some of the elementary properties of the suitably normalized Frobenius solutions which were introduced in Fulton [10] and Fulton and Langer [14]. It will be noted that, in most of the common cases (Bessel quations, Confluent Hypergeometric equations, Whittaker equations) rather standard normalizations of well known special functions have to be abandoned in order to achieve the desired analytic properties of the Frobenius solutions (particularly, entire
behaviour in \(\lambda\) needed for the fundamental definition of a single Titchmarsh-Weyl m-function, the corresponding scalar spectral function, and for determination of eigenfunction expansions of the problems considered in this paper (all of which have simple spectrum).

We consider in this paper the Sturm-Liouville equation (1.1) on the half line \((0, \infty)\) under the following assumptions (see [10, 14]):

**Assumption 1: Near \(x = 0\):**

**Case I:** For all \(x \in (0, \infty)\),

\[
q(x) = \frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n, \quad q_n \text{ real for all } n, \tag{2.1}
\]

where the series is convergent in \((0, \infty)\), and where

\[-\frac{1}{4} \leq q_0 < \infty. \quad \text{and } q_0, q_1 \text{ not both zero.} \tag{2.2}\]

or **Case II:** There exists \(a > 0\) such that \(q(x)\) is given by (2.1) for \(x \in (0, a]\) where the series is convergent in \((0, a]\) and where (2.2) holds, and in the interval \([a, \infty)\) we have \(q \in L^1_{loc}[a, \infty)\),

and

**Assumption 2: Near \(x = \infty\):**

\[
l \lim_{x \to \infty} q(x) = 0, \tag{2.3}\]

The assumptions near \(x = 0\) ensure that the indicial roots near the regular singular point \(x = 0\) are both real; it follows that the endpoint \(x = 0\) is either \(\text{LC/N or LP/N}\), and the assumption near \(x = \infty\) ensure that the endpoint \(x = \infty\) is \(\text{LP/O-N}\) with cutoff \(\Lambda = 0\) in the terminology of [15]. Under the above assumptions it was proved in [10, Theorems 4.2, 4.3, 5.3, 5.4] and [14, Theorem 4.5] that the eigenfunction expansion associated with (1.1) (in both the LP and LC cases at \(x = 0\) assumes the form (1.2), with a suitably normalized Frobenius solution \(\phi(\cdot, \lambda)\).

We now give the formulas for all cases of Frobenius solutions which can occur at \(x = 0\) under the assumptions (2.1)-(2.2); these are the solutions which were utilized in [10, 14]. The indicial equation for the R.S.P. \(x = 0\) for the Sturm-Liouville equation (1.1) with potential (2.1),

\[
- y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n\right) y(x) = \lambda y(x), \quad x \in (0, \infty). \tag{2.4}
\]

is

\[
r^2 - r - q_0 = r^2 - r - \left(\nu^2 - \frac{1}{4}\right) = \left(r - \left(\frac{1}{2} + \nu\right)\right) \cdot \left(r - \left(\frac{1}{2} - \nu\right)\right) \tag{2.5}
\]

where we have set

\[q_0 = \nu^2 - \frac{1}{4}, \quad \nu \geq 0\]

for convenience. This gives rise to the following cases of Frobenius solutions:

**Case I:** \(-\frac{1}{4} < q_0 < \infty, \quad q_0 = \nu^2 - \frac{1}{4} \neq \frac{M-1}{4}, \quad M = 1, 2, \ldots\) (This is Case I A in [10]). In this case,

\[
y_1(x, \lambda) = x^{\frac{1}{2} + \nu} \left(1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n\right), \tag{2.6}
\]

\[
y_2(x, \lambda) = x^{\frac{1}{2} - \nu} \left(1 + \sum_{n=1}^{\infty} b_n(\lambda)x^n\right), \tag{2.7}
\]
where \( a_n(\lambda), b_n(\lambda) \) are polynomials in \( \lambda \) of degree \([\frac{q}{2}])\), and
\[
W_x (y_1(\cdot; \lambda), y_2(\cdot; \lambda)) = -2\nu. \tag{2.8}
\]

**Case II A:** \( q_0 = \frac{M-1}{4}, M \) odd: \( M = 2\ell + 1, \ell = 0, 1, \ldots \), that is, \( q_0 = \ell(\ell + 1) \).
In [10] this is Case IC for \( M \) odd and it includes Case II (for \( \ell = 0 \)). In this case,
\[
y_1(x, \lambda) = x^{\ell+1} \left( 1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n \right),
\]
\[
y_2(x, \lambda) = K_\ell(\lambda) y_1(x; \lambda) \ln x + x^{-\ell} \left( 1 + \sum_{n=1}^{\infty} d_n(\lambda)x^n \right), \tag{2.9}
\]
where \( a_n(\lambda), d_n(\lambda) \) are polynomials in \( \lambda \) of degree \([\frac{q}{2}])\), \( K_\ell(\lambda) \) is a polynomial of degree \( \ell \), and
\[
W_x (y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = -(2\ell + 1). \tag{2.10}
\]

**Case II B:** \( q_0 = \frac{M^2-1}{4}, M \) even: \( M = 2N, N = 0, 1, \ldots \), that is, \( q_0 = N^2 - \frac{1}{4} \).
In [10] this is Case IC for \( M \) even and it includes Case IB (for \( N = 0 \)). In this case,
\[
y_1(x, \lambda) = x^{\frac{1}{2}+N} \left( 1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n \right),
\]
\[
y_2(x, \lambda) = y_1(x, \lambda) \ln x + \sum_{n=1}^{\infty} d_n(\lambda)x^{\frac{1}{2}+n}, \text{ if } N = 0
\]
\[
y_2(x, \lambda) = K_N(\lambda) y_1(x; \lambda) \ln x + x^{\frac{1}{2}-N} \left( 1 + \sum_{n=1}^{\infty} d_n(\lambda)x^n \right), \text{ if } N \geq 1 \tag{2.12}
\]
where \( a_n(\lambda), d_n(\lambda) \) are polynomials in \( \lambda \) of degree \([\frac{q}{2}])\), \( K_N(\lambda) \) is a polynomial of degree \( N \), and
\[
W_x (y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = \begin{cases} -2N & \text{if } N \geq 1, \\ 1 & \text{if } N = 0. \end{cases} \tag{2.13}
\]

In each of the above cases the first Frobenius solution \( y_1(\cdot, \lambda) \) is the principal solution at \( x = 0 \) for all \( \lambda \in (-\infty, \infty) \). The Frobenius solutions as normalized above satisfy the following properties (see [10, Theorem 2.1]):

(i) \( y_1(\cdot, \cdot), y_2(\cdot, \cdot) \) and their derivatives are entire functions for each \( x \in (0, \infty) \) and satisfy for all \( \lambda \in \mathbb{C}, x \in (0, \infty) \) the relations
\[
y_i(x, \lambda) = y_i(x, \lambda), \quad y'_i(x, \lambda) = \overline{y'_i(x, \lambda)}, \quad i = 1, 2.
\]

(ii) \( y_1(\cdot, \lambda) \in L_2(0, x_0) \) for \( 0 < x_0 < \infty \) and for all \( \lambda \in \mathbb{C} \).

(iii) \( W_x (y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = C \neq 0 \) where \( C \in \mathbb{R} \), independent of \( \lambda \).

It follows that a fundamental system of solutions near \( x = 0 \) which is entire in \( \lambda \) and satisfies property (i), together with the normalization
\[
W_x (\phi(\cdot, \lambda), \theta(\cdot, \lambda)) = 1 \text{ for all } \lambda \in \mathbb{C}, \tag{2.15}
\]
can be selected by taking
\[
\phi(x, \lambda) := y_1(x, \lambda), \quad \theta(x, \lambda) := y_2(x, \lambda)/C, \tag{2.16}
\]
where \( C \) is the real constant in \([2.8], 2.11\), or \([2.12]\). In the LP cases at \( x = 0 \) only \( \phi(\cdot, \lambda) \) satisfies the property (ii) of square integrability near \( x = 0 \), so in all LP cases it is the first Frobenius solution which is used to write the eigenfunction expansion in the form \([2.2]\).

The LC cases at \( x = 0 \) are Case I with \( q_0 \in (-\frac{1}{4}, 0) \cup (0, \frac{1}{4}) \), Case IIA with \( q_0 = 0(\ell = 0) \), and Case IIB with \( q_0 = \frac{1}{2}(N = 0) \). In this paper we limit our consideration of LC boundary conditions at \( x = 0 \) to the Friedrichs LC boundary condition (see [5.2] below); in this case it is the first Frobenius solution \( \phi \) (the principal solution) which is selected and used in the eigenfunction expansion \([2.2]\).
3 Preliminaries

In this section we collect together some useful results which relate solutions of the Sturm-Liouville equation (1.1) to solutions of the companion first order system (1.6). The proofs of these results (though sometimes tedious) require only straightforward algebraic manipulation making use of these two equations, and no special assumptions on the potential \( q(x) \); so we omit the proofs.

1. If \( y \) is any solution of the SL-equation, then \( (y')^2 - 2yy'' \) is a solution of the first order system (1.6).

2. If we let a fundamental system of the Sturm-Liouville equation (2.4) be defined by the initial conditions at any \( x_0 > 0 \)
   \[
   \begin{bmatrix}
   u(x_0, \lambda) \\
   u'(x_0, \lambda)
   \end{bmatrix}
   =
   \begin{bmatrix}
   1 \\
   0
   \end{bmatrix},
   \tag{3.1}
   \]
   then a corresponding fundamental system of solutions of equation (1.6) is
   \[
   U = [U_1, U_2, U_3] = \begin{bmatrix}
   (u')^2 & u'v' & (v')^2 \\
   -2uv' & -u'v + uv' & -2vv'
   \end{bmatrix}.
   \tag{3.2}
   \]

3. If \( \{\phi(x, \lambda), \theta(x, \lambda)\} \) are the Frobenius solutions defined in Section 2 (in all the cases) and normalized by (2.10) so as to ensure that \( W_x(\phi(-, \lambda), \theta(-, \lambda)) = 1 \), then a corresponding fundamental system of solutions of equation (1.6) is
   \[
   U = [U_1, U_2, U_3] = \begin{bmatrix}
   (\theta')^2 & \theta'\phi' & (\phi')^2 \\
   -2\theta\theta' & -[\theta'\phi + \theta\phi'] & -2\phi\phi'
   \end{bmatrix}.
   \tag{3.3}
   \]

4. An indefinite inner product on the solution space of equation (1.6) may be defined by
   \[
   \langle U_1, U_2 \rangle := 2(P_1R_2 + P_2R_1) - Q_1Q_2 = \text{const}, \quad \text{independent of } x \in [0, \infty)
   \tag{3.4}
   \]
   where \( U_k = (P_k, Q_k, R_k), k = 1, 2 \).

5. For any solution \( U = (P,Q,R)^T \) of equation (1.6),
   \[
   \frac{d}{dx} \langle U, U \rangle = \frac{d}{dx} [4PR - Q^2] = 0,
   \]
   i.e.
   \[
   4PR - Q^2 = \text{const}, \quad \text{independent of } x \in [0, \infty)
   \tag{3.5}
   \]

6. If \( U_1 \) and \( U_2 \) are any two solutions of equation (1.6) represented in the form,
   \[
   U_j = \begin{bmatrix}
   P_j \\
   Q_j \\
   R_j
   \end{bmatrix}
   = a_j \begin{bmatrix}
   (\theta')^2 \\
   -2\theta\theta' \\
   \theta^2
   \end{bmatrix} + b_j \begin{bmatrix}
   \theta'\phi' \\
   -\theta'\phi + \theta\phi' \\
   \theta\phi
   \end{bmatrix} + c_j \begin{bmatrix}
   (\phi')^2 \\
   -2\phi\phi' \\
   \phi^2
   \end{bmatrix}
   \tag{3.6}
   \]
in terms of the Frobenius solutions \( \{\phi(-, \lambda), \theta(-, \lambda)\} \) of section 2, then we have
   \[
   \langle U_1, U_2 \rangle := 2(P_1R_2 + P_2R_1) - Q_1Q_2 = 2(a_1c_2 + c_1a_2) - b_1b_2
   \tag{3.7}
   \]
   In particular,
   \[
   \langle U_1, U_1 \rangle := 4P_1R_1 - Q_1^2 = 4a_1c_1 - b_1^2.
   \tag{3.8}
   \]

7. Similarly, if these same solutions, \( U_1 \) and \( U_2 \), of equation (1.6) are represented in the form,
   \[
   U_j = \begin{bmatrix}
   \tilde{P}_j \\
   \tilde{Q}_j \\
   \tilde{R}_j
   \end{bmatrix}
   = \tilde{a}_j \begin{bmatrix}
   (u')^2 \\
   -2uu' \\
   u^2
   \end{bmatrix} + \tilde{b}_j \begin{bmatrix}
   uu'v' \\
   -uv' + u'v \\
   uv
   \end{bmatrix} + \tilde{c}_j \begin{bmatrix}
   (v')^2 \\
   -2vv' \\
   v^2
   \end{bmatrix}
   \tag{3.9}
   \]
in terms of the solutions defined in (3.1)-(3.2) we have
\[ \langle U_1, U_2 \rangle := 2(\tilde{P}_1 \tilde{R}_2 + \tilde{P}_2 \tilde{R}_1) - \tilde{Q}_2 \tilde{Q}_1 = 2(\tilde{a}_1 \tilde{c}_2 + \tilde{c}_1 \tilde{a}_2) - \tilde{b}_1 \tilde{b}_2. \] (3.10)

In particular,
\[ \langle U_1, U_1 \rangle := 4 \tilde{P}_1 \tilde{R}_1 - \tilde{Q}_1 = 4\tilde{a}_1 \tilde{c}_1 - \tilde{b}_1^2. \] (3.11)

It follows from (3.7), (3.10) and (3.8), (3.11) that we must also have
\[ 2(a_1 c_2 + c_1 a_2) - b_1 b_2 = 2(\tilde{a}_1 \tilde{c}_2 + \tilde{c}_1 \tilde{a}_2) - \tilde{b}_1^2, \quad \text{and} \quad 4a_1 c_1 - \tilde{b}_1^2 = 4\tilde{a}_1 \tilde{c}_1 - \tilde{b}_1^2. \] (3.12)

8. If \( y \) is any solution of the SL equation (1.1) and \( U = (P,Q,R)^T \) is any solution of the companion system (1.6) then
\[ \frac{d}{dx}[Py^2 + Qyy' + R(y')^2] = 0, \] (3.13)
i.e.,
\[ P(x,\lambda)y^2(x,\lambda) + Q(x,\lambda)y(x,\lambda)y'(x,\lambda) + R(x,\lambda)(y'(x,\lambda))^2 = \text{constant, independent of } x. \] (3.14)

4 A Spectral Density Function Characterization of Al-Naggar and Pearson

In this section we consider the Sturm-Liouville problem
\[ -y''(x) + \left( \frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n \right) y(x) = \lambda y(x), \quad x \in [A,\infty), \quad A > 0, \] (4.1)
\[ y(A) = 0. \] (4.2)

We shall assume that Assumption 1, Case I, holds, so that the above potential \( q \) is continuous in \((0,\infty)\) and also has a continuous derivative. In addition we make the following assumption:

Assumption 3: Near \( x = \infty \):

For \( x_0 > 0 \) we have either
\[ q \in L_1(x_0,\infty) \] (4.3)
or
\[ q' \in L_1(x_0,\infty), \quad q \in AC_{loc}[x_0,\infty), \quad \text{and} \quad \lim_{x \to \infty} q(x) = 0. \] (4.4)

Under the assumption (4.3) or the assumption (4.4) it was established in Fulton, Pearson and Pruess [12, Thm1 and Cor 2] that the initial value problem (1.6)-(1.7) has a unique solution for all \( \lambda \in (0,\infty) \). Henceforth we denote this unique solution by
\[ U_1(x,\lambda) = \begin{bmatrix} P_1(x,\lambda) \\ Q_1(x,\lambda) \\ R_1(x,\lambda) \end{bmatrix}, \] (4.5)
that is, \( U_1 \) is the unique solution (under Assumption 3) for which
\[ \lim_{x \to \infty} U_1(x,\lambda) = \begin{bmatrix} P_1(\infty,\lambda) \\ Q_1(\infty,\lambda) \\ R_1(\infty,\lambda) \end{bmatrix} = \begin{bmatrix} \sqrt{\lambda} \\ 0 \\ \sqrt{\lambda} \end{bmatrix}, \quad \text{for } \lambda \in (0,\infty). \]

The assumptions (4.3) and (4.4) were used in [12] [13] to obtain spectral density function characterizations of the type (1.5) when the left endpoint is regular. Al-Naggar and Pearson [1] [2] also obtained a spectral density function characterization of this type when the left endpoint is regular, using a different
approach. Their approach was based on the determination of intervals of a.c. spectrum by locating those intervals of the real \( \lambda \)-axis where subordinate solutions do not exist. The purpose of this section is to present their analysis as it applies to the problem (1.1)–(1.2) and under the additional Assumption 3 on the half line \([A, \infty)\), \(A > 0\), and show that it also guarantees a.c. spectrum for \( \lambda \in (0, \infty) \) and yields a spectral density function formula of the type (1.3) (see (4.30) below and [12, Cor 4]); this route to the spectral density function characterization represents an alternative to the analysis in [12, 13]. As we shall see, the approach of Al-Naggar and Pearson has a major advantage in that it extends nicely to obtain a corresponding spectral density function characterization of the type (1.5) for the doubly singular equation (1.1) on \((0, \infty)\). This will be done in the next section.

In [11, 2] the analysis is focused on the third order ordinary differential equation (see (4.13) below) satisfied by the third component of a solution of Appell’s first order system; here, we modify the approach slightly so as to focus attention on the system (1.6), so that we can properly exploit the results from [12] on uniqueness of the above solution \( U_1 \) satisfying the initial condition (1.7).

Letting \( \{u(\cdot, \lambda), v(\cdot, \lambda)\} \) be the fundamental system of solutions of (4.1) defined by the initial conditions (3.1) at \( x_0 = A \), the Titchmarsh-Weyl \( m \)-function associated with the problem (1.1)–(1.2) is defined by

\[
\Psi_A(\cdot, \lambda) := u(\cdot, \lambda) + M_A(\lambda)v(\cdot, \lambda) \in L_2(A, \infty), \quad \text{for all } Im(\lambda) \neq 0.
\]

Then, as is well known, this \( m \)-function is a Nevanlinna function and therefore admits the representation

\[
m_A(z) = \alpha + \beta z + \int_{-\infty}^{\infty} \left( \frac{1}{t-z} - \frac{t}{1+t^2} \right) d\rho_A(t), \quad \alpha \in (-\infty, \infty), \quad \beta \geq 0,
\]

where the inversion integral for \( \rho_A \) is the Titchmarsh-Kodaira formula

\[
\rho_A(\lambda) = \lim_{\epsilon \searrow 0} \frac{1}{\pi} \int_0^\lambda Im[m_A(\lambda + i\epsilon)]d\lambda.
\]

Since the Assumption 3 ensures a.c. spectrum for \( \lambda \in (0, \infty) \) we may differentiate (4.8) to obtain the spectral density function as

\[
f_A(\lambda) := \rho_A'(\lambda) = \lim_{\epsilon \searrow 0} \frac{1}{\pi} Im[m_A(\lambda + i\epsilon)]
\]

We now proceed to transform (4.9) into the form (1.3); after some analysis this yields (4.30) in Theorem 1 below. In the sequel it will be helpful to make use of the fundamental system of solutions of Appell’s system (1.6) given in (3.2) in terms of the solutions \( \{u(\cdot, \lambda), v(\cdot, \lambda)\} \) of equation (4.1) fixed by the initial conditions (3.1) with \( x_0 = A \)

**Lemma 1.** Assume the potential \( q \) satisfies Assumption 3.

(i) For all \( \lambda \in (0, \infty) \) let \( U_1 \) be the unique solution defined at \( x = \infty \) in (1.5). Then using the indefinite inner product on the solution space of (1.6) defined in (3.7) we have

\[
\langle U_1, U_1 \rangle = 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4.
\]

(ii) If the solution \( U_1 \) is represented in the form (3.9), say

\[
U_1(x, \lambda) = \begin{bmatrix} P_1(x, \lambda) \\ Q_1(x, \lambda) \\ R_1(x, \lambda) \end{bmatrix} = \tilde{a} \begin{bmatrix} (u')^2 \\ -2uu' \\ u^2 \end{bmatrix} + \tilde{b} \begin{bmatrix} u'u' \\ -[uv' + u'v] \\ uv \end{bmatrix} + \tilde{c} \begin{bmatrix} (v')^2 \\ -2vv' \\ v^2 \end{bmatrix}
\]

then

\[
4\tilde{a}\tilde{b} - (\tilde{c})^2 = 4.
\]

**Proof.** (i) To get the constant 4 observe from (3.5) and the initial condition (1.7) that

\[
4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = \lim_{x \to \infty} 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4\sqrt{\lambda} \cdot \left( \frac{1}{\sqrt{\lambda}} \right) = 4.
\]
(ii) The conversion of the indefinite inner product in terms of the coefficients \( \{ \tilde{a}, \tilde{b}, \tilde{c} \} \) is the property \([3.7]\) and \([3.8]\); this is readily proved by substitution of the components of \( U_1 \) into the inner product formula and use of the wronskian relation \( W_x(u(-,\lambda), v(-,\lambda)) = 1 \). \( \square \)

It can be shown that the third component, \( R(x, \lambda) \), of a solution of Appell's system \([1.6]\) satisfies the third order equation of \([2\text{, p. 6584, Equa. 5}]\),

\[
\frac{d^3 R}{dx^3} + 4(\lambda - q(x)) \frac{dR}{dx} - 2q'(x)R = 0.
\] (4.13)

**Remark** In Appell's paper this third order equation is \([3\text{, p. 213, Equa (5)}]\). Also, a general solution of (4.13) can be obtained from a suitably normalized solution \( R_1(x, \lambda) \) as in \([2, \text{Lemma 2, p. 6587}]\). Here we generalize this technique to obtain from the given solution \( R_1, R_2, R_3 \) an alternative form of the solutions of (4.13), of a solution of Appell’s system (1.6) satisfies the third order equation of \([2, \text{p. 6584, Equa. 5}]\),

\[
\frac{d^3 R}{dx^3} + 4(\lambda - q(x)) \frac{dR}{dx} - 2q'(x)R = 0.
\] (4.13)

**Remark** In Appell’s paper this third order equation is \([3\text{, p. 213, Equa (5)}]\). Also, a general solution of (4.13) can be obtained from a suitably normalized solution \( R_1(x, \lambda) \) as in \([2, \text{p. 6587, Lemma 2}]\). Here we generalize this technique to obtain from the given solution \( U_1, U_2, U_3 \), two other linearly independent solutions. This is the content of the following lemma.

**Lemma 2.** Let \( U_1 = (P_1, Q_1, R_1)^T \) be the unique solution of (1.6) defined at \( x = \infty \) by the initial condition (1.7). Then we can write the general solution of (1.6) in the form

\[
U = \begin{bmatrix} P \\ Q \\ R \end{bmatrix} = \beta_1 U_1 + \beta_2 U_2 + \beta_3 U_3,
\] (4.14)

where

\[
U_2(x, \lambda) = \begin{bmatrix} P_1 \cos 2\gamma + (Q_1/R_1) \sin 2\gamma - (2/R_1) \cos 2\gamma \\ Q_1 \cos 2\gamma + 2 \sin 2\gamma \\ R_1 \cos 2\gamma \end{bmatrix},
\] (4.15)

\[
U_3(x, \lambda) = \begin{bmatrix} P_1 \sin 2\gamma - (Q_1/R_1) \cos 2\gamma - (2/R_1) \sin 2\gamma \\ Q_1 \sin 2\gamma - 2 \cos 2\gamma \\ R_1 \sin 2\gamma \end{bmatrix},
\] (4.16)

and

\[
\gamma(x) = \int_{x_0}^x 1/R_1(t, \lambda) \, dt
\]

for some \( x_0 > 0 \).

**Proof.** The fact that

\[
R(x, \lambda) := R_1(x, \lambda)[\beta_1 + \beta_2 \cos 2\gamma + \beta_3 \sin 2\gamma]
\]

is a general solution of (4.13) follows as in \([2, \text{Lemma 2, p. 6587}]\). Since (4.13) is satisfied by the third component of any solution of (1.6), we can generate a general solution for (1.6) by computing \( Q(x, \lambda) = -dR/dx \) and then \( P(x, \lambda) = [-dQ/dx + 2(\lambda - q)R]/2 \) and expressing these solutions of (1.6) in terms of \( P_1, Q_1, R_1 \). This gives the result (4.14). Alternatively, a direct substitution of \( U_2 \) and \( U_3 \) into (1.6) and use of the formulas for \( P_1', Q_1' \) and \( R_1' \) will verify that \( U_2 \) and \( U_3 \) are solutions of (1.6). \( \square \)

**Corollary.** (i) The general solution (4.14) in Lemma 2 satisfies

\[
\langle U, U \rangle = 4PR - Q^2 = 4((\beta_1)^2 - (\beta_2)^2 - (\beta_3)^2).
\] (4.17)

Similarly, if

\[
\tilde{U} = (\tilde{P}, \tilde{Q}, \tilde{R}) = \tilde{\beta}_1 U_1 + \tilde{\beta}_2 U_2 + \tilde{\beta}_3 U_3,
\]

we have for the inner product that

\[
\langle U, \tilde{U} \rangle = 2(P\tilde{R} + R\tilde{P}) - \overline{QQ}
\]

\[
= 4(\tilde{\beta}_1\beta_1 - \tilde{\beta}_2\beta_2 - \tilde{\beta}_3\beta_3).
\] (4.18)

(ii) The solutions \( \{U_1, U_2, U_3\} \) in Lemma 1 are mutually orthogonal with respect to the indefinite inner product defined in \([3.4]\).
The proof of (4.18) is similar. 

(ii) Taking $U = U_1$, which satisfies the normalization (4.10), and $\tilde{U} = U_2$ in (4.18) we have from (4.18) that $\langle U_1, U_2 \rangle = 4(1 \cdot 0 - 0 \cdot 1 - 0 \cdot 0) = 0$. Similarly, $\langle U_1, U_3 \rangle$ and $\langle U_2, U_3 \rangle$ are zero. 

**Remark.** The third component, $R_1$, of (4.11) satisfies the third order equation (4.13) and since $R_1(x, \lambda) \to 1/\sqrt{\lambda} > 0$, it is in fact the same quadratic form as $Y(x, \lambda)$ which was employed in [2, Lemma3 and Thm2].

The following lemma gives a limit relation involving the solution, $U_1$, and the solutions from Lemma 2 which are orthogonal to it.

**Lemma 3.** We assume the potential $q$ satisfies Assumption 3. 

(i) For the solution $U_1$ of the initial value problem (1.6)-(1.7), let $U_2$ and $U_3$ be the linearly independent solutions of Lemma 1 which are generated by using $(P_1, Q_1, R_1)^T$ in (4.15) and (4.16). Then, for any linear combination 

$$U = \begin{pmatrix} P \\ Q \\ R \end{pmatrix} = \beta_2 U_2 + \beta_3 U_3$$

we have for all $x_0 > 0$, 

$$\lim_{N \to \infty} \frac{\int_{x_0}^N R(x, \lambda) \, dx}{\int_{x_0}^N R_1(x, \lambda) \, dx} = 0. \tag{4.19}$$

(ii) The representation (4.11) for $U_1$ has $\tilde{a}(\lambda) > 0$ and $\tilde{c}(\lambda) > 0$ for all $\lambda \in (0, \infty)$.

**Proof (i).** The solutions $U_2$ and $U_3$ in (4.15) and (4.16) have $R_2 = R_1(x, \lambda) \cos(2\gamma(x))$ and $R_3 = R_1(x, \lambda) \sin(2\gamma(x))$, where 

$$\gamma(x) = \int_{x_0}^x [1/R_1(t, \lambda)] \, dt,$$

for all $x > 0$. The fact that $R_1(x) > 0$ for all $x > 0$ follows from (4.20) below. Consequently, it suffices to prove that (4.19) holds for these two choices of $R$. For $R_2$ we have 

$$\int_{x_0}^N R_1 \cos 2\gamma \, dx = \int_{x_0}^N 0.5(R_1)^2 \frac{d}{dx} \sin 2\gamma \, dx$$

$$= 0.5(R_1)^2 \sin 2\gamma \bigg|_{x_0}^{x_0} + \int_{x_0}^N R_1 Q_1 \sin 2\gamma \, dx.$$

Since $Q_1(x) \to 0$ as $x \to \infty$ we can prove that 

$$\lim_{N \to \infty} \frac{\int_{x_0}^N R_1 Q_1 \sin 2\gamma \, dx}{\int_{x_0}^N R_1 \, dx} = 0.$$

Given $\epsilon > 0$, pick $x_\epsilon$ sufficiently large that $|Q_1(x)| < \epsilon$ for $x \geq x_\epsilon$. Then we have 

$$\left| \int_{x_0}^N R_1 Q_1 \sin 2\gamma \, dx \right| \leq M \int_{x_0}^{x_\epsilon} R_1 \, dx + \epsilon \int_{x_\epsilon}^N R_1 \, dx,$$

where $M$ is a bound on $Q_1$ in $[x_0, x_\epsilon]$. Now pick $N$ sufficiently large that 

$$\frac{M \int_{x_\epsilon}^N R_1 \, dx}{\int_{x_0}^N R_1 \, dx} < \epsilon,$$
which is possible since \( \int_{x_0}^{\infty} R_1 \, dx = \infty \). Then the above quotient is less than \( 2\epsilon \). For the boundary term we have

\[
[R_1(N, \lambda)]^2 = [R_1(x_0, \lambda)]^2 + \int_{x_0}^{N} 2R_1 R_1' \, dx
\]

\[
= [R_1(x_0, \lambda)]^2 - \int_{x_0}^{N} 2R_1 Q_1 \, dx,
\]

so

\[
\lim_{N \to \infty} \frac{[R_1(N, \lambda)]^2}{\int_{x_0}^{N} R_1 \, dx} = 0,
\]

by employing the same argument. The proof for \( R_3 \) is similar.

(ii) In the representation (4.11) for \( U_1 \) we have

\[
R_1(x, \lambda) = \tilde{a}u(x, \lambda)^2 + \tilde{b}u(x, \lambda)v(x, \lambda) + \tilde{c}v(x, \lambda)^2.
\]

To see that \( \tilde{a} > 0 \) and \( \tilde{c} > 0 \) for all \( \lambda \in (0, \infty) \) we first observe from (4.12) that \( 4\tilde{a}\tilde{c} - (\tilde{b})^2 = 4 \) requires \( \tilde{a} \) and \( \tilde{c} \) to be of the same sign; and this must hold for all \( \lambda \in (0, \infty) \) since they are continuous and cannot pass through zero (which would violate (4.12)). Factoring out \( \tilde{a} \) we have

\[
R_1(x, \lambda) = \tilde{a}[u(x, \lambda)^2 + (\tilde{b}/\tilde{a})u(x, \lambda)v(x, \lambda) + (\tilde{c}/\tilde{a})v(x, \lambda)^2]
\]

with the coefficients of \( u^2 \) and \( v^2 \) positive. Therefore \( R_1 \) admits a factorization of the form

\[
R_1(x, \lambda) = \tilde{a}[(u(x, \lambda) + \alpha v(x, \lambda))(u(x, \lambda) + \bar{\alpha}v(x, \lambda))]
\]

\[
= \tilde{a}|u(x, \lambda) + \alpha v(x, \lambda)|^2,
\]

where \( \alpha = \alpha_1 + i\alpha_2 \) must satisfy (by (4.12))

\[
\alpha_1 = -\tilde{b}/(2\tilde{a}) \quad \text{and} \quad \alpha_2 = (\bar{\tilde{c}}/\tilde{a}) - [(\tilde{b})^2/(4(\tilde{a})^2)] = 1/(\tilde{a})^2.
\]

Since \( \tilde{a}, \tilde{b}, \) and \( \tilde{c} \) are real, we must have either \( \alpha_2 = 1/\tilde{a} \) or \( \alpha_2 = -1/\tilde{a} \); but either way the factorization remains the same with \( \alpha \) and \( \tilde{a} \) switched. Since \( |u - \alpha v|^2 > 0 \), it follows from the above factorization that \( \tilde{a}(\lambda) > 0 \) for all \( \lambda \in (0, \infty) \); otherwise, \( \lim_{x \to \infty} R_1(x, \lambda) \leq 0 \) contradicting the fact that \( R_1(\infty, \lambda) = 1/\sqrt{\lambda} > 0 \). Hence, also \( \tilde{c}(\lambda) > 0 \) for all \( \lambda \in (0, \infty) \).

Since the definition of \( \alpha_2 \) must be \( \pm 1/\tilde{a}(\lambda) \) from (4.21) and since this indeterminacy is actually immaterial, we choose to take \( \alpha_2 = 1/\tilde{a}(\lambda) \), so that

\[
\alpha(\lambda) := \frac{-\tilde{b}}{2\tilde{a}} + i \frac{1}{\tilde{a}}.
\]

Using the fundamental system \( \{u(\cdot, \lambda), v(\cdot, \lambda)\} \) we now define the complex-valued solution of (1.1) for real \( \lambda \in (0, \infty) \),

\[
\psi_A(x, \lambda) := u(x, \lambda) + \alpha(\lambda)v(x, \lambda).
\]

The key idea of Al-Naggar and Pearson, which enables identification of a.c. spectrum, is embodied in the following requirement:

**Definition.** The general Sturm-Liouville equation (1.1) satisfies *Condition A*, for a given real value of \( \lambda \), if and only if there exists a complex-valued solution \( y(x, \lambda) \) of (1.1) for which

\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} y(x, \lambda)^2 \, dx}{\int_{x_0}^{N} |y(x, \lambda)|^2 \, dx} = 0 \quad \text{for} \quad x_0 > 0.
\]

(4.24)
We now prove that equation (4.11) satisfies Condition A for all \( \lambda \in (0, \infty) \).

**Lemma 4.** Assume \( q(x) \) in (4.1) satisfies Assumptions 3. Then for \( x_0 > 0 \) and all \( \lambda \in (0, \infty) \)

\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} \psi_A(x, \lambda)^2 \, dx}{\int_{x_0}^{N} |\psi_A(x, \lambda)|^2 \, dx} = 0. \tag{4.25}
\]

**Proof:** Since equation (4.13) is satisfied by all linear combinations of \( v(\cdot, \lambda)^2, u(\cdot, \lambda)v(\cdot, \lambda) \) and \( u(\cdot, \lambda)^2 \) (see [2, Lemma 1, p. 6584]), it follows that \( \psi_A(\cdot, \lambda)^2 \) is a solution of (4.13) and since it is complex-valued, also that \( \Re \psi_A(\cdot, \lambda)^2 \) and \( \Im \psi_A(\cdot, \lambda)^2 \) satisfy (4.13). Accordingly, it follows that there exist solutions \( U_2 = (P_2, Q_2, \Re(\psi_A^2))^T \) and \( U_3 = (P_3, Q_3, \Im(\psi_A^2))^T \) of the first order system (1.6), since any real solution \( R \) of (4.13) can be used to generate a solution of (1.6) having \( R \) as its third component; e.g., let \( Q = -R' \) and \( P = -Q'/2 - (\lambda - q)R \). From (4.20) and (4.23) we readily deduce the following representations of \( R_1(\cdot, \lambda), \Re[\psi_A(\cdot, \lambda)^2], \) and \( \Im[\psi_A(\cdot, \lambda)^2] \) of the form (4.11) (or, the third component of (4.11)):

\[
R_1(x, \lambda) = \bar{\alpha}u^2 + 2\tilde{a}\alpha_1 uv + \tilde{a}(\alpha_1^2 + \alpha_2^2)v^2 \quad \Re[\psi_A(x, \lambda)]^2 = u^2 + 2\alpha_1 uv + (\alpha_1^2 - \alpha_2^2)v^2 \quad \Im[\psi_A(x, \lambda)]^2 = 2\alpha_2 uv + 2\alpha_1\alpha_2v^2.
\]

It now follows from these formulas that the above solutions \( U_2 \) and \( U_3 \) associated with \( \Re[\psi_A(\cdot, \lambda)^2] \) and \( \Im[\psi_A(\cdot, \lambda)^2] \) are orthogonal to \( U_1 \) in the sense of the inner product defined in (3.7), i.e., we have

\[
\langle U_1, U_2 \rangle = 2[\bar{\alpha}(\alpha_1^2 - \alpha_2^2) + \tilde{a}(\alpha_1^2 + \alpha_2^2)] - 4\tilde{a}\alpha_1^2 = 0,
\]

and

\[
\langle U_1, U_3 \rangle = 2[\bar{\alpha}(2\alpha_1\alpha_2) + 0] - 4\tilde{a}\alpha_1\alpha_2 = 0.
\]

Hence it follows from Lemma 3(i) that for all \( x_0 > 0 \)

\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} \Re[\psi_A(x, \lambda)]^2 \, dx}{\int_{x_0}^{N} R_1(x, \lambda) \, dx} = 0
\]

and

\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} \Im[\psi_A(x, \lambda)]^2 \, dx}{\int_{x_0}^{N} R_1(x, \lambda) \, dx} = 0,
\]

from which (4.25) follows. \( \blacksquare \)

Assuming the Sturm-Liouville equation (1.1) has a potential \( q \) which is LP at \( x = \infty \) and regular at a finite left endpoint, Al-Naggar and Pearson obtain the following results in [1, Lemma 1 and Thm.2] (where the fundamental system \( \{u, v\} \) is defined by initial conditions at the left endpoint so that \( v \) satisfies a general regular boundary condition and \( W_x(u(\cdot, \lambda), v(\cdot, \lambda) = 1) \):

**Lemma 5 (Al-Naggar and Pearson).** Let \( I \subset (-\infty, \infty) \) be an interval on which Condition A holds for the general equation (4.1), and let the fundamental system \( \{u(\cdot, \lambda), v(\cdot, \lambda)\} \) be defined by the initial conditions (3.7) at \( x_0 = 0 \).

Then

(1) There exists a complex valued function \( M(\lambda) \) on \( I \) which is uniquely defined by the properties:

(a) \( \Im[M(\lambda)] > 0 \) and (b) \( \lim_{N \to \infty} \frac{\int_{x_0}^{N} (u(x, \lambda) + M(\lambda)v(x, \lambda))^2 \, dx}{\int_{x_0}^{N} |u(x, \lambda) + M(\lambda)v(x, \lambda)|^2 \, dx} = 0 \).

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(ii) For $\lambda \in I$ the function $M$ in (i) is the boundary value of the Titchmarsh-Weyl $m$-function defined by (4.6), that is,

$$M(\lambda) = \lim_{\epsilon \downarrow 0} [m_A(\lambda + i\epsilon)].$$

**Proof.** Statements (i) and (ii) are, respectively, Lemma 1 and Theorem 2 from [1].

We now apply these results to the problem (4.1)-(4.2).}

**Lemma 6.** Assume that for the problem (4.1)-(4.2) Assumption 3 holds. Then with $\alpha(\lambda)$ defined by (4.22) we have for all $\lambda \in (0, \infty)$

$$\alpha(\lambda) = \lim_{\epsilon \downarrow 0} [m_A(\lambda + i\epsilon)].$$

**Proof.** By the uniqueness of $M(\lambda)$, and the fact for all $\lambda \in I = (0, \infty)$ $\alpha(\lambda)$ has positive imaginary part (see (4.22) and Lemma 3(ii)) and $\psi_A(x, \lambda)$ satisfies property (b) in Lemma 5(i) (see Lemma 4) it follows from Lemma 5(ii) with $I = (0, \infty)$ that for all $\lambda \in (0, \infty)$ we must have (4.26).

We are now ready to prove the representation of $f_A(\lambda)$ in the form (1.5).

**Theorem 1** Assume the potential $q$ is given as in (4.1) and that Assumption 3 holds. Let $\alpha(\lambda)$ be defined as in (4.22) and $\psi_A(\cdot, \lambda)$ as in (4.23). Then the spectral function defined by (4.8) for the problem (4.1)-(4.2) is absolutely continuous for $\lambda \in (0, \infty)$ and the corresponding spectral density function admits the following representations for $\lambda \in (0, \infty)$:

$$f_A(\lambda) := \rho'(\lambda) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} Im[m(\lambda + i\epsilon)]$$

$$= \frac{\alpha_2(\lambda)}{\pi}$$

$$= \frac{1}{\pi \tilde{a}(\lambda)}$$

$$= \frac{1}{\pi [P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda) v(x, \lambda) v'(x, \lambda) + R_1(x, \lambda) (v'(x, \lambda))^2]}$$

**Proof:** The statement (4.28), and the absolute continuity of the spectral function $\rho$, follows from Lemma 6 by taking imaginary parts on each side of equation (4.26). The statement (4.29) follows from the definition of $\alpha_2$ in (4.22). To obtain (4.30) substitute $U_1 = (P_1, Q_1, R_1)^T$ from the representation (4.11) in terms of $\{u(x, \lambda), v(x, \lambda)\}$ and collect coefficients of $\tilde{a}(\lambda)$, $\tilde{b}(\lambda)$ and $\tilde{c}(\lambda)$ to obtain

$$Pv^2 + Qvv' + R(v')^2 = \tilde{a}(\lambda) |W_x(v, u)|^2 = \tilde{a}(\lambda).$$

**Remark.** Putting $x = 0$ in (4.30) yields $f_A(\lambda) = 1/(\pi R_1(A, \lambda))$ which was a main result of Theorem 2 in [2].

The following well known spectral density function formula, due to Titchmarsh [23], 1946, and Weyl [24], 1910, in the case of the assumption (4.3) (and due to Pearson [19, 11] in the case of assumption (4.4)) also follows readily from Theorem 1:

**Corollary.** Under the assumptions of Theorem 1 we have for all $\lambda \in (0, \infty)$

$$f_A(\lambda) = \lim_{x \to \infty} \frac{1}{\pi \sqrt{\alpha(v(x, \lambda))^2 + \frac{1}{\sqrt{\alpha}}(v'(x, \lambda))^2}}.$$

**Proof:** The Assumption 3 ensures (see [12 Thm 2]) that the solutions $v$ and $u$ defined by the initial conditions (3.1) are bounded for sufficiently large $x$. Hence, making use of the initial condition (1.7)
which $U_1$ satisfies, we have

$$
P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + R_1(x, \lambda)(v'(x, \lambda))^2
$$

$$=
\lim_{x \to \infty} [P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + R_1(x, \lambda)(v'(x, \lambda))^2]
$$

$$=
\lim_{x \to \infty} Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + \lim_{x \to \infty} [P_1(x, \lambda)(v(x, \lambda))^2 + R_1(x, \lambda)(v'(x, \lambda))^2]
$$

$$= 0 + \lim_{x \to \infty} [\lambda(v(x, \lambda))^2 + \frac{1}{\lambda}(v'(x, \lambda))^2],
$$

so it follows that \((4.30)\) gives rise to the characterization \((4.31)\).

**Remark.** In \([12]\) we made use of the formula \((4.31)\) to establish \((4.30)\). Here, by linking the spectral density function first to the m-function, and following the approach of Al-Naggar and Pearson, we have obtained a direct proof of \((4.30)\), from which the older result \((4.31)\) follows as a consequence.

## 5 Generalization of a Spectral Density Function Characterization to Doubly Singular problems

In this section we consider the Sturm-Liouville problem

$$
\tau y := -y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n\right) y(x) = \lambda y(x), \quad x \in (0, \infty),
$$

$$\quad W_0((y(\cdot, \lambda), \phi(\cdot)), 0) = \lim_{x \to 0} W_x((y(\cdot, \lambda), \phi(\cdot)), 0) = 0, \quad \text{if } x = 0 \text{ is LC ,}
$$

where $\phi(x, 0)$ is the first Frobenius solution for $\lambda = 0$ given in \((4.10)\). Since this is also the principal solution at $x = 0$ in all (LC and LP) cases, the boundary condition \((5.2)\) is the Friedrichs boundary condition in the LC cases at $x = 0$ and selects $\phi(x, \lambda)$ for all $\lambda \in C$; this boundary condition is also automatically satisfied by $\phi(x, \lambda)$ in all the LP cases at $x = 0$. In this section we adopt the Assumption 1 and 2 from Section 2, and the Assumption 3 from Section 4. Our aim is to extend the spectral density function characterization in Theorem 1 (under the above 3 assumptions) to obtain the formula \((1.5)\) for the doubly singular problem \((5.1)-(5.2)\). The Assumption 1 ensures that $x = 0$ is a singular point of type LP/N or LC/N; the Assumption 2 ensures that $x = \infty$ is a singular point of type LP/O-N with cutoff value $\Lambda = 0$; and the Assumption 3 ensures that we have a.c. spectrum in $(0, \infty)$. The underlying self-adjoint operator associated with \((5.1)-(5.2)\) has the domain

$$
D(A) := \left\{ f \in L_2(0, \infty) \mid f(x) \in AC^1_{loc}(0, \infty), \quad \tau f \in L_2(0, \infty), \quad \lim_{x \to 0} W_x(f(\cdot), \phi(\cdot), 0) = 0 \right\}
$$

\((5.3)\)

in the LC cases at $x = 0$, and

$$
D(A) := \left\{ f \in L_2(0, \infty) \mid f(x) \in AC^1_{loc}(0, \infty), \quad \tau f \in L_2(0, \infty) \right\}
$$

\((5.4)\)

in the LP cases at $x = 0$. The associated eigenfunction expansion theory which obtains the eigenfunction expansion in the form \((1.2)\) for both of the above cases was given in \([10]\) and \([13]\), and explicit formulas for the corresponding Titchmarsh-Weyl m-function and associated scalar spectral function were obtained in \([14]\) for all cases of the special potential

$$q(x) = \frac{q_0}{x^2} + \frac{q_1}{x}, \quad q_0 \quad \text{and} \quad q_1 \quad \text{satisfying (2.2).}
$$

\((5.5)\)

Here the Titchmarsh-Weyl m-function is defined as in \([10][14]\) by

$$
\Psi(\cdot, \lambda) := \theta(\cdot, \lambda) - m(\lambda) \phi(\cdot, \lambda) \in L_2(x_0, \infty), \quad x_0 > 0, \quad \text{for all } Im(\lambda) \neq 0.
$$

\((5.6)\)
where φ(·, λ) and θ(·, λ) are the first and second Frobenius solutions normalized as in (2.16). We now repeat some basic information from [14] concerning the Titchmarsh-Weyl m-functions defined by (5.6). In the LC cases at x = 0 the m-function defined by (5.6) is a Nevanlinna function (that is, a function of class \( N_0 \)), and therefore admits an integral representation of the form (4.7), and the inversion integral for ρ in terms of m is a Titchmarsh-Kodaira formula like (4.8). The eigenfunction expansion for the problem (5.1)-(5.2) when x = 0 is LC has the form (1.2) where φ(·, λ) is the first Frobenius solution in (2.16), and ρ is the spectral function obtained from the above m-function.

In the LP cases at x = 0, the m-function defined by (5.6) is a generalized Nevanlinna function of class \( N_\kappa \) for some \( \kappa \geq 1 \) (see [14, p. 188]) and it follows using the theory of Krein and Langer [16] for these functions (see [14] Thm 3.5 and Lemma 4.1)) that they admit the representation

\[
m(z) = (1 + z^2)^n \int_{-\infty}^{\infty} \left( \frac{1}{t - z} - \frac{t}{1 + t^2} \right) d\sigma(t) + \sum_{j=0}^{m} \alpha_j z^j
\]

where \( n, m \geq 1 \), \( \alpha_j \in (\infty, \infty) \), \( \alpha_m \neq 0 \) if \( m > 0 \), and where \( \sigma \) is a measure on \( \mathbb{R} \) satisfying

\[
\int_{-\infty}^{\infty} \frac{d\sigma(t)}{1 + t^2} < \infty.
\]

The spectral function for the associated self-adjoint operator \( A \) in (5.4) is then defined interms of \( \sigma \) as

\[
\rho(\lambda) := \int_0^{\lambda} \left( 1 + s^2 \right)^n d\sigma(s), \quad \lambda \in (-\infty, \infty).
\]

While the Titchmarsh-Kodaira formula is well known for \( N_0 \) functions, it was only recently established in various cases with two LP endpoints and simple spectrum by Gesztesy and Zinchenko [16] and Fulton and Langer [14]. For the case of equation (5.1), where generalized Nevanlinna functions of class \( N_\kappa \) arise, we quote this result, and also relate it to the classical real-variable definition of Levitan and Levinson (see [14] Thm 4.7 and 4.8)):

**Theorem 2** (Fulton and Langer). Consider equation (5.1) with \( x = 0 \) of LP type and suppose Assumptions 1 and 2 hold. If \( \lambda, \lambda_0 \) are points of \( \rho \)-measure zero (not discrete eigenvalues of the associated self-adjoint operator \( A \)), then the spectral function defined by (5.7) has the representation

\[
\rho(\lambda) - \rho(\lambda_0) = \lim_{\epsilon \to 0^+} \frac{1}{\pi} \int_{\lambda_0}^{\lambda} \text{Im} \left[ m(\mu + i\epsilon) \right] d\mu \tag{5.8}
\]

\[
= \lim_{b \to \infty} \sum_{\lambda_j \in (\lambda_0, \lambda) \cap \sigma(A_b)} \frac{1}{\int_0^{b} |\phi(x, \lambda_j)|^2 dx}.
\]

Note: When (5.1) is of LC type at \( x = 0 \) we have \( n = 0 \) in (5.7) and a standard Nevanlinna representation of \( m(\lambda) \), for which the inversion formula is also (5.8).

Here, \( A_b \) is the corresponding truncated self-adjoint operator on \( (0, b] \) with any regular boundary condition at \( x = b \). It follows from [14] Thm 4.5] that for the LP cases at \( x = 0 \) the function defined by (5.7) or (5.8) is the spectral function which arises in the eigenfunction expansion (1.2). For proofs of convergence results and Parseval relation we refer to [10, 14].

**Remark.** The above theorem justifies the use of the second formula in (5.8) for the computation of the spectral function \( \rho \) as was implemented in the software package \texttt{SLEDGE} when both endpoints are of LP type. For Sturm-Liouville problems satisfying Assumptions 1,2 of Section 2, \texttt{SLEDGE} [15] Equa (1.13) does in fact normalize the \( \rho \)-solution as in (2.6), (2.9) and (2.12).

If we make the Assumption 3 in addition to the assumptions 1 and 2 of Section 2, the spectrum is a.c. on \( (0, \infty) \). In the case when the left endpoint is regular, it was shown under Assumption 3 in [12] Thm 1 and Cor 2] that the initial value problem (1.6)-(1.7) at \( x = \infty \) has a unique solution for each of the cases (6.3) and (6.4); also, that the spectral density function has the form (1.5) (see [12, Cor 4]
The eigenfunction expansion associated with the underlying self-adjoint operator $A$ when $x = 0$ is $\text{LP}$ has the form (1.2) where $\phi(\cdot, \lambda)$ is the first Frobenius solution in (2.16), and $\rho$ is the spectral function defined in (5.7) or (5.8). In both cases ($\text{LC}$ and $\text{LP}$ at $x = 0$) the spectral density function is given by (5.9) in terms of the $m$-function which is defined in (5.6) above relative to the suitably normalized Frobenius solutions.

We proceed now to transform (5.9) to the form (1.5); after some analysis this yields (5.30) in Theorem 3 below. Since many of the necessary lemmas which are required are the same as in Section 4, we list and prove only those lemmas which undergo some change as a result of allowing the left endpoint $x = 0$ to be a singular endpoint satisfying Assumptions 1,2. We also adopt the notational convention that Lemma $n^*$ in this section represents the analog of Lemma $n$ in Section 4.

In the sequel it will be helpful to make use of the fundamental system of solutions of Appell’s system (1.6) given in (3.3) in terms of the suitably normalized Frobenius solutions $\{\phi(\cdot, \lambda), \theta(\cdot, \lambda)\}$ of equation (5.1) fixed by the definition (2.16).

LEMMA 1*. Assume that for equation (5.1) Assumption 1, Case I, and Assumption 2,3 hold.

(i) Same as Lemma 1(i); this yields

$$\langle U_1, U_1 \rangle = 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4. \quad (5.10)$$

(ii) If the solution $U_1$ is represented in the form (3.3), say

$$U_1(x, \lambda) = \begin{bmatrix} P_1(x, \lambda) \\ Q_1(x, \lambda) \\ R_1(x, \lambda) \end{bmatrix} = a^* \begin{bmatrix} (\theta')^2 \\ -2\theta\theta' \\ \theta^2 \end{bmatrix} + b^* \begin{bmatrix} \theta'\phi' \\ -[\theta\phi' + \theta'\phi] \\ \theta\phi \end{bmatrix} + c^* \begin{bmatrix} (\phi')^2 \\ -2\phi\phi' \\ \phi^2 \end{bmatrix} \quad (5.11)$$

then

$$4a^*c^* - (b^*)^2 = 4. \quad (5.12)$$

PROOF. (ii) The conversion of the indefinite inner product in terms of the coefficients $\{a^*, b^*, c^*\}$ is the property (3.7) and (5.8); this is readily proved by substitution of the components of $U_1$ into the inner product formula and use of the wronskian relation $W_2(\phi(\cdot, \lambda), \theta(\cdot, \lambda)) = 1$.

LEMMA 3*. Assume that for equation (5.1) Assumption 1, Case I, and Assumption 2,3 hold.

(i) Same as Lemma 3(i).

(ii) The representation (5.11) for $U_1$ has $a^*(\lambda) > 0$ and $c^*(\lambda) > 0$ for all $\lambda \in (0, \infty)$.

PROOF: (ii) In the representation (5.11) for $U_1$ we have

$$R_1(x, \lambda) = a^*\theta(x, \lambda)^2 + b^*\theta(x, \lambda)\phi(x, \lambda) + c^*\phi(x, \lambda)^2.$$

To see that $a^* > 0$ and $c^* > 0$ for all $\lambda \in (0, \infty)$ we first observe from (5.12) that $4a^*c^* - (b^*)^2 = 4$ requires $a^*$ and $c^*$ to be of the same sign; and this must hold for all $\lambda \in (0, \infty)$ since they are continuous and cannot pass through zero (which would violate (5.12)). Factoring out $a^*$ we have

$$R_1(x, \lambda) = a^*[(\theta(x, \lambda) - \xi\phi(x, \lambda))(\theta(x, \lambda) - \xi\phi(x, \lambda))]$$

with the coefficients of $\theta^2$ and $\phi^2$ positive. Therefore $R_1$ admits a factorization of the form

$$R_1(x, \lambda) = a^*[(\theta(x, \lambda) - \xi\phi(x, \lambda))]^2,$$

(5.13)
where \( \xi = \xi_1 + i\xi_2 \) must satisfy (by (5.12))
\[
\xi_1 = -b^*/(2a^*) \quad \text{and} \quad \xi_2^2 = (c^*/a^*) - [(b^*)^2/(4(a^*)^2)] = 1/(a^*)^2.
\]
(5.14)

Since \( a^*, b^*, \) and \( c^* \) are real, we must have either \( \xi_2 = 1/a^* \) or \( \xi_2 = -1/a^* \); but either way the factorization remains the same with \( \xi \) and \( \xi \) switched. Since \( |\theta - \xi\phi|^2 > 0 \), it follows from the above factorization that \( a^*(\lambda) > 0 \) for all \( \lambda \in (0, \infty) \); otherwise, \( \lim_{x \to \infty} R_1(x, \lambda) \leq 0 \) contradicting the fact that \( R_1(\infty, \lambda) = 1/\sqrt{\lambda} > 0 \). Hence, also \( c^*(\lambda) > 0 \) for all \( \lambda \in (0, \infty) \).

Since the definition of \( \xi_2 \) must be \( \pm 1/a^*(\lambda) \) from (5.14) and since this indeterminacy is actually immaterial, we choose to take \( \xi_2 = 1/a^*(\lambda) \), so that
\[
\xi(\lambda) := -\frac{b^*}{2a^*} + i\frac{1}{a^*}.
\]
(5.15)

Using the Frobenius solutions normalized by (2.10) we now define the complex-valued solution of (5.1) for real \( \lambda \in (0, \infty) \), by
\[
\psi(x, \lambda) := \theta(x, \lambda) - \xi(\lambda)\phi(x, \lambda).
\]
(5.16)

We now prove the following lemma that equation (5.1) satisfies Condition A for all \( \lambda \in (0, \infty) \).

**Lemma 4.** Assume \( q(x) \) satisfies Assumption 1, Case I, and Assumptions 2, 3. Then for \( x_0 > 0 \) and all \( \lambda \in (0, \infty) \)
\[
\lim_{N \to \infty} \frac{\int_{x_0}^N \psi(x, \lambda)^2 \, dx}{\int_{x_0}^N |\psi(x, \lambda)|^2 \, dx} = 0.
\]
(5.17)

**Proof:** Since equation (4.13) is satisfied by all linear combinations of \( \phi(\cdot, \lambda)^2, \theta(\cdot, \lambda)\phi(\cdot, \lambda) \) and \( \theta(\cdot, \lambda)^2 \) (see \( \mathcal{L} \) Lemma 1, p. 6584), it follows that \( \psi(\cdot, \lambda)^2 \) is a solution of (4.13) and since it is complex-valued, also that \( \text{Re} \left[ \psi(\cdot, \lambda)^2 \right] \) and \( \text{Im} \left[ \psi(\cdot, \lambda)^2 \right] \) satisfy (4.13). Accordingly, it follows that there exist solutions \( U_2 = (P_2, Q_2, \text{Re}(\psi^2))^T \), \( U_3 = (P_3, Q_3, \text{Im}(\psi^2))^T \) of the first order system (1.6), since any real solution \( R \) of (4.13) can be used to generate a solution of (1.6) having \( R \) as its third component; e.g., let \( Q' = -R' \) and \( P = -Q'/2 - (\lambda - q)R \). From (5.13) and (5.16) we readily deduce the following representations of \( R_1(\cdot, \lambda), \text{Re} \left[ \psi(\cdot, \lambda)^2 \right], \) and \( \text{Im} \left[ \psi(\cdot, \lambda)^2 \right] \) of the form (5.11) (or, the third component of (5.11)):
\[
R_1(x, \lambda) = a^*\theta^2 - 2a^*\xi_1\theta\phi + a^*(\xi_1^2 + \xi_2^2)\phi^2
\]
\[
\text{Re} \left[ \psi(x, \lambda)^2 \right] = \theta^2 - 2\xi_1\theta\phi + (\xi_1^2 - \xi_2^2)\phi^2
\]
\[
\text{Im} \left[ \psi(x, \lambda)^2 \right] = -2\xi_2\theta\phi + 2\xi_1\xi_2\phi^2.
\]

It now follows from these formulas that the above solutions \( U_2 \) and \( U_3 \) associated with \( \text{Re} \left[ \psi(\cdot, \lambda)^2 \right] \) and \( \text{Im} \left[ \psi(\cdot, \lambda)^2 \right] \) are orthogonal to \( U_1 \) in the sense of the inner product defined in (3.7), i.e., we have
\[
\langle U_1, U_2 \rangle = 2[a^*(\xi_1^2 - \xi_2^2) + a^*(\xi_1^2 + \xi_2^2)] - 4a^*\xi_1^2 = 0,
\]
and
\[
\langle U_1, U_3 \rangle = 2[a^*(2\xi_1\xi_2) + 0] - 4a^*\xi_1\xi_2 = 0.
\]
Hence it follows from Lemma 3(i) that for all \( x_0 > 0 \)
\[
\lim_{N \to \infty} \frac{\int_{x_0}^N \text{Re}[\psi(x, \lambda)]^2 \, dx}{\int_{x_0}^N R_1(x, \lambda) \, dx} = 0
\]
and
\[
\lim_{N \to \infty} \frac{\int_{x_0}^N \text{Im}[\psi(x, \lambda)]^2 \, dx}{\int_{x_0}^N R_1(x, \lambda) \, dx} = 0.
\]
from which (5.17) follows. □

**Lemma 5** (Al-Naggar and Pearson). We assume for equation (5.1) that Assumption 1, Case I, and Assumptions 2,3 hold. Let \( I \subset (-\infty, \infty) \) be an interval on which Condition A holds. Then

(i) There exists a complex valued function \( M(\lambda) \) on \( I \) which is uniquely defined by the properties:

\[
\begin{align*}
(a) \quad \text{Im}[M(\lambda)] & > 0 \quad \text{and} \quad (b) \quad \lim_{N \to \infty} \frac{\int_{x_0}^{N} (\theta(x, \lambda) - M(\lambda)\phi(x, \lambda))^2 \, dx}{\int_{x_0}^{N} (\theta(x, \lambda) - M(\lambda)\phi(x, \lambda))^2 \, dx} = 0, \quad \text{for all} \quad x_0 > 0.
\end{align*}
\]

where \( \{\phi(\cdot, \lambda), \theta(\cdot, \lambda)\} \) are the Frobenius solutions defined in (2.16).

**Proof:** The proof is the same as that for Lemma 1 in [1]. The proof of this lemma does not depend in any essential way on the choice of the fundamental system of equation (5.1). □

Unfortunately, the corresponding statement (ii) from Lemma 5 does not carry over immediately to the doubly singular problem (5.1)-(5.2) by borrowing information from [1]: particularly, the proof of Theorem 2 in [1] makes use of asymptotic behaviour of solutions which are fixed by initial conditions at a regular left endpoint, and therefore do not apply to the Frobenius solutions \( \{\phi, \theta\} \). The Titchmarsh-Weyl \( m \)-function (5.6) was first introduced in the papers [16, 10, 14]; and it wasn’t discovered to be a generalized Nevanlinna function in the LP case at \( x = 0 \) until the 2010 paper [14]. A direct generalization of Theorem 2 of [1] for cases when the left endpoint is singular remains unknown. However, we can recover the analogue of part (ii) of Lemma 5 by making appeal to the uniqueness result in Lemma 5*(i) and gleaning information on the boundary behaviour of \( m(z) \) from known information on the boundary behaviour of \( m_A(z) \). This is the objective of Lemma 6*. To this end, it will be helpful to introduce notation for the boundary values of the “regular” and “doubly singular” Titchmarsh-Weyl functions \( m_A(\lambda) \) and \( m(\lambda) \) and for the corresponding \( \Psi \)-functions defined in (5.10) and (5.6).

**Definition.** Associated with the \( \mathfrak{m} \)-functions, \( m_A(\lambda) \) and \( m(\lambda) \), for the problem with regular left endpoint and for the doubly singular problem, respectively, we define for all \( x \in (0, \infty) \) and all \( \lambda \in (0, \infty) \):

\[
\begin{align*}
m_A^+(\lambda) & := \lim_{\epsilon \downarrow 0} m_A(\lambda + i\epsilon), \\
\Psi_A^+(x, \lambda) & := \lim_{\epsilon \downarrow 0} \Psi_A(\lambda + i\epsilon) = u(x, \lambda) + m_A^+(\lambda)v(x, \lambda), \\
m^+(\lambda) & := \lim_{\epsilon \downarrow 0} m(\lambda + i\epsilon), \\
\Psi^+(x, \lambda) & := \lim_{\epsilon \downarrow 0} \Psi(\lambda + i\epsilon) = \theta(x, \lambda) - m^+(\lambda)\phi(x, \lambda),
\end{align*}
\]

**Lemma 6***. We assume for equation (5.1) that Assumption 1, Case I, and Assumptions 2,3 hold. Then

(i) for all \( x \in (0, \infty) \) and all \( z \) with \( \text{Im} \, z \neq 0 \)

\[
\Psi(x, \lambda) = \frac{\Psi_A(x, z)}{-\phi'(A, z) + m_A(z)\phi(A, z)}.
\]

(ii) For all \( x \in (0, \infty) \) and all \( \lambda \in (0, \infty) \)

\[
\Psi^+(x, \lambda) = \frac{\Psi_A^+(x, \lambda)}{-\phi'(A, \lambda) + m_A^+(\lambda)\phi(A, \lambda)}.
\]

(iii) For \( x_0 > 0 \) and all \( \lambda \in (0, \infty) \)

\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} (\Psi(x, \lambda))^2 \, dx}{\int_{x_0}^{N} (\Psi^+(x, \lambda))^2 \, dx} = 0.
\]
(iv) For all \( \lambda \in (0, \infty) \)
\[
\text{Im } m_+(\lambda) = \frac{\text{Im } m^+_\lambda(\lambda)}{|m^A_\lambda(\lambda)\phi(A,\lambda) - \phi'(A,\lambda)|^2} > 0. \tag{5.25}
\]

(v) For all \( \lambda \in (0, \infty) \) the complex valued function \( \xi(\lambda) \) defined in (5.16) is the boundary value of the Titchmarsh-Weyl m-function, that is,
\[
\xi(\lambda) = \lim_{\epsilon \downarrow 0} m(\lambda + i\epsilon). \tag{5.26}
\]

PROOF. For (i) make use of the fact that for \( Imz \neq 0 \) both \( \Psi_A(x, z) = u(x, \lambda) + m_A(\lambda)v(x, \lambda) \) and \( \Psi(x, z) = \theta(x, \lambda) - m(\lambda)\phi(x, \lambda) \) are in \( L_2(x_0, \infty) \), and therefore linearly dependent. Using \( W_x(\phi, \theta) = W_x(\phi, \Psi) = 1 \), the relation of linear dependence is found to be
\[
\Psi(x, z) = \frac{\Psi_A(x, z)}{W_x(\phi, u + m_A(v))},
\]
and (5.22) follows on evaluation of the denominator at \( x = A \) making use of the initial conditions (5.1). For (ii) put \( z = \lambda + i\epsilon \) in (5.22) and pass \( \epsilon \to 0 \). For (iii) put (5.23) into (5.24) and factor the constant terms out of the integrals to get the equivalent statement
\[
\lim_{N \to \infty} \frac{\int_{x_0}^{N} \Psi^+_A(x, \lambda)^2 \, dx}{\int_{x_0}^{N} |\Psi^+_A(x, \lambda)|^2 \, dx} = 0.
\]

But \( \Psi^+_A(x, \lambda) \) is known to satisfy Condition A by Lemma 5(ii), Lemma 6, and Lemma 4 with (i.e. by Theorem 2 of [1]) applied to the problem (4.1)-(4.2). Hence it follows that (5.23) also holds for all \( \lambda \in (0, \infty) \) and all \( x_0 > 0 \); in other words, \( \Psi^+(x, \lambda) \) also satisfies Condition A. For (iv) use
\[
m^+(\lambda) = W_x(\theta(\cdot, \lambda), \Psi^+(\cdot, \lambda))
\]
and substitute the right hand side of (5.22) for \( \Psi^+(x, \lambda) \), evaluating \( W_x(\theta, u) \) and \( W_x(\phi, v) \) at \( x = A \) using the initial conditions (3.1), to obtain for all \( \lambda \in (0, \infty) \)
\[
m^+(\lambda) = \frac{\theta(A, \lambda)m^A_\lambda(\lambda) - \theta'(A, \lambda)}{\phi(A, \lambda)m^A_\lambda(\lambda) - \phi'(A, \lambda)}.
\]
Then (5.23) follows by taking imaginary parts on both sides. The right hand side of (5.26) is positive for all \( \lambda \in (0, \infty) \) because the numerator is positive by Theorem 1 (equation (4.28)), and the denominator never becomes zero (by separating real and imaginary parts and observing that the cases \( \phi(A, \lambda) = 0 \) and \( \phi(A, \lambda) \neq 0 \) both yield a positive denominator). To prove (v) we observe first that for all \( \lambda \in (0, \infty) \), \( m^+(\lambda) \) has positive imaginary part (by (5.25)) and \( \Psi^+(x, \lambda) \) satisfies (by (5.24)) property (b) in Lemma 5*(i). Similarly, the function \( \xi \) defined in (5.15) has positive imaginary part (see Lemma 3(ii) ) for all \( \lambda \in (0, \infty) \) and the solution \( \psi(x, \lambda) \) defined in (5.16) satisfies (see Lemma 4*) property (b) in Lemma 5*(i). Hence by the uniqueness of the function \( M(\lambda) \) satisfying the two properties of Lemma 5*(i), the functions \( m^+(\lambda) \) and \( \xi(\lambda) \) must be identical, that is, (5.26) holds.

We are now ready to prove the representation of \( f(\lambda) \) in the form (1.16). This represents the “doubly singular” analogue of the spectral density function characterization of Theorem 1.

Theorem 3 We assume that Assumption 1, Case I, and Assumptions 2,3 hold. Let \( \xi(\lambda) \) be defined as in (5.15) and \( \psi(\cdot, \lambda) \) as in (5.16). Then the spectral function defined by (5.8) for the problem (5.1)-(5.2) (in both the LC and LP cases at \( x = 0 \)) is absolutely continuous for \( \lambda \in (0, \infty) \) and the
corresponding spectral density function admits the following representations for \( \lambda \in (0, \infty) \):

\[
f(\lambda) := \rho'(\lambda) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \text{Im}[m(\lambda + i\epsilon)]
\]

(5.27)

\[
= \frac{\xi_2(\lambda)}{\pi} 
\]

(5.28)

\[
= \frac{1}{\pi a^*(\lambda)} 
\]

(5.29)

\[
= \frac{1}{\pi [P_1(x, \lambda)(\phi(x, \lambda))^2 + Q_1(x, \lambda)\phi(x, \lambda)\phi'(x, \lambda) + R_1(x, \lambda)(\phi'(x, \lambda))^2]} .
\]

(5.30)

**Proof:** The statement (5.28), and the absolute continuity of the spectral function \( \rho \), follows from Lemma 6 by taking imaginary parts of each side of (5.26). The statement (5.29) follows from the definition of \( \xi_2 \) in (5.15). To obtain (5.30) substitute \( U_1 = (P_1, Q_1, R_1)^T \) from the representation (5.11) in terms of \( \{\theta(x, \lambda), \phi(x, \lambda)\} \) and collect coefficients of \( a^*(\lambda) \), \( b^*(\lambda) \) and \( c^*(\lambda) \) to obtain

\[
P(\phi)^2 + Q\phi\phi' + R(\phi')^2 = a^*(\lambda)[W_\lambda(\phi, \theta)]^2 = a^*(\lambda). 
\]

6 Some Examples with Explicitly Known Spectral Density Functions

In this section we give the explicit formulas from [10, 14] for the Frobenius solution \( \phi(\cdot, \lambda) \), the Titchmarsh-Weyl m-function, and the spectral density function for some examples of the special potential (5.5). We restrict attention to those cases which will be used as test problems for the numerical algorithms in Sections 8 and 9.

**Example 1:** \( q_0 = -a, a > 0; q_1 = \ell(\ell + 1) \) Hydrogen Atom

\[
- y'' + \left(-\frac{a}{x} + \frac{\ell(\ell + 1)}{x^2}\right) y = \lambda y \quad a > 0, \quad 0 < x < \infty. 
\]

(6.1)

The first Frobenius solution with normalization (2.9) is

\[
\phi(x, \lambda) = x^{\ell+1}[1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n] 
\]

\[
= x^{\ell+1}e^{ix\sqrt{\lambda}}M(\ell + 1 - \beta, 2\ell + 2, -2ix\sqrt{\lambda}) 
\]

\[
= \frac{1}{(-2i\sqrt{\lambda})^{\ell+1}}M_{\beta, \ell+\frac{1}{2}}(-2ix\sqrt{\lambda}), 
\]

(6.2)

with \( \beta := ia/2\sqrt{\lambda} \) for all \( \lambda \in \mathbb{C} \). Here \( M \) is the confluent hypergeometric function of first kind and \( M \) is the corresponding Whittaker function of first kind. The coefficients \( a_n(\lambda) \) are polynomials in \( \lambda \) of degree \( [n/2] \) which are generated from the recurrence relation

\[
a_n(\lambda) = -\frac{a}{n(n + 2\ell + 1)}a_{n-1}(\lambda) - \frac{\lambda}{n(n + 2\ell + 1)}a_{n-2}(\lambda), 
\]

and the first three are

\[
a_1 = \frac{a}{2\ell + 2}, 
\]

\[
a_2(\lambda) = \frac{a^2 - 2(\ell + 1)\lambda}{2!(2\ell + 2)(2\ell + 3)}, 
\]

\[
a_3(\lambda) = \frac{-a^3 + (6\ell + 8)a\lambda}{3!(2\ell + 2)(2\ell + 3)(2\ell + 4)}, 
\]

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The Titchmarsh-Weyl m-function arising from (5.6) is
\[
m_{\ell}(\lambda) = k_{\ell}(\lambda) \left[ -a \log(-2i\sqrt{\lambda}) - a\Psi(1-ia/(2\sqrt{\lambda})) - 2\gamma a + i\sqrt{\lambda} \right] + p_{\ell}(\lambda),
\] (6.3)
where \(\Psi\) is the psi or digamma function, \(\gamma\) is Euler's constant,
\[
k_{\ell}(\lambda) := \frac{1}{[(2\ell + 1)]!^2} \prod_{j=1}^{\ell} (4\lambda j^2 + a^2),
\]
and where \(p_{\ell}(\lambda)\) is a polynomial of degree \(\ell\) (see [10, 17]). We take \(0 \leq \arg(\lambda) < 2\pi\), so that the branch cut for \(\sqrt{\lambda}\) and \(m_{\ell}\) is on the positive real \(\lambda\)-axis.

The associated spectral density function arising from (5.9) is
\[
f_{\ell}(\lambda) := \lim_{\epsilon \to 0} \frac{\text{Im}[m_{\ell}(\lambda + i\epsilon)]}{\pi} = k_{\ell}(\lambda) \left[ \frac{a}{1 - e^{-\pi a/\sqrt{\lambda}}} \right].
\] (6.4)

Example 2: \([q_0 = -a, a < 0; q_1 = \ell(\ell + 1)]\) Repulsive Coulomb
\[
-\gamma'' + \left( -\frac{a}{x} + \frac{\ell(\ell + 1)}{x^2} \right) y = \lambda y, \quad a < 0, \quad 0 < x, \infty
\] (5.5)
The first Frobenius solution with normalization (2.6) is (same as (6.2) with \(a < 0\))
\[
\phi(x, \lambda) = x^{\ell+1}[1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n]
\] = \[
x^{\ell+1}e^{ix\sqrt{\lambda}}M(\ell + 1 - \beta, 2\ell + 2, -2ix\sqrt{\lambda})
\] = \[
\frac{1}{(-2\pi i)^{\ell+1}}\mathcal{M}_{\beta,\ell+\frac{1}{2}}(-2ix\sqrt{\lambda}),
\] (6.6)
where \(\beta := ia/2\sqrt{\lambda}\), and \(a < 0\). The recurrence relation and first three coefficients, \(a_n(\lambda)\), are the same as in Example 1 with \(a < 0\). The Titchmarsh-Weyl m-function arising from (5.6) is
\[
m_{\ell}(\lambda) = k_{\ell}(\lambda) \left[ -a \log(-2i\sqrt{\lambda}) - a\Psi(1-ia/(2\sqrt{\lambda})) - 2\gamma a + i\sqrt{\lambda} \right] + p_{\ell}(\lambda),
\] (6.7)
where \(a < 0\), and \(k_{\ell}(\lambda), p_{\ell}(\lambda)\) are the same, with \(a < 0\), as given above for the hydrogen atom. The branch cut is taken again on the positive real \(\lambda\)-axis.

The associated spectral density function arising from (5.9) is
\[
f_{\ell}(\lambda) = k_{\ell}(\lambda) \left( \frac{|a|}{\exp(|a|\pi/\sqrt{\lambda}) - 1} \right),
\] (6.8)

Example 3: \([q_0 = \nu^2 - 1/4, \nu \neq M/2, M = 0, 1, 2 \ldots; q_1 = 0]\) Bessel Equation of Non-integer Order
\[
-\gamma'' + \frac{\nu^2 - 0.25}{x^2} y = \lambda y, \quad \nu > 0, \ \nu \neq N/2, N = 1, 2, \ldots,
\] (6.9)
The first Frobenius solution with normalization (2.6) is
\[
\phi(x, \lambda) := x^{\nu+0.5} \left[ 1 + \sum_{j=1}^{\infty} \frac{(-1)^j \lambda^j x^{2j}}{j!(\nu + 1)j2^j} \right] = 2^{\nu} \Gamma(\nu + 1)\lambda^{-\nu/2}x^{1/2}J_{\nu}(\sqrt{\lambda}x)
\] (6.10)
The Titchmarsh-Weyl m-function arising from (5.6) is
\[ m(\lambda) = -\pi \frac{1}{2^{\nu+1} \Gamma^2(\nu + 1) \cdot \sin(\nu \pi)} \lambda^{-\nu} \cdot e^{-i\nu\pi} \lambda^\nu \]  \hspace{1cm} (6.11)
where \( 0 \leq \arg(\lambda) < 2\pi \), so that the branch cut for \( \lambda^\nu \) is on the positive real \( \lambda \)-axis.

The associated spectral density function arising from (5.9) is
\[ f_\nu(\lambda) = \frac{\lambda^\nu}{2^{\nu+1} \Gamma^2(\nu + 1)}. \]  \hspace{1cm} (6.12)

**Example 4:** \([q_0 = N^2 - 1/4, N = 0, 1, 2, \ldots ; q_1 = 0]\) Bessel Equation of Integer Order

The first Frobenius solution with normalization (2.12) is
\[ \phi(x, \lambda) := x^{N+0.5} \left[ 1 + \sum_{j=1}^{\infty} \frac{(-1)^j \lambda^j x^{2j}}{j!(N + 1, 2)^{2j}} \right] = \lambda^N (N + 1) \lambda^{-N/2} x^1 x J_N(\sqrt{\lambda} x), N = 0, 1, 2, \ldots . \]  \hspace{1cm} (6.14)

The Titchmarsh-Weyl m-function arising from (5.6) is
\[ m_0(\lambda) = -\log(-2i\sqrt{\lambda}) + \gamma - 2\ell n2, \]  
\[ m_N(\lambda) = \frac{\lambda^N}{2^{2N}(N!)^2} m_0(\lambda) + \frac{\lambda^N H_{N+1}}{2^{2N+1}(N!)^2}, N \geq 1. \]  \hspace{1cm} (6.15)
where \( 0 \leq \arg(\lambda) < 2\pi \), so that the branch cut for \( m_0 \) is on the positive real \( \lambda \)-axis.

The associated spectral density function arising from (5.9) is
\[ f_N(\lambda) = \frac{\lambda^N}{2^{2N+1}(N!)^2}. \]  \hspace{1cm} (6.16)

### 7 Numerical Methods

In this section and the following two sections we describe some new numerical methods for obtaining approximations to the spectral density function (1.4) and then the spectral function, by making use of the new representation (5.30) in Theorem 3, and compare their performance with SLEDGE. For general information and discussion of numerical methods for Sturm-Liouville problems we refer to Pryce’s book [21] and for spectral function computation using SLEDGE we refer to our previous papers [20, 6, 15].

Many numerical methods for (1.1) break down near a singular point at \( x = 0 \). However, when we take this singular point to be a regular singular point, it admits a convergent Frobenius expansion, and then a finite number of leading terms in the sum can be used as an initial approximation near \( x = 0 \). For equation (2.4) the indicial equation is (2.5) and the principal solution is the first Frobenius solution with the larger indicial root,
\[ r_1 = \nu := 0.5 + 0.5 \sqrt{1 + 4q_0}. \]

This solution has the general form
\[ \phi(x, \lambda) = \sum_{n=0}^{\infty} a_n x^{n+\nu}, \]  \hspace{1cm} (7.1)
and the general recurrence formula is
\[ a_1 = \frac{q_1 a_0}{\nu(\nu + 1) - q_0}. \]
and for $n > 1$

$$a_n = \frac{-\lambda a_{n-2} + q_1 a_{n-1} + \sum_{k=0}^{n-2} q_k + 2a_{n-2-k}}{(\nu + n - 1)(\nu + n) - q_0}.$$ 

The choice for $a_0$ fixes the normalization of $\phi(\cdot, \lambda)$, and in this paper we have made the simple choice $a_0 = 1$ in all the cases (2.6), (2.9) and (2.12); this ensures that the properties (i), (ii), (iii) of section 2 hold in all the cases of Assumption 1.

We note that there is a risk of loss of significance in the computation of $a_n(\lambda)$ for very large $\lambda$, because for moderate $n$ the powers of $\lambda$ in the numerator of $a_n$ build up faster than the denominator does. We have found that keeping

$$x < x_0(\lambda) := |q_0|/\sqrt{\lambda}$$

and using the truncated Frobenius series (to full machine precision) only on $(0, x_0(\lambda)]$ works well. For $x > x_0(\lambda)$ we use the methods from [12] and [13] for regular problems. In brief, the algorithm is as follows:

(i) For a given $\lambda$ choose a ‘matching point’ $x(\lambda)$.
(ii) Use the first Frobenius solution (7.1) (this is the principal solution near zero) on the interval $(0, x(\lambda)]$ to produce values for solution and its derivative (usually to machine precision) at $x(\lambda)$.
(iii) Apply standard methods to numerically estimate $y$ for (5.1) on the interval $[x(\lambda), x(\lambda)]$ satisfying initial conditions from (i). Because of the oscillation in $y$ for $\lambda > 0$, we use a piecewise trigonometric approximation to $y$.
(iv) Approximate the solution $P(x, \lambda), Q(x, \lambda)$, and $R(x, \lambda)$ of the initial value problem (1.6)-(1.7) at the matching point $x(\lambda)$ using one of the approaches described below.
(v) Substitute the estimates from (iii), (iv) into

$$f_x(\lambda) := \frac{1}{\pi[P(x, \lambda)y(x, \lambda)^2 + Q(x, \lambda)y(x, \lambda)y'(x, \lambda) + R(x, \lambda)y'(x, \lambda)^2]}.$$ 

(7.3)

to produce an approximation to the exact spectral density, $f(\lambda)$, given in Theorem 3, equation (5.30).

The two papers [12] and [13] derive two very different approaches to the numerical computation of $(P(b, \lambda), Q(b, \lambda)$, and $R(b, \lambda)$). In [12] we constructed a family of recurrence formulas that generated successively more accurate approximations to $P$, $Q$, and $R$ and hence to $f(\lambda)$. For fixed $x > 0$ define for each positive integer $j$ the family of functions

$$P_j^2(\lambda) := \frac{1}{\pi[P_jy^2 + Q_jyy' + R_jy'^2]}.$$ 

(7.4)

From [11] for $j = 1$ we define

$$P_1 := \sqrt{\lambda}, \quad Q_1 := 0, \quad R_1 := 1/\sqrt{\lambda}.$$ 

(7.5)

From [12] the next formula in the family for $j = 2$ is defined by

$$P_2 := \sqrt{\lambda - q(x)}, \quad Q_2 := -q'(x)/[2(\lambda - q(x))^{3/2}], \quad R_2 := 1/\sqrt{\lambda - q(x)}.$$ 

(7.6)

The final member that we use is $j = 3$, also defined in [12] as:

$$P_3 := P_2 + 0.25 \gamma_2 + 0.125 \gamma_1^2/\gamma_0$$
$$Q_3 := Q_2 - \frac{d}{dx} \left\{ -0.25 \gamma_2^2 \gamma_2 + 0.125 \gamma_0 \gamma_1^2 \right\}$$
$$R_3 := R_2 - 0.25 \gamma_2 + 0.125 \gamma_0 \gamma_1^2$$

(7.7)

where

$$\gamma_k := \frac{d^k}{dx^k} \left[ \frac{1}{\sqrt{\lambda - q(x)}} \right]$$

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for $k = 0, 1, 2$. For regular problems on $[A, \infty)$, $A > 0$, it is shown in (12) that each member of this family converges to the spectral function $f_A(\lambda)$ as $x \to \infty$. For the hydrogen atom potential (1.1) on $[A, \infty)$ the theory of (12) implies that

$$f_A(\lambda) - F^\dagger_A(\lambda) = O(1/x^{2j-1}) \text{ as } x \to \infty. \quad (7.8)$$

This method requires knowledge of derivatives of the potential $q(x)$.

In (12) we constructed explicit approximations to the solutions of (1.6) with known residual terms that arise during the construction; in particular, replace $P(x, \lambda)$, $Q(x, \lambda)$, and $R(x, \lambda)$ with estimates of the form

$$P_N(x) := \sqrt{\lambda} + \sum_{j=1}^N a_j/x^j$$

$$Q_N(x) := \sum_{j=1}^N b_j/x^{j+1}$$

$$R_N(x) := 1/\sqrt{\lambda} + \sum_{j=1}^N c_j/x^j,$$

where $\{a_j\}$, $\{b_j\}$, and $\{c_j\}$ will depend on $\lambda$ but not $x$. The resulting sums are substituted into (1.6) and the coefficients chosen to match terms of like powers. Then we put the computed coefficients into (7.9) and define the family of approximations

$$f^N_N(\lambda) := \frac{1}{\pi} [P_N(x, \lambda)y(x, \lambda)^2 + Q_N(x, \lambda)y(x, \lambda)y'(x, \lambda) + R_N(x, \lambda)y'(x, \lambda)^2]. \quad (7.10)$$

Specifically, the $N$th residuals are defined as

$$\left( \begin{array}{c} \phi^P_N \\ \phi^Q_N \\ \phi^R_N \end{array} \right) := \left( \begin{array}{ccc} P'_N & 0 \\ Q'_N & 0 \\ R'_N & 0 \end{array} \right) - \left( \begin{array}{ccc} 0 & \lambda - q & 0 \\ -2 & 0 & 2(\lambda - q) \\ 0 & -1 & 0 \end{array} \right) \cdot \left( \begin{array}{c} P_N \\ Q_N \\ R_N \end{array} \right)$$

and we attempt to make these small, as $x \to \infty$, by the choice of coefficients in (7.9). All potentials in the examples of the previous section have the form (7.5), that is,

$$q(x) = A/x + B/x^2,$$

where $A = q_1$ and $B = q_0$ and (7.5) is satisfied. It is straightforward to show that

$$\phi^P_N = \sum_{j=1}^N \frac{-ja_j - \lambda b_j + Ab_{j-1} + Bb_{j-2}}{x^{j+1}} + \frac{Bb_{N-1} + Ab_N}{x^{N+1}} + \frac{Bb_N}{x^{N+3}}$$

$$\phi^Q_N = \sum_{j=1}^N \frac{-(j-1)b_{j-2} - 2a_j - 2\lambda c_j + 2Ac_{j-1} + 2Bc_{j-2}}{x^j} + \frac{2A + 2B/x}{x^2}$$

$$\phi^R_N = \sum_{j=1}^N \frac{-jc_j + b_j}{x^{j+1}}.\quad (7.12)$$

If we require the coefficients to satisfy

$$ja_j + \lambda b_j = Ab_{j-1} + Bb_{j-2} \quad (7.12)$$

$$a_j - \lambda c_j = (j - 1)b_{j-2}/2 - Ac_{j-1} - Bc_{j-2} + [A\delta_{j1} + B\delta_{j2}]/\sqrt{\lambda} \quad (7.13)$$

$$b_j - jc_j = 0, \quad (7.14)$$
for \( j = 1, 2, \ldots, N \), then the residuals simplify to

\[
\phi_N^P = \frac{A_b N + B_{b_{N-1}}}{x^{N+2}} + \frac{B_{b_N}}{x^{N+3}}
\]

(7.15)

\[
\phi_N^Q = \frac{-N b_{N-1} + 2 A c_N + 2 B_{c_{N-1}}}{x^{N+1}} + \frac{2 B_{c_N} - (N + 1)b_N}{x^{N+2}}
\]

(7.16)

\[
\phi_N^R = 0.
\]

(7.17)

If we adopt the convention that coefficients with nonpositive subscripts have zero values, then the solution of (7.12)–(7.14) can be written, for \( 1 \leq j \leq N \),

\[
a_j = \frac{(t_1 + t_2)}{2}
\]

\[
c_j = \frac{(t_1 - t_2)}{(2\lambda)}
\]

\[
b_j = j c_j,
\]

where

\[
t_1 = [(A_{b_{j-1}} + B_{b_{j-2}})/j
\]

and

\[
t_2 = 0.5(j - 1)b_{j-2} - A c_{j-1} - B c_{j-2} - [A\delta_{j1} + B\delta_{j2}]/\sqrt{\lambda}.
\]

Since the derivatives of the residuals do not change sign once \( x \) is sufficiently large, the theory of [12] implies for that

\[
f(\lambda) - f_N^x(\lambda) = O(1/x^{N+1})
\]

(7.18)

as \( x \to \infty \).

To numerically estimate the spectral density function \( f(\lambda) \), we would usually use the methods (7.4) from [12] because they require knowledge of only the first few derivatives of \( q(x) \). But when \( q \) has the required special forms, the method (7.10) from [13], often more efficient, can also be used.

8 Numerical Estimation of the Spectral Density Function \( f(\lambda) \)

In this section we test our implementation of the various numerical methods from the previous section on the examples listed in section 6, for which exact formulas are known for the spectral density function. Then we also test a more interesting example from quantum chemistry for which exact formulas are not known.

For the hydrogen atom potential, Example 1 (equation (6.1)) with \( a = 1 \), Table 8.1 has numerical output when \( \ell = 1 \) for many \( \lambda \) with the methods \( F^1_x, F^2_x, F^3_x, \) and \( f^6_x \) using the notation of the previous section. Table 8.2 shows the analogous data when \( \ell = 2 \). Shown are only the errors: absolute when the answer is less than one and relative otherwise. A tolerance of \( 10^{-14} \) was used for the numerical integration of the initial value problem for (6.1), starting at \( x_0(\lambda) \) from (7.2). Consequently, table entries this small represent errors in \( y \) as well as errors due to finite \( x \). Note that for a fixed accuracy, generally larger matching points \( x \) are needed when \( \lambda \) is smaller. As expected, the higher order methods \( F^3 \) and \( f^6 \) are much superior.
The next choice is the Bessel Equation, Example 3 (equation (6.9)), with $\nu = 1/3$:

$$q(x) = -5/(36x^2). \quad (8.1)$$

The error behavior is similar to that in the previous tables.
Table 8.3. Numerical Error: \( q(x) = -5/(36x^2) \)

| \( \lambda \) | \( x = x(\lambda) \) | \( F^1_x \) | \( F^2_x \) | \( F^3_x \) | \( f^6_x \) |
|--------------|-----------------|----------|----------|----------|----------|
| 0.1 | 320.0 | -3.26(-7) | 4.61(-11) | 3.21(-14) | 5.37(-14) |
| 0.2 | 225.0 | 1.22(-6) | -1.13(-10) | 1.59(-13) | 6.86(-14) |
| 0.4 | 160.0 | -5.18(-7) | 7.31(-11) | 4.90(-14) | 8.34(-14) |
| 1 | 100.0 | 2.34(-6) | -3.48(-10) | 2.85(-13) | 1.12(-13) |
| 2 | 71.0 | 3.30(-6) | -4.93(-10) | 3.92(-13) | 1.47(-13) |
| 4 | 50.0 | 3.71(-6) | -5.53(-10) | 4.38(-13) | 1.63(-13) |
| 10 | 32.0 | -1.51(-6) | 2.14(-10) | 1.49(-13) | 2.49(-13) |
| 20 | 22.5 | 5.26(-6) | -7.86(-10) | 6.76(-13) | 2.85(-13) |
| 40 | 16.0 | -1.78(-6) | 2.51(-10) | 1.58(-13) | 2.76(-13) |
| 100 | 10.0 | 5.92(-6) | -8.26(-10) | 7.22(-13) | 2.83(-13) |
| 200 | 7.0 | -5.92(-6) | 9.12(-10) | -1.74(-13) | 2.95(-13) |
| 400 | 5.0 | 5.92(-6) | -8.82(-10) | 7.36(-13) | 2.97(-13) |
| 1000 | 3.2 | -1.78(-6) | 2.51(-10) | 1.54(-13) | 2.72(-13) |
| 2000 | 2.2 | -5.78(-6) | 8.89(-10) | -1.65(-13) | 2.91(-13) |
| 4000 | 1.6 | -1.78(-6) | 2.51(-10) | 1.70(-13) | 2.88(-13) |
| 10000 | 1.0 | 5.92(-6) | -8.82(-10) | 5.98(-12) | 2.63(-13) |

In the papers of Bain et al [4], Brändas et al [5], and Engdahl et al [7, 8, 9] can be found a potential with a “barrier” near \( x = 2 \) and decaying rapidly to zero as \( x \to \infty \):

\[
q(x) = \frac{\ell(\ell + 1)}{x^2} - \frac{a}{x} + 15x^2 e^{-x}.
\] (8.2)

For this example we have \( q_0 = \ell(\ell + 1) \), \( q_1 = -a \), \( q_2 = q_3 = 0 \), and for \( k \geq 2 \)

\[
q_{k+2} = (-1)^k \frac{15}{(k - 2)!}.
\]

For \( a = 1 \), Table 8.4 displays the results for several values of \( x \) to show the rapid convergence as \( x \to \infty \). A tolerance of \( 10^{-14} \) was used for the numerical integration of \( y \).

Table 8.4. \( F^3_x \) Estimates for Barrier Potential \([8.2]\) with \( a = 1 \).

| \( x \) | \( \ell = 0 \) | \( \ell = 1 \) | \( \ell = 2 \) | \( \ell = 0 \) | \( \ell = 1 \) | \( \ell = 2 \) |
|--------|-----------------|----------|----------|----------|----------|----------|
| \( \lambda = 7 \) | 0.1428909355 | 0.019804657 | 0.0004166628 | 1.686525464 | 1.728282916 | 0.1242771047 |
| 5.0 | 0.142829890 | 0.019801387 | 0.0004162081 | 1.686646374 | 1.728086680 | 0.1242724151 |
| 10.0 | 0.142829143 | 0.019801395 | 0.0004162075 | 1.686647533 | 1.728085796 | 0.1242728883 |
| 15.0 | 0.142829149 | 0.019801396 | 0.0004162075 | 1.686647559 | 1.728085772 | 0.1242723721 |
| 20.0 | 0.142829149 | 0.019801396 | 0.0004162075 | 1.686647559 | 1.728085772 | 0.1242723721 |
| \( \lambda = 10 \) | 5.0 | 0.1499374819 | 4.314112367 | 2.8784054557 | 2.558971562 | 11.31991552 | 17.27075628 |
| 10.0 | 0.1499374819 | 4.314112204 | 2.8784044730 | 2.558971266 | 11.31991563 | 17.27075635 |
| 15.0 | 0.1499374882 | 4.314112311 | 2.8784043230 | 2.558971293 | 11.31991552 | 17.27075623 |
| 20.0 | 0.1499374882 | 4.314112307 | 2.8784043230 | 2.558971293 | 11.31991552 | 17.27075628 |
| 25.0 | 0.1499374882 | 4.314112307 | 2.8784043240 | 2.558971293 | 11.31991552 | 17.27075628 |

9 Numerical Estimation of the Spectral Function \( \rho(\lambda) \)

Associated with the density function \( f(\lambda) \) is the associated spectral function defined by

\[
\rho(\lambda) := \int_0^\lambda f(\mu) d\mu.
\] (9.1)
In [11] for problems regular at \( x = 0 \) we estimated \( \rho \) using \( F^1 \) and compared with the package SLEDGE [20, 15]; generally the \( \rho(\lambda) \) computation using a quadrature routine for (9.1) and the \( F^1 \) formula ran considerably faster than SLEDGE, but still had the drawback that rather large \( x \)-intervals were required for the \( F^1 \) calculation. Here we apply the methods of this paper for computing \( \rho \) by estimating \( f \) in (9.1), and performing a quadrature, to the examples in section 6 for which exact answers are known, and again compare with SLEDGE.

The SLEDGE software for estimating \( \rho(\lambda) \) is based on the Levitan-Levinson characterization of the spectral function as a limit of step spectral functions over a finite interval approximation (second formula in (5.8)); this is a totally different approach than the present approach of this paper which relies on the family of \( F^j \)-approximants, together with the quadrature in (9.1). For the case of two singular endpoints, the performance of SLEDGE for computing the spectral function on examples having explicit formulas for the spectral function was reported on in [15]. As reported there, one of the major weaknesses of the SLEDGE package is obtaining high accuracy in the \( \rho(\lambda) \) calculation when \( \lambda \) is large; this is due primarily to the fact that SLEDGE does not rely on asymptotic approximations for the eigenvalues and eigenfunction norm reciprocals, but computes them numerically as required for implementing the \( \rho_\beta(\lambda) \)-formula in (5.8). Experience in using SLEDGE on doubly singular problems is that very large computing times are required due to the computation of large numbers of eigenvalue - eigenfunction norm pairs, and that there is significant loss of accuracy when \( \lambda \) becomes sufficiently large. As the timing and accuracy data of this section shows, doubly singular problems can be handled with high accuracy and much reduced computing times by making use of the \( F^j_2 \)-approximants and the \( f^N_2 \)-approximants of this paper, along with the quadratures for computing \( \rho(\lambda) \) in (9.1); this represents a major improvement in computational technique over the SLEDGE algorithm for spectral function computation.

Following SLEDGE, we assume approximations are sought for a finite set of \( \lambda \)-values in the continuous spectrum, \( (0, \infty) \), ordered so that

\[
0 < \lambda_1 < \lambda_2 < \ldots < \lambda_m.
\]

Then with \( \rho(0) \) given (or computed via SLEDGE) we estimate

\[
\rho(\lambda_1) = \rho(0) + \int_0^{\lambda_1} f(\mu) \, d\mu
\]

and for \( j = 2, 3, \ldots, m \)

\[
\rho(\lambda_j) = \rho(\lambda_{j-1}) + \int_{\lambda_{j-1}}^{\lambda_j} f(\mu) \, d\mu
\]

(9.2)

using an adaptive quadrature code with \( f \) replaced by \( F^j_2 \) or \( f^N_2 \) approximations. Here we report some timing and accuracy data for the four examples listed in section 6.

The spectral functions on \( (0, \infty) \) for these examples are known in closed form by putting the exact spectral density functions from (5.4), (6.8), (6.12), and (6.16) into (9.1) and performing an exact integration. The resulting closed form formulas for \( \rho(\lambda) \) were used for the four examples to compare with the numerical approximations and to generate the ‘exact’ error; the errors are taken as absolute if the exact value of \( \rho(\lambda) \) is less than one, and relative otherwise.

For the Bessel equation of order 1, Example 4 (equation (6.13 with \( N = 1 \)), we used \( N = 7 \) in the approximation (7.10) (that is, the scheme from [13, Sec 4]). Output data for six \( \lambda \)-values is displayed in Table 9.1. The quadrature tolerance was \( 10^{-8} \) and the tolerance for the initial value problem was \( 10^{-9} \).

Note that, at this tolerance, all the apparent error arises from the first integration interval and is passed on through the sum in (9.2).

| \( x \) | \( \lambda = 1 \) | \( \lambda = 2 \) | \( \lambda = 4 \) | \( \lambda = 10 \) | \( \lambda = 20 \) | \( \lambda = 40 \) |
|---|---|---|---|---|---|---|
| 6.00 | 0.063318042 | 0.25068042 | 1.00068041 | 6.25068041 | 25.00068041 | 100.00068041 |
| 12.00 | 0.06254252 | 0.2504252 | 1.0004252 | 6.2504252 | 25.0004252 | 100.0004252 |
| 24.00 | 0.06250266 | 0.2500266 | 1.0000266 | 6.2500266 | 25.0000266 | 100.0000266 |
| 36.00 | 0.06250000 | 0.2500000 | 1.0000000 | 6.2500000 | 25.0000000 | 100.0000000 |
The data for estimating $f(\lambda)$ in section 8 showed that as $\lambda$ gets larger, smaller values of the matching point $x = x(\lambda)$ are needed for a given accuracy. The data in Table 9.1 for $\rho$ exhibit this phenomena. Hence, from efficiency considerations in order to compute $\rho(\lambda)$ we want the choice of matching point $x$ to vary with the integer $N$, or even better, pointwise with $\lambda$. For $q(x) = 0.75/x^2$ it can be shown that the absolute error in $f(\lambda)$ for a given $N$ is proportional to

$$
\frac{1}{x^{N+2}\lambda^{N-1/2}}.
$$

This suggests that taking $x \sim 1/\lambda^{(2N-1)/(2N+4)}$ would be a good heuristic for the matching point. Similarly, for the family of approximants, $F^N$, from (7.4)–(7.7) the corresponding form for the absolute error in $f(\lambda)$ is

$$
\frac{1}{x^{2N}\lambda^{N-1/2}},
$$

so that $x \sim 1/\lambda^{(2N-1)/(4N)}$ would be an appropriate matching point. The latter is roughly $1/\sqrt{\lambda}$. As mentioned earlier, these formulas would change for a different $q$. Also, the heuristic would differ for relative errors. A similar analysis for the general potential $q(x) = A/x + B/x^2$ suggests a good first value of matching point would be

$$
x = x(\lambda) := |A|/(2\lambda) + \sqrt{A^2/(4\lambda^2) + |B|/\lambda}.
$$

(9.3)

We have written a research code, called AutoB, for which the only inputs required are the set of $\lambda$ points, the $\rho(0)$ value, and the accuracy desired. If $q$ has the form of (7.11) or the form of similar potentials in (13), then we use the appropriate $f_N^B$ formula in (7.10) with $N$ chosen to be a function of the accuracy sought. Otherwise, we use $F^3$ from (7.4) which requires knowledge of derivatives of $q$. We report the performance of AutoB on the four examples in section 6 using (9.3) as the initial choice of matching point. Given a prescribed tolerance $\tau$, for each $\lambda$ the matching point $x$ is then increased until

$$
|\text{error estimate}| \leq \max\{1,|\text{output value}|\} \tau
$$

holds. Estimates at various $\tau$ were sought for the following set of sixteen $\lambda$ values:

$$
\{0.1, 0.2, 0.4, 1, 2, 4, 10, 20, 40, 100, 200, 400, 1000, 2000, 4000, 10000\}.
$$

(9.4)

The error shown is the maximum (relative when the ‘exact’ $\rho > 1$, absolute otherwise) over the set of sixteen $\lambda$ values. For many of these runs the heuristics were overly conservative, but the times are nevertheless quite small. For the Bessel equation of order $3/4$, Example 3 (equation (6.9) with $\nu = 1/3$), the relatively large computing times were due to difficulties near $\lambda = 0$.

### Table 9.2. AutoB results for several tolerances and Four Potentials on $(0,\infty)$.

| Potential | $\tau = 10^{-4}$ | $\tau = 10^{-6}$ | $\tau = 10^{-8}$ | $\tau = 10^{-10}$ |
|-----------|----------------|----------------|----------------|----------------|
|           | error | time | error | time | error | time | error | time | error | time |
| 1. Ex4($\nu=1$) | 1.30(−7) | 0.28 | 1.50(−9) | 0.50 | 1.92(−12) | 1.06 | 1.73(−13) | 2.46 |
| 2. Ex1($\ell=1$) | 1.78(−6) | 0.42 | 7.88(−7) | 0.84 | 1.50(−8) | 3.11 | 7.93(−11) | 18.50 |
| 3. Ex2($\ell=1$) | 2.49(−6) | 0.37 | 3.37(−7) | 0.74 | 8.54(−9) | 3.95 | 1.10(−10) | 20.97 |
| 4. Ex3($\nu=1/3$) | 9.57(−5) | 0.49 | 1.04(−6) | 3.00 | 1.52(−8) | 41.95 | 1.13(−10) | 894.77 |

For comparison, output from the SLEDGE program is shown for the Bessel equation of order Example 4 with $\nu = 1$, Example 4 (equation (6.13) in Table 9.3. Since SLEDGE is known to have difficulty with large values of $\lambda$, we ran the program at various choices of $\tau$ only on the first $n \lambda$-values from (9.3) with $n = 1, 2, \ldots, 9$. The final line ($n = 16$) is output from AutoB using all sixteen $\lambda$ values up to $\lambda = 10000$. Clearly, AutoB is much more reliable than SLEDGE. Similar results were observed for other doubly singular potentials.
Table 9.3. SLEDGE output for the Bessel equation of order 1 ($q(x) = \frac{0.75}{x^2}$)

| $n$ | $\tau = 10^{-3}$ | $\tau = 10^{-4}$ | $\tau = 10^{-5}$ | $\tau = 10^{-6}$ |
|-----|------------------|------------------|------------------|------------------|
|     | time (sec)       | time (sec)       | time (sec)       | time (sec)       |
| 1   | 1.31(-4) 0.02   | 3.87(-5) 0.09    | 9.74(-6) 0.50    | 9.92(-6) 1.58    |
| 2   | 6.86(-4) 0.02   | 1.24(-5) 0.23    | 1.07(-5) 1.31    | 9.87(-6) 8.43    |
| 3   | 2.72(-4) 0.14   | 1.32(-5) 0.34    | 2.95(-5) 2.34    | 6.70(-6) >96.53 |
| 4   | 2.71(-4) 0.16   | 1.79(-4) 0.50    | 3.20(-5) 8.45    | 6.70(-6) >177.28 |
| 5   | 7.16(-4) 0.19   | 1.79(-4) 0.70    | 3.20(-5) 16.40   |                   |
| 6   | 1.92(-3) 0.21   | 1.79(-4) 1.71    | 3.20(-5) 29.51   |                   |
| 7   | 7.04(-3) 0.96   | 1.83(-4) 7.67    | 8.65(-5) 51.64   |                   |
| 8   | 1.47(-2) 1.83   | 1.83(-4) 11.39   | 2.18(-4) 75.87   |                   |
| 9   | 2.23(-2) 12.00  | 3.31(-4) 20.48   | 2.83(-4) >465.99 |                   |

AutoB

|     | time (sec)       | time (sec)       | time (sec)       | time (sec)       |
| 16  | 3.69(-6) 0.18   | 1.30(-7) 0.28    | 5.74(-9) 0.36    | 1.50(-9) 0.50    |

To illustrate the superiority of the new code AutoB over SLEDGE we also ran comparisons on timing and accuracy the Hydrogen Atom potential with $\ell = 1$, Example 1 (equation (6.1)). The output values for $\rho(\lambda)$ obtained for each of the sixteen $\lambda$ values in (9.4) for four choices of the tolerance levels are displayed in Table 9.4. The $>$ in the time needed for SLEDGE indicates that it stopped (too much time) before the user requested input accuracy was achieved. Since SLEDGE could not achieve $10^{-5}$-accuracy over the whole range of $\lambda$-values, no SLEDGE runs for tighter tolerances are listed. As the data shows, SLEDGE has much difficulty to compute highly accurate results for large values of $\lambda$, while the new codes are capable of quite high accuracy in much less computing time. Similar testing for the Hydrogen Atom potential using the $F_j^x$ approximants was also done in the thesis of Mark Schuster [22].

Table 9.4: Comparison of SLEDGE with AutoB for Hydrogen problem with $\ell = 1$.

| $\lambda$ | Exact  | SLEDGE | AutoB | AutoB | AutoB | AutoB |
|-----------|--------|--------|-------|-------|-------|-------|
| 0.1       | 0.005621362 | 0.0056 | 0.0056 | 0.0056214 | 0.005621362 |
| 0.2       | 0.010067470 | 0.0100 | 0.0100 | 0.01007 | 0.010067470 |
| 0.4       | 0.022334389 | 0.0222 | 0.0223 | 0.0223345 | 0.022334389 |
| 1.0       | 0.087358065 | 0.0874 | 0.0873 | 0.087358065 | 0.087358065 |
| 2.0       | 1.298717032 | 1.2987 | 1.2987 | 1.298717032 | 1.298717032 |
| 4.0       | 1.661656722 | 1.6616 | 1.6616 | 1.661656722 | 1.661656722 |
| 10.0      | 8.206942681 | 8.2069 | 8.2069 | 8.206942681 | 8.206942681 |
| 20.0      | 38.9811754  | 38.981 | 38.981 | 38.9811754 | 38.9811754 |
| 40.0      | 194.5884791 | 194.59 | 194.59 | 194.5884791 | 194.5884791 |
| 100.0     | 1719.215348 | 1719.2 | 1719.2 | 1719.215348 | 1719.215348 |
| 200.0     | 9188.295022 | 9188.3 | 9188.3 | 9188.295022 | 9188.295022 |
| 400.0     | 49923.13741 | 49923.1 | 49923.1 | 49923.13741 | 49923.13741 |
| 1000.0    | 2475962.250 | 247596.2 | 247596.2 | 2475962.250 | 2475962.250 |
| 2000.0    | 1234411.32 | 1234411.3 | 1234411.3 | 1234411.32 | 1234411.32 |
| 4000.0    | 6176672.30 | 6176672.3 | 6176672.3 | 6176672.30 | 6176672.30 |
| 10000.0   | 310797243.9 | 310797243.9 | 310797243.9 | 310797243.9 | 310797243.9 |

Remark. High accuracy in the spectral function computation for the Bessel equation on $(0, \infty)$, Examples 3 and 4, was also achieved in [13, Sec 4]; this, however, was done by inserting asymptotic formulas for the eigenvalues and eigenfunction norm reciprocals for the Bessel equation on $(0, b]$ into the SLEDGE code (bypassing the SLEDGE computation of these quantities); but, of course, this was not an automatic procedure applicable to other problems with two singular endpoints.
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