Computing the spectral function for singular Sturm–Liouville problems

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Abstract

Algorithms for computing Sturm–Liouville spectral density functions are developed based on several mathematical characterizations. Convergence and error bounds are derived and methods are tested on several examples. The results are compared with those from the existing software package SLEDGE.

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1. Introduction

In this paper the singular Sturm–Liouville problem

\[
\begin{align*}
-U'' + q(x)U &= \lambda U, \quad x \in [a, \infty) \\
U(a) \cos \alpha + U'(a) \sin \alpha &= 0,
\end{align*}
\]

(1.1)

is studied when $q$ belongs to Weyl’s limit point case and generates some continuous spectrum.
New formulas from Pearson [20] for the spectral function and for the spectral density function over the range of continuous spectrum are further developed and implemented numerically; the results demonstrate that higher accuracy and considerably reduced execution times are possible with this approach than with the existing software package SLEDGE [25].

Two cases of new formulas for the spectral density function are given for each of the following cases:

(i) $q \in L_1(a, \infty)$ and (ii) $q = V_1 + V_2$, where $V_1 \in L_1(a, \infty)$ and $V_2$ is a continuous function of bounded variation on $[a, \infty)$, with $\lim_{x \to \infty} V_2(x) = 0$.

We make the general assumption (iii) $q$ is limit point at $\infty$ and $q$ is oscillatory at $\infty$ for $\lambda \in (A, \infty)$ and nonoscillatory at $\infty$ for $\lambda \in (-\infty, A)$. This includes the special cases (i) and (ii), for which $A = 0$.

Under these assumptions the spectrum of the singular problem (1.1) over $[a, \infty)$ is discrete in $(-\infty, A)$ and the continuous spectrum is contained in $(A, \infty)$. Further assumptions, implicit in our method of discretization of (1.1) by a step function approximation to $q$ as in SLEDGE, are $q \in C^4[a, b]$ for the first level of a Richardson’s $h^2$-extrapolation over successive meshes, $q \in C^6[a, b]$ for two levels of extrapolations, etc. Here the right endpoint $b$ is necessarily finite, but may be large depending on the problem and the user’s accuracy request.

For all $\lambda \in \| \mathbb{C} \|$ (the set of complex numbers) let $y(\cdot, \lambda)$ and $u(\cdot, \lambda)$ be the solutions of (1.1) defined at $x = a$ by the initial conditions:

$$
\begin{pmatrix} y(a, \lambda) & u(a, \lambda) \\
 y'(a, \lambda) & u'(a, \lambda) \end{pmatrix} = \begin{pmatrix} -\sin \alpha & \cos \alpha \\
 \cos \alpha & \sin \alpha \end{pmatrix}.
$$

As in SLEDGE we will need to make use of the solutions $y(\cdot, \lambda)$ and $u(\cdot, \lambda)$ only for real values of $\lambda$; but for the Weyl–Titchmarsh approach to defining the spectral function complex values of $\lambda$ are required.

The software package SLEDGE [25] makes use of the Levitan–Levinson approach to defining the spectral function $\rho^2(\cdot)$ associated with the singular problem (1.1) as in (4.3) and (4.4) below. By truncating to a finite interval $[a, b]$, the eigenvalues and eigenfunction norms for the finite interval problem with Dirichlet boundary condition at $b$ ((4.1) in Section 4 below with $x = b$) can be computed for a fixed choice of $b$ and an initial mesh to produce an approximation to $\rho^2_b(\lambda)$ over the range of $\lambda$ desired. The mesh and the $b$ value are adjusted until convergence occurs to sufficient accuracy, and the result is returned as an approximation to $\rho^2$. See [25,8–11] for background information, examples and applications. This approach typically requires the calculation of an enormous number of eigenvalue/eigenfunction pairs, often in the tens to hundreds of thousands. Hence, the desirability of alternate methods.

In the next section, we discuss a characterization of the spectral density function that goes back to Weyl and Titchmarsh for the case (i) of $q \in L_1(a, \infty)$. In Section 3, we give new formulas of Pearson [20] for both cases (i) and (ii) along with error bounds depending on the length of the interval $[a, b]$ of the approximating regular problem. In Section 4, we give some background results on averaging of spectral measures, which are then utilized in Section 5 to prove new formulas for approximating the spectral density functions for both cases (i) and (ii). The proof of Theorem 1 in Section 5 establishes that Pearson’s new formulas are valid characterizations of the spectral density functions for both cases. The basic numerical algorithms are described in Section 6. Error analysis for the algorithms is found in Section 7. Section 8 contains several numerical examples illustrating the theory and the practicality of the approach.

The characterization of the spectral density function for the cases (i) and (ii) given here includes a large class of the problems SLEDGE can handle. For problems in Liouville normal form on $[a, \infty)$ with left endpoint regular, and satisfying assumption (iii), SLEDGE requires only that the potential $q$ have power
behavior near $+\infty$ (for classification [11] and generation of the initial mesh) and, for applicability of the Richardson $h^2$-extrapolation, that $q \in C^4$. (If the latter does not hold, then Aitken extrapolation is used as a backup.) The same assumptions are needed for the codes presented here. Of course, the assumptions (i) and (ii) necessarily restrict the class of problems the current codes can handle. However, the only LNF potentials $q$ which SLEDGE has been tested on which do not satisfy the assumptions of being in $L_1(a, \infty)$ or a sum of an $L_1(a, \infty)$ function and a BV$(a, \infty)$ function are (1) periodic potentials or perturbations of them, (2) potentials which give rise to eigenvalues embedded in the continuous spectrum (most of the examples in [8]), and (3) potentials which behave like $\sin(kx)/x$ or $\cos(kx)/x$ with $0 < \beta \leq 1$. The original SLEDGE test set [27] contains four potentials which do not satisfy assumptions (i) and (ii) (after normalizing $q$ so that $q \to 0$ as $x \to \infty$): the Gelfand–Levitan potential (#PF36), the potentials $\cos x$ (#PF40) and $\cos x + k/x^2$ (#PF196 and #PF197) and the Wigner–von Neumann potential (#PF98). In addition all the problems in [8] which were constructed to have embedded eigenvalues fail to satisfy the assumptions (i) or (ii). However, work is in progress to extend the present methods so as to include these types of potentials. Although mathematical theory is currently lacking, the two codes described here have been run on the Gelfand–Levitan example and the Wigner–von Neumann example with quite reasonable results.

In addition, it is anticipated to extend the methods presented here to include problems not in LNF with one endpoint regular and one endpoint satisfying assumption (iii), and to problems with two singular endpoints, one satisfying assumption (iii) and one which is nonoscillatory for all $\lambda$ (LP or LC). When this is finished, virtually all the problems which SLEDGE can handle will be covered by the new methods.

2. A characterization of Weyl and Titchmarsh for the spectral density function

For $q \in L_1$ Titchmarsh [31, Section 5.7] made use of the Liouville Integral Equation to obtain, for his solution, $\phi(x, \lambda)$, which is the solution $-y(x, \lambda)$ defined in (1.2), the asymptotic behavior for large $x$ and fixed $s = \sqrt{\lambda} \in (0, \infty)$:

$$\phi(x, \lambda) = a(\lambda) \cos sx + b(\lambda) \sin sx + O\left(\int_x^\infty |q| \, dt\right), \quad (2.1)$$

$$\phi'(x, \lambda) = -sa(\lambda) \sin sx + sb(\lambda) \cos sx + O\left(\int_x^\infty |q| \, dt\right), \quad (2.2)$$

where

$$a(\lambda) = \sin z - \frac{1}{s} \int_0^\infty \sin(st) q(t) \phi(t, \lambda) \, dt, \quad (2.3)$$

and

$$b(\lambda) = -\frac{\cos z}{s} + \frac{1}{s} \int_0^\infty \cos(st) q(t) \phi(t, \lambda) \, dt. \quad (2.4)$$

He obtained the formula for $f(\lambda) = \rho'(\lambda)$ for the continuous range of the spectrum, $[0, \infty)$, as

$$f^2(\lambda) := \frac{1}{\pi \sqrt{\lambda}[a^2(\lambda) + b^2(\lambda)]}. \quad (2.5)$$
From (2.1) and (2.2) a simple calculation shows that
\[
\frac{1}{\pi[(1/s)(\phi'(x, \lambda))^2 + s(\phi(x, \lambda))^2]} = \frac{1}{\pi s[a^2(\lambda) + b^2(\lambda) + o(1)]}
\]
as \(x \to \infty\) for all \(\lambda \in (0, \infty)\), so it follows that
\[
f^2(\lambda) = \lim_{b \to \infty} \frac{1}{\pi[(1/s)(y'(b, \lambda))^2 + s(y(b, \lambda))^2]}
\]
for the \(y(x, \lambda)\) defined in (1.2). Compare also Brown et al. [5, p. 336]. Eastham [7] has also obtained higher-order terms in the asymptotic expansions (2.1) and (2.2) and higher order asymptotics for \(\rho^2(\lambda)\) as \(\lambda \to \infty\).

**Problem 1.** It is sometimes possible to make use of (2.5) directly for specific equations for which large \(x\) asymptotics are known in terms of special functions. For example, consider the Bessel equation of order \(v, v \geq 0, \text{ on } [1, \infty)\) with \(z = 0\),
\[
-y'' + \frac{v^2 - 1/4}{x^2}y = \lambda y, \quad y(1) = 0, \quad y'(1) = 1.
\]
The solution of this initial value problem is
\[
y(x, \lambda) = \frac{\pi}{2} \sqrt{x}[ -Y_v(s)J_v(sx) + J_v(s)Y_v(sx)],
\]
where \(s = \sqrt{\lambda}\). Making use of the asymptotic formulas for \(J_v(sx)\) and \(Y_v(sx)\), we find
\[
y(x, \lambda) = a(\lambda) \cos(sx - (v + 1)\pi/2) + b(\lambda) \sin(sx - (v + 1)\pi/2) + O(1/x)
\]
as \(x \to \infty\), where \(a(\lambda) = -\sqrt{\pi/(2s)}Y_v(s)\) and \(b(\lambda) = \sqrt{\pi/(2s)}J_v(s)\). It follows from (2.1)–(2.2) and (2.5) that
\[
f^0(\lambda) = \frac{2}{\pi^2[J_v^2(s) + Y_v^2(s)]}.
\]
Similarly, for the Neumann boundary condition at \(x = 1 (\pi = \pi/2)\) we find
\[
f^{\pi/2}(\lambda) = \frac{2}{\pi^2[[J_v(s)/2 + sJ_v'(s)]^2 + [Y_v(s)/2 + sY_v'(s)]^2]}.
\]
This problem is one of the test problems for our numerical codes and will be compared with SLEDGE on timing and accuracy in Section 8 for both Dirichlet and Neumann boundary conditions. Since Bessel function software can be used to compute the quantities in (2.10) and (2.11) to machine precision, these examples provide an independent check on the accuracy of the numerical codes. For these cases we have \(A = 0\) and \(\rho(A) = 0\).

Our numerical approach to computing the limit in (2.6) is to approximate \(q\) by a piecewise constant function and employ piecewise circular or hyperbolic trigonometric functions to estimate \(y\) and \(y'\) for large \(x\). This is similar in spirit to the underlying integrator used in SLEDGE [25], but differs in that \(y\) here is the solution of an initial value problem instead of an eigenvalue problem. The basic \(O(h^2)\) error
bounds for \( \max_{x \in [a,b]} |y(x) - \hat{y}(x)| \) are, however, well known for the initial value problem [22]. The computation of the spectral function for (1.1) then proceeds by a quadrature using
\[
\rho^2(\lambda) = \rho^2(\Lambda) + \int_{\lambda}^\Lambda f^2(\mu) \, d\mu. \tag{2.12}
\]
Here \( \rho^2(\Lambda) \) is the sum of the reciprocals of the norms of the discrete eigenfunctions \( y(x, \lambda_n) \) for \( \lambda_n < \Lambda \), which can be computed using SLEDGE.

3. New characterizations of the spectral density function

**Lemma 3.1.** Assume \( q \in L_1(a, \infty) \).

(i) If \( y(x, \lambda) \) is the solution defined by (1.2) we put
\[
\Phi(x, \lambda) := \frac{1}{\sqrt{\lambda}} [y'(x, \lambda)]^2 + \sqrt{\lambda} |y(x, \lambda)|^2. \tag{3.1}
\]
Then
\[
\Phi(x_2, \lambda) - \Phi(x_1, \lambda) = \int_{x_1}^{x_2} q(t) \frac{2y(t, \lambda)y'(t, \lambda)}{\sqrt{\lambda}} \, dt. \tag{3.2}
\]
(ii) Defining for all \( b \in (a, \infty) \) and all \( \lambda > 0 \)
\[
F_b^2(\lambda) := \frac{1}{\pi\Phi(b, \lambda)}, \tag{3.3}
\]
we have from (2.6), (3.1) and (3.2) that
\[
f^2(\lambda) := \lim_{b \to \infty} F_b^2(\lambda) = \frac{1}{\pi[\Phi(a, \lambda) + (2/\sqrt{\lambda}) \int_a^\infty q(t)y(t, \lambda)y'(t, \lambda) \, dt]}, \tag{3.4}
\]
where, by (1.2), \( \Phi(a, \lambda) = \cos^2 \pi/\sqrt{\lambda} + \sqrt{\lambda} \sin^2 \pi \).

(iii) We also have the bound
\[
|\Phi(x, \lambda)| \leq \Phi(a, \lambda) \exp \left( \int_{a}^{x} \frac{|q(t)|}{\sqrt{\lambda}} \, dt \right). \tag{3.5}
\]
(iv) The solution \( y \) and its derivative \( y' \) (and \( |yy'| \)) are bounded over \( [a, \infty) \).

(v) We have the following error bounds as \( b \to \infty \)
\[
|\Phi(b, \lambda) - \Phi(\infty, \lambda)| = O \left( \int_{b}^{\infty} |q| \, dt \right), \quad b \to \infty, \tag{3.6}
\]
\[
|F_b(\lambda) - F(\infty)(\lambda)| = O \left( \int_{b}^{\infty} |q| \, dt \right), \quad b \to \infty \tag{3.7}
\]
uniformly for \( \alpha \in [0, \pi) \).
(vi) If, in addition to \( q \in L_1(a, \infty) \), we assume \( \lim_{x \to \infty} q(x) = 0 \) and \( q' \) is of one sign for sufficiently large \( x \), then we have the error bounds

\[
|\Phi(b, \lambda) - \Phi(\infty, \lambda)| = O(|q(b)|), \quad b \to \infty,
\]

\[
|F_b(\lambda) - F_\infty(\lambda)| = O(|q(b)|), \quad b \to \infty
\]

uniformly for \( x \in [0, \pi) \).

**Proof.** For (i)

\[
\Phi'(x, \lambda) = 2y'y''/\sqrt{\lambda} + 2\sqrt{\lambda}yy' = 2y'(q - \lambda)y/\sqrt{\lambda} + 2\sqrt{\lambda}yy' = q[2y'/\sqrt{\lambda}].
\]

For (ii) put \( x_1 = a \) and \( x_2 = b \) in (3.2) and pass \( b \to \infty \) in (3.3). For (iii) observe that with \( A := 1/\sqrt{\lambda} \) and \( B := \sqrt{\lambda} \) we have

\[
0 \leq \left( \sqrt{\lambda}y' - \sqrt{B}|y| \right)^2 \leq \Phi(x, \lambda) - 2|yy'|
\]

and therefore

\[
2|yy'| \leq \Phi(x, \lambda)
\]

for all \( x \in [a, \infty) \). Using this in (3.2) and putting \( x_1 = a \) we have

\[
\Phi(x, \lambda) \leq \Phi(a, \lambda) + \frac{1}{\sqrt{\lambda}} \int_a^x |q|\Phi(t, \lambda) \, dt.
\]

The bound (3.5) now follows from Gronwall’s inequality.

For (iv) we observe that the quantities \( y'^2/\sqrt{\lambda} \), \( \sqrt{\lambda}y^2 \), and \( 2|yy'| \) are all bounded by \( \Phi(x, \lambda) \), which is bounded on \([a, \infty) \) by

\[
\Phi(a, \lambda) \exp \left( \int_a^\infty \frac{|q|}{\sqrt{\lambda}} \, dt \right).
\]

For (v) we have from (3.2) that

\[
|\Phi(b, \lambda) - \Phi(\infty, \lambda)| = \left| \int_b^\infty q \frac{2yy'}{\sqrt{\lambda}} \, dt \right|.
\]

Putting bound (3.11) in the integrand and applying the bound in (3.13) gives the result. Here \( \Phi(a, \lambda) \) can be bounded independently of \( x \). The same bound for \( |F_b(\lambda) - F_\infty(\lambda)| \) follows readily from (3.3).

For (vi) we may integrate by parts in the right-hand side of (3.14), obtaining

\[
\int_b^\infty q^2yy' \, dt = q(b)y^2(b, \lambda) - \int_b^\infty q'y^2 \, dt.
\]
Under the assumptions, both terms on the right are $O(|q(b)|)$ since $y$ is bounded by (3.13) independently of $\alpha \in [0, \pi)$. □

**Lemma 3.2.** Assume $q = V_1 + V_2$, where $V_1 \in L_1(a, \infty)$ and $V_2$ is a continuous function of bounded variation on $[a, \infty)$, with $\lim_{x \to \infty} V_2(x) = 0$.

(i) If $y(x, \lambda)$ is the solution defined by (1.2) we put

$$\phi(x, \lambda) := y^2(x, \lambda) + (\lambda - V_2(x))y^2(x, \lambda).$$

Then for all $x \in (a, \infty)$

$$\phi(x_2, \lambda) - \phi(x_1, \lambda) = 2 \int_{x_1}^{x_2} V_1 y y' \, dt - \int_{x_1}^{x_2} y^2 \, dV_2(t).$$

(ii) Defining

$$F_b(\lambda) := \frac{\sqrt{\lambda}}{\pi[(y'(b, \lambda))^2 + (\lambda - V_2(b))(y(b, \lambda))^2]} = \frac{\sqrt{\lambda}}{\pi \phi(b, \lambda)}$$

we have

$$f^2(\lambda) := \lim_{b \to \infty} F_b^2(\lambda) = \frac{\sqrt{\lambda}}{\pi[\phi(a, \lambda) + 2\int_a^\infty V_1(t)yy' \, dt - \int_a^\infty (y(t, \lambda))^2 \, dV_2(t)]}.$$  \hfill (3.18)

Note: The Weyl–Titchmarsh formulas (2.5) and (2.6) do not apply to conclude at this point that the right-hand side of (3.18) is a spectral density function; however, this follows from Theorem 1(ii) and Lemmas 3.2 and 3.3 below.

(iii) The separation of the potential $q$ into the parts $V_1$ and $V_2$ is nonunique, and it is always possible to redefine $V_1$ and $V_2$ for a given $\lambda$ so as to ensure that $\lambda - V_2 \geq c = c(\lambda) > 0$ for all $x \in (a, \infty)$. Also, since $V_2$ is continuous and of bounded variation, we can write $V_2 = U_2 - W_2$, where $U_2$ and $W_2$ are continuous, nondecreasing and bounded, and without loss of generality, $W_2(a) = 0$. Then we have

$$|\phi(x, \lambda)| \leq |\phi(a, \lambda)| \exp \left( \frac{W_2(x)}{c} + \frac{1}{\sqrt{c}} \int_a^x |V_1(t)| \, dt \right).$$  \hfill (3.19)

(iv) The solution $y$ and its derivative $y'$ (and $|yy'|$) are bounded over $[a, \infty)$.

(v) We have the following error bounds as $b \to \infty$

$$|\phi(b, \lambda) - \phi(\infty, \lambda)| = O \left( \int_b^\infty |V_1| \, dt + \int_b^\infty dW_2 + \int_b^\infty dU_2 \right), \quad b \to \infty,$$

$$|F_b(\lambda) - F_\infty(\lambda)| = O \left( \int_b^\infty |V_1| \, dt + \int_b^\infty dW_2 + \int_b^\infty dU_2 \right), \quad b \to \infty$$

uniformly for $\alpha \in [0, \pi)$.

(vi) If, in addition to $V_1 \in L_1(a, \infty)$, we assume $\lim_{x \to \infty} V_1(x) = 0$ and $V_1'$ is of one sign for sufficiently large $x$, then we have the error bounds

$$|\phi(b, \lambda) - \phi(\infty, \lambda)| = O \left( |V_1(b)| + \int_b^\infty dW_2 + \int_b^\infty dU_2 \right), \quad b \to \infty.$$  \hfill (3.22)
\[ |F_b(\lambda) - F_\infty(\lambda)| = O \left( |V_1(b)| + \int_b^\infty dW_2 + \int_b^\infty dU_2 \right), \quad b \to \infty \quad (3.23) \]

uniformly for \( x \in [0, \pi) \).

**Proof.** For (i) we observe that Lemma 3.1(i) gives
\[
(y^2(x_2, \lambda) + \lambda y^2(x_2, \lambda)) - (y^2(x_1, \lambda) + \lambda y^2(x_1, \lambda)) = \int_{x_1}^{x_2} 2qy'y \, dt. \quad (3.24)
\]

Adding \(-V_2(x_2)y^2(x_2, \lambda) + V_2(x_1)y^2(x_1, \lambda)\) to both sides gives
\[
\phi(x_2, \lambda) - \phi(x_1, \lambda) = \int_{x_1}^{x_2} 2qyy' \, dt - \int_{x_1}^{x_2} d(V_2 y^2) = \int_{x_1}^{x_2} 2V_1 yy' \, dt - \int_{x_1}^{x_2} y^2 \, dV_2.
\]

For (ii) put \( x_1 = a \) and \( x_2 = b \) in (3.16) and pass \( b \to \infty \) in (3.17).

For (iii) observe that
\[
0 \leq \left( |y'| - \sqrt{\lambda - V_2} |y| \right)^2 \leq \phi(x, \lambda) - 2 \sqrt{\lambda - V_2} |yy'|
\]
and therefore
\[
2|y'y| \leq \frac{\phi(x, \lambda)}{\sqrt{c}} \quad (3.26)
\]
for all \( x \in [a, \infty) \). We also have for all \( x \in [a, \infty) \)
\[
y^2 \leq \frac{\phi(x, \lambda)}{c} \quad \text{and} \quad y'^2 \leq \phi(x, \lambda).
\]

Using (3.26) and (3.27) in (3.16) and putting \( x_1 = a \) we have
\[
\phi(x, \lambda) \leq \phi(a, \lambda) + \int_a^x \left| V_1 \right| \frac{\phi(t, \lambda)}{\sqrt{c}} \, dt - \int_a^x y^2 \, dU_2 + \int_a^x y^2 \, dW_2
\leq \phi(a, \lambda) + \int_a^x \left| V_1 \right| \frac{\phi(t, \lambda)}{\sqrt{c}} \, dt + \int_a^x \frac{\phi(t, \lambda)}{c} \, dW_2.
\]

The bound (3.19) now follows from an extension of Gronwall’s inequality.

For (iv) we observe that the quantities \( 2 \sqrt{c} |yy'|, cy^2, \) and \( y'^2 \) are all bounded by \( \phi(x, \lambda) \), which is bounded on \([a, \infty)\) by
\[
\phi(a, \lambda) \exp \left( \frac{W_2(\infty)}{c} + \frac{1}{\sqrt{c}} \int_a^\infty \left| V_1(t) \right| \, dt \right). \quad (3.28)
\]

For (v) we have from (3.16) that
\[
|\phi(b, \lambda) - \phi(\infty, \lambda)| = \left| \int_b^\infty V_1 2yy' \, dt - \int_b^\infty dU_2 + \int_b^\infty dW_2 \right|. \quad (3.29)
\]
Putting bound (3.26) in the integrand and applying the bound in (3.28) gives the result. Here \( \phi(a, \lambda) \) can be bounded independently of \( \alpha \). The same bound for \(|F_b(\lambda) - F_\infty(\lambda)|\) follows readily from (3.17). For (vi) we may integrate by parts in the first term on the right of (3.29), obtaining

\[
\int_b^\infty V_1 y' \, dt = V_1(b) y^2(b, \lambda) - \int_b^\infty V'_1 y^2 \, dt.
\]  

Under the assumptions, both terms on the right are \( O(|V_1(b)|) \) since \( y^2 \) is bounded by (3.28) independently of \( \alpha \). □

4. Averaging of spectral measures

In this section we list some general results on averaging of spectral measures and state a necessary and sufficient condition for a function \( f(\alpha) \) to be a spectral density function for the spectral measure associated with the singular problem (1.1). Consider first the regular Sturm–Liouville problem over \([a, x]\) for \( x > a \),

\[
\begin{cases}
-U'' + q(t)U = \lambda U, & t \in [a, x], \\
U(a) \cos \alpha + U'(a) \sin \alpha = 0, & \alpha \in [0, \pi), \\
U(x) = 0.
\end{cases}
\]

(4.1)

From standard Weyl–Titchmarsh theory we have that for \( \lambda \in \mathbb{C} \)

\[
m_x(\lambda) := -\frac{u(x, \lambda)}{y(x, \lambda)},
\]

(4.2)

where \( y(\cdot, \lambda) \) and \( u(\cdot, \lambda) \) are the solutions defined by (1.2) is a Herglotz (or Pick–Nevanlinna) function for all \( x \in (a, \infty) \) which has poles on the eigenvalues \( \{\lambda_{nx}\}_{n=0}^\infty \) of problem (4.1), and that the corresponding spectral measure, \( \mu_x \), for the regular problem on \([0, x]\) is defined by the right-continuous step spectral function

\[
\rho^x_\lambda := \sum_{\lambda_{nx} \leq \lambda} \frac{1}{\int_a^x |y(t, \lambda_{nx})|^2 \, dt}, \quad \lambda \in (-\infty, \infty).
\]

(4.3)

Here the spectral measure has point masses on the eigenvalues and is given by \( \mu_x^\lambda(\lambda_1, \lambda_2) = \rho^x_\lambda(\lambda_2) - \rho^x_\lambda(\lambda_1) \) for any real numbers \( \lambda_1 < \lambda_2 \). Under the assumption that \( q \) is in the limit point case at \( \infty \), the corresponding spectral function of the singular problem (1.1) over \([a, \infty)\) may be defined using the approach of Levitan [17] and Levinson [16] as

\[
\rho^\lambda := \lim_{x \to \infty} \rho^x_\lambda(\lambda)
\]

at points of continuity of \( \rho^\lambda \), and by making \( \rho^\lambda \) right continuous at points of discontinuity. The corresponding spectral measure of any interval \((\lambda_1, \lambda_2]\) for the singular problem (1.1) is then given in terms of the spectral function by \( \mu^\lambda((\lambda_1, \lambda_2]) = \rho^\lambda(\lambda_2) - \rho^\lambda(\lambda_1) \). It is also well known that the Weyl–Titchmarsh \( m \)-function for the singular problem (1.1),

\[
m(\lambda) := \lim_{x \to \infty} m_x(\lambda), \quad \text{for } \text{Im}(\lambda) \neq 0,
\]

(4.5)
gives rise to the same spectral function (4.4) by means of the Titchmarsh–Kodaira definition
\[
\rho^2(\lambda) := \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\lambda} \frac{\text{Im}(m^2(u + i\varepsilon))}{\pi} \, du.
\] (4.6)

In order to establish that the limit function \( f^2(\cdot) \) in (3.18) and (5.4) below, are spectral density functions for the measure \( \mu^2 \) associated with the spectral function \( \rho^2 \) defined by (4.4) we require the following lemmas. These results will be more fully developed and generalized in a forthcoming paper. First we state what is meant by \( f^2 \) being a spectral density function for the measure \( \mu^2 \):

**Definition.** We say that the spectral measure \( \mu^2 \) associated with the spectral function \( \rho^2 \) has the spectral density function \( f^2(\cdot) \) on an interval \((\lambda_1, \lambda_2)\) if and only if
\[
\mu^2(B) = \int_B f^2(\lambda) \, d\lambda
\] (4.7)
for all Borel subsets of \((\lambda_1, \lambda_2)\).

For the case of \( q \in L_1(a, \infty) \) the spectral function \( \rho^2 \) is known to be absolutely continuous in \((0, \infty)\), and
\[
f^2(\lambda) := \lim_{\varepsilon \to 0^+} \frac{\text{Im}(m^2(\lambda + i\varepsilon))}{\pi}
\] (4.8)
is the most classical example of a spectral density function for the associated spectral measure \( \mu^2 \) for any subinterval of \((0, \infty)\), and the spectral measure is absolutely continuous on any subinterval of \((0, \infty)\). The same is also true under the assumption (ii) of \( q = V_1 + V_2 \). In the following lemmas, we identify another way of taking limits so as to produce a spectral density function \( f^2(\cdot) \) for the spectral measure \( \mu^2 \) under the general assumption (iii). We shall also assume the potential satisfies the assumption (i) [Lemma 3.1 assumptions] or assumption (ii) [Lemma 3.2 assumptions]. These additional restrictions are sufficient to rule out discrete eigenvalues in the range of continuous spectrum \([A, \infty)\); for the case of the assumption (ii) well known large-x asymptotics of the solutions, for example, make it impossible for \( L^2 \) solutions to exist for \( \lambda \in (0, \infty) \) [19, Lemma 2.18, p. 114]. Accordingly, the statements in (i) and (iii) of Lemma 3.1 below will be true for unrestricted values of the \( \lambda \) variable. Generally, the goal is to be able to represent the spectral function over the range \((-\infty, \infty)\) in the form
\[
\rho^2(\lambda) = \begin{cases} 
\sum_{\lambda_n \leq \lambda} \int_a^\infty \frac{1}{|y(t, \lambda_n)|^2} \, dt & \text{for } \lambda \leq A, \\
\rho^2(A) + \int_A^\lambda f^2(\mu) \, d\mu & \text{for } \lambda > A,
\end{cases}
\] (4.9)
where \( \lambda_n \) are discrete eigenvalues of the singular problem on \([a, \infty)\), and where \( f^2(\cdot) \) is a spectral density function over the continuous range of spectrum \((A, \infty)\).

**Lemma 4.1.** (i) Let \( \overline{\rho}_b^2(\lambda) \) be defined on \((-\infty, \infty)\) by
\[
\overline{\rho}_b^2(\lambda) = \frac{1}{b-a} \int_a^b \int_{-\infty}^{\lambda} \frac{d\rho^2_x(\lambda')}{dx} \, dx.
\] (4.10)
Then
\[
\lim_{b \to \infty} \overline{\mu}_b^z(\lambda_2) - \overline{\mu}_b^z(\lambda_1) = \lim_{b \to \infty} \frac{1}{b-a} \int_a^b \int_{\lambda_1}^{\lambda_2} 1 \, d\rho_x^z(\lambda') \, dx = \lim_{b \to \infty} \frac{1}{b-a} \int_a^b \mu_x^z((\lambda_1, \lambda_2]) \, dx = \rho^z(\lambda_2) - \rho^z(\lambda_1),
\]
(4.11)
where \( \mu_x^z((\lambda_1, \lambda_2]) \) is the measure associated with the right-continuous step spectral function \( \rho_x^z \) defined by (4.3), and the limit function is the right-continuous function \( \rho^z \) defined by (4.4).

(ii) For \( \lambda \in [A, \infty) \) and \( b \in (a, \infty) \) define
\[
\int_{b-a}^b \left[ \sum_{a < z_j \leq b} (u^z(z_j, \lambda))^2 \right] \, dx,
\]
where \( a < z_1 < \cdots < z_M \leq b \) are the zeros of \( y^z \) in \( (a, b) \). Then
\[
\overline{\mu}_b^z(\lambda_2) - \overline{\mu}_b^z(\lambda_1) = \int_{\lambda_1}^{\lambda_2} f_b^z(\lambda') \, d\lambda',
\]
(4.13)
which means that \( f_b^z \) can be viewed as a spectral density function for the averaged measure, \( \mu_x^z \), associated with the right-continuous averaged spectral function \( \overline{\mu}_b^z(\lambda) \) defined by (4.10). It is easy to see that \( f_b^z \) is itself piecewise continuous in \( (0, \infty) \) except for jump discontinuities at the points \( \lambda_j \) for which \( z_j(\lambda_j) = f(b) \) (or \( y(b, \lambda_j) = 0) \).

(iii) For all real \( \lambda_2 > \lambda_1 > A \) we have
\[
\rho^z(\lambda_2) - \rho^z(\lambda_1) = \lim_{b \to \infty} \int_{\lambda_1}^{\lambda_2} f_b^z(\lambda') \, d\lambda'.
\]
(4.14)

Proof. We give a rough argument for part (i). Part (iii) follows readily from (i) and (ii). For part (ii) the idea of the proof can be found in [20]. For the interval \( (\lambda_1, \lambda_2) \) statement (4.11) is equivalent to
\[
\lim_{b \to \infty} \overline{\mu}_b^z((\lambda_1, \lambda_2]) = \lim_{b \to \infty} \frac{1}{b-a} \int_a^b \mu_x^z((\lambda_1, \lambda_2]) \, dx = \mu_x^z((\lambda_1, \lambda_2]).
\]
(4.15)
Since \( m_x^z(\lambda) \) converges uniformly to \( m^z(\lambda) \) on compact \( \lambda \)-sets in the upper half \( \lambda \)-plane, it follows for intervals \( (\lambda_1, \lambda_2) \) that the corresponding measure \( \mu_x^z((\lambda_1, \lambda_2]) \to \mu^z((\lambda_1, \lambda_2]) \) as \( x \to \infty \), provided that the endpoints \( \lambda_1 \) and \( \lambda_2 \) are not discrete points of \( \mu^z \). Hence we also have the convergence in (4.15).

Lemma 4.2. For fixed \( b \in (a, \infty) \) and \( \lambda \in (A, \infty) \) we have
\[
\int_0^\pi f_b^z(\lambda) \, d\lambda = 1.
\]
(4.16)

Proof. Let \( \lambda \in (A, \infty) \) be fixed. Let \( z_j(\lambda) = z_j(x, \lambda) \) be the \( j \)th zero of \( y^z \) in \( (a, b) \). First consider the case for which \( b = z_N(0, \lambda) \) for some fixed integer \( N \). Since for all \( x \in (0, \pi) \) the zeros of \( y^z(x, \lambda) \) and
\[ y^0(x, \lambda) \text{ interlace we have} \]
\[ a = z_0(0, \lambda) < z_1(x, \lambda) < z_1(0, \lambda) < \cdots < z_{j-1}(0, \lambda) < z_j(x, \lambda) < z_j(0, \lambda) < \cdots < z_N(0, \lambda) = b. \quad (4.17) \]

Moreover, \( z_j(x, \lambda) \) varies continuously from \( z_j(0, \lambda) \) to \( z_j(0, \lambda) \) as \( x \) varies from 0 to \( \pi \). The proof is accomplished by using this fact to integrate the \( z \)-derivative of \( z_j(x, \lambda) \) over \( [0, \pi] \), giving
\[
\frac{1}{b-a} \sum_{j=1}^{N} \int_{0}^{\pi} \frac{dz_j}{dx}(x, \lambda) \, dx = \frac{1}{b-a} \sum_{j=1}^{N} \int_{z_{j-1}(0,\lambda)}^{z_j(0,\lambda)} 1 \, dz_j(x, \lambda) \]
\[ = \frac{1}{b-a} \sum_{j=1}^{N} (z_j(0, \lambda) - z_{j-1}(0, \lambda)) \]
\[ = \frac{b-a}{b-a} = 1. \quad (4.20) \]

This completes the proof since
\[
\frac{dz_j}{dx}(x, \lambda) = (u^z(z_j(x, \lambda), \lambda))^2. \quad (4.21) \]

To establish (4.21) we observe that from (1.2) we have the relations of linear dependence
\[
y^0(x, \lambda) = y^0(x, \lambda) \cos x - u^0(x, \lambda) \sin x,
\]
\[
u^z(x, \lambda) = u^0(a, \lambda) \cos x + y^0(x, \lambda) \sin x
\]
from which we obtain
\[
\cot x = \frac{u^0(z_j(x, \lambda), \lambda)}{y^0(z_j(x, \lambda), \lambda)} \quad (4.22)
\]
and on differentiation with respect to \( x \)
\[
\frac{dz_j}{dx}(x, \lambda) = \left( \frac{y^0(z_j(x, \lambda), \lambda)}{\sin x} \right)^2. \quad (4.23)
\]

On the other hand, substituting \( u^0(z_j(x, \lambda), \lambda) \) from (4.22) into the above formula for \( u^z \) gives
\[
(u^z(z_j(x, \lambda), \lambda))^2 = \left( \frac{y^0(z_j(x, \lambda), \lambda)}{\sin x} \right)^2,
\]
so (4.21) follows.

Next, to handle an arbitrary choice of \( b \), select \( N \) so that \( z_{j-1}(0, \lambda) < b < z_N(0, \lambda) \), and \( z_b \in (0, \pi) \) so that \( z_N(z_b, \lambda) = b \), and revise the above argument performing the integrations (4.18) over \( z_{j-1}(z_b, \lambda) \) to \( z_j(z_b, \lambda) \). \( \square \)

**Lemma 4.3.** Let \( (\lambda_1, \lambda_2) \subset [A, \infty) \) and suppose that
\[
f^z(\lambda) := \lim_{b \to \infty} f^z_b(\lambda) \quad (4.25)
\]
Theorem 5.1. Assume \( q \in L_1(a, \infty) \). Then \( \Lambda = 0 \). We have for all \( \lambda \in (0, \infty) \)

\[
    f^\lambda(\lambda) := \frac{1}{\pi[\Phi(a, \lambda) + (2/\sqrt{\lambda}) \int_a^\infty qyy' \, dt]}
    = \lim_{b \to \infty} f^\lambda_b(\lambda)
\]

uniformly for \( \alpha \in [0, \pi] \).

(ii) Assume \( q = V_1 + V_2 \), where \( V_1 \in L_1(a, \infty) \) and \( V_2 \) is a continuous function of bounded variation on \([a, \infty)\), with \( \lim_{x \to \infty} V_2(x) = 0 \). Then \( \Lambda = 0 \). We have for all \( \lambda \in (0, \infty) \)

\[
    f^\lambda(\lambda) := \frac{\sqrt{\lambda}}{\pi[\Phi(a, \lambda) + 2 \int_a^\infty V_1(t)yy' \, dt - \int_a^\infty (y(t, \lambda))^2 \, dV_2]}
    = \lim_{b \to \infty} f^\lambda_b(\lambda)
\]

uniformly for \( \alpha \in [0, \pi] \).
Corollary 5.1. The functions \( f^z(\cdot) \) defined in Theorem 5.1 are spectral density functions for the measure \( \mu^z \) over any interval \( (\lambda_1, \lambda_2) \subset [A, \infty) \).

Proof. To see that the required normalization condition (4.26) of Lemma 4.3 holds, we observe from Lemma 4.2 that
\[
\int_0^\pi f^z(\lambda) \, d\lambda = \lim_{b \to \infty} \int_0^\pi f^z_b(\lambda) \, d\lambda = 1. \tag{5.5}
\]
The result now follows from Lemma 4.2. \( \square \)

For the proof of Theorem 5.1 we require the following

Lemma 5.1. For each \( z \in [0, \pi) \) and \( \lambda > A \) let \( N^z_b(\lambda) \) be the number of zeros of \( y^z(x, \lambda) \) in the interval, \( a < x \leq b \). We have the following asymptotic limit as \( b \to \infty \).

(i) If \( q \in L_1(a, \infty) \), then for all \( \lambda > 0 \),
\[
\lim_{b \to \infty} \frac{N^z_b(\lambda)}{b - a} = \frac{\sqrt{\lambda}}{\pi}. \tag{5.6}
\]

(ii) If \( q = V_1 + V_2 \), where \( V_1 \in L_1(a, \infty) \) and \( V_2 \) is a continuous function of bounded variation on \( [a, \infty) \), with \( \lim_{x \to \infty} V_2(x) = 0 \), then (5.6) holds.

The use of Prüfer and modified Prüfer transformations to count the number of zeros of a solution, or the number of eigenvalues of a regular Sturm–Liouville problem less than \( \lambda \), is a well-established tool in the theory of one-dimensional Sturm–Liouville equations (for example [31] Chapter [7] or [1]). Here we make use of a modified Prüfer transformation which is adapted to the case when \( \lambda \) is in the continuous spectrum.

Proof. Let \( N^z_b(\lambda) \) be the number of zeros of \( y^z(\cdot, \lambda) \) in \( (0, b] \). We consider first the case \( z = 0 \). Between two consecutive zeros of \( y^0(\cdot, \lambda) \), \( \tan \theta := y'(x, \lambda) / \sqrt{\lambda} y(x, \lambda) \) varies in \( (-\infty, \infty) \), and therefore
\[
\theta(x, \lambda) := \arctan \left( \frac{y'(x, \lambda)}{\sqrt{\lambda} y(x, \lambda)} \right) \tag{5.7}
\]
decreases by \( \pi \).

Since \( a = z_0 < z_1 < \cdots < z_N < b < z_{N+1} \) are the zeros of \( y^0(\cdot, \lambda) \), it follows that \( N = N^0_b(\lambda) \) satisfies
\[
\int_a^b \theta'(x, \lambda) \, dx = \sum_{j=0}^{N-1} \int_{z_j}^{z_{j+1}} \theta'(x, \lambda) \, dx + \int_{z_N}^b \theta'(x, \lambda) \, dx
\]
\[
= - N \pi + \int_{z_N}^b \theta'(x, \lambda) \, dx
\]
\[
= \int_a^b \left[ -\sqrt{\lambda} + \frac{\sqrt{\lambda} q y^2}{(y')^2 + \lambda y^2} \right] \, dx. \tag{5.8}
\]
For part (i), when \( q \in L_1(a, \infty) \), this yields
\[
N^0_b(\lambda) = \sqrt{\dot{\lambda}}(b-a) \pi + O(1) + O \left( \int_a^\infty |q| \, dx \right)
\]
as \( b \to \infty \), or
\[
\frac{N^0_b(\lambda)}{b-a} - \sqrt{\dot{\lambda}} = O \left( \frac{1}{b-a} \right),
\]
(5.9)
as \( b \to \infty \), so (5.6) follows. Since the zeros of \( y^2 \) and \( y^0 \) interlace for \( \lambda \neq 0 \), \( N^2_b (\lambda) \) is either \( N^0_b (\lambda) \) or \( N^0_b (\lambda) + 1 \), so we have for all \( \lambda \in [0, \pi] \) that
\[
\frac{N^2_b (\lambda)}{b-a} - \sqrt{\dot{\lambda}} = O \left( \frac{1}{b-a} \right),
\]
(5.10)
and the limit in (5.6) is uniform over \( \lambda \in [0, \pi] \).

For part (ii) we observe that, after an integration by parts in the integral involving \( V_2 \),
\[
\left| \int_a^b \frac{q y^2}{(y')^2 + \dot{\lambda} y^2} \, dt \right| = \left| \int_a^b \frac{V_1 y^2}{(y')^2 + \dot{\lambda} y^2} \, dt + V_2(b) \int_a^b \frac{y^2}{(y')^2 + \dot{\lambda} y^2} \, dt - \int_a^b \psi(t) \, dV_2(t) \right|
\leq \frac{1}{\dot{\lambda}} \left( \int_a^\infty |V_1(t)| \, dt \right) + \frac{V_2(b)(b-a)}{\dot{\lambda}} + \frac{1}{\dot{\lambda}} \int_a^b (t-a) \, d(U_2(t) + W_2(t)),
\]
(5.11)
where
\[
\psi(t) := \int_a^t \frac{y^2(s)}{(y'(s))^2 + \dot{\lambda} y^2(s)} \, ds.
\]
Using (5.11) in (5.8) yields
\[
N^0_b(\lambda) = \frac{\sqrt{\dot{\lambda}}(b-a)}{\pi} + O(1) + O(|V_2(b)|(b-a)) + O \left( \int_a^b (t-a) \, d(U_2(t) + W_2(t)) \right)
\]
as \( b \to \infty \), or
\[
\frac{N^0_b(\lambda)}{b-a} - \sqrt{\dot{\lambda}} = O \left( \frac{1}{b-a} + V_2(b) + \frac{1}{b-a} \int_a^b (t-a) \, d(U_2(t) + W_2(t)) \right).
\]
(5.12)
Since \( N^0_b(\lambda) \) and \( N^0_b(\lambda) \) can differ only by one, it follows that (5.12) also holds for \( N^0_b(\lambda) \). Since the quantities in the O-symbol tend to zero as \( b \to \infty \), the convergence in (5.6) is uniform over \( \lambda \in [0, \pi] \). □

**Remark.** Formula 5.6 is the limit of the averaged number of zeros of the solution \( y^2(\cdot, \lambda) \) over the interval \([a, b]\) as the interval length tends to \( \infty \); this corresponds to the so-called “integrated density of states” (i.d.s.) for one-dimensional Sturm–Liouville problems. Many authors have developed formulas for the
asymptotic density of zeros under various assumptions, for example [2]. There is also a large body of
literature dealing with extensions and generalizations of i.d.s. to partial differential equations (see [29]).

Proof of Theorem 5.1(i). For simplicity we take \( a = 0 \). From (3.2) with \( x_1 = 0 \) and \( x_2 = z_j \) where \( z_j = z_j(\lambda) \) is the \( j \)th zero of \( y(x, \lambda) \) in \((a, b]\) we have

\[
(y'(z_j, \lambda))^2 = \sqrt{\lambda} \Phi(z_j, \lambda) = \frac{\sqrt{\lambda}}{\pi \cdot F_{z_j}(\lambda)}.
\]

(5.13)

Hence

\[
f_b^2(\lambda) = \frac{1}{b} \sum_{0 < z_j < b} \frac{1}{(y'(z_j, \lambda))^2}
\]

\[
= \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j < b} F_{z_j}(\lambda)
\]

\[
= \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j < b} f^2(\lambda)
\]

\[
+ \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j < b} (F_{z_j}(\lambda) - f^2(\lambda))
\]

\[
= \frac{N^2_b(\lambda) \pi}{b \sqrt{\lambda}} f^2(\lambda)
\]

\[
+ \frac{N^2_b(\lambda) \pi}{b \sqrt{\lambda}} \mathcal{O} \left( \int_0^\infty |q| \, dt \right)
\]

\[
+ \frac{\pi}{b \sqrt{\lambda}} (N^2_b(\lambda) - N^2_{\lambda b}(\lambda)) \mathcal{O} \left( \int_0^\infty |q| \, dt \right)
\]

(5.14)

uniformly for \( \lambda \in [0, \pi) \), where we have made use of the estimates (3.6) which are also uniform in \( \lambda \). To see that the constant in the \( \mathcal{O} \)-symbol for the second term is independent of \( z_j \), put the bound (3.13) into (3.14) to get

\[
|\Phi(z_j, \lambda) - \Phi(\infty, \lambda)| \leq \frac{\Phi(a, \lambda)}{\lambda} \left( \int_0^\infty |q| \, dt \right)^2
\]

(5.15)

and similarly for \( |F_{z_j}(\lambda) - F_{\infty}(\lambda)| \). Similarly, the constant in the \( \mathcal{O} \)-symbol for the third term is independent of \( z_j \). The first-term converges to \( f^2 \) by application of Lemma 5.1(i). Applying Lemma 5.1(i) to the second
and third terms we find they are, respectively, $O(1/ \sqrt{b})$ and $O(\int_0^\infty |q| \, dt)$, and so they tend to zero as $b \to \infty$. \hfill \Box

Note: Error bounds for $|f^x_b(\lambda) - f^x(\lambda)|$ from the above proof are $O(1/b) + O(1/ \sqrt{b}) + O(\int_0^\infty |q| \, dt)$ by making use of (5.10) for the first term. Using $b^\epsilon$ in place of $\sqrt{b}$, the corresponding bounds are $O(1/b) + O(1/b^{1-\epsilon}) + O(\int_0^\infty |q| \, dt)$. The observed rates of convergence in Table 4 in Section 8 below indicate roughly $O(1/b)$ convergence (FP0) of $f^x_b$ to $f^x$ for the examples tried.

Proof of Theorem 5.1(ii). For simplicity we take $a = 0$. From (3.16) and (3.17) with $x_1 = 0$ and $x_2 = z_j$ where $z_j = z_j(\lambda)$ is the $j$th zero of $y(x, \lambda)$ in $(a, b]$ we have

$$(y'(z_j, \lambda))^2 = \sqrt{\lambda} \phi(z_j, \lambda) = \frac{\sqrt{\lambda}}{\pi F_{z_j}(\lambda)}. \quad (5.16)$$

Hence

$$f^x_b(\lambda) = \frac{1}{b} \sum_{0 < z_j \leq b} \frac{1}{(y'(z_j, \lambda))^2}$$
$$= \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j \leq b} F_{z_j}(\lambda)$$
$$= \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j \leq b} f^x(\lambda) + \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j \leq b} (F_{z_j}(\lambda) - f^x(\lambda))$$
$$= \frac{N^x_b(\lambda) \pi}{b \sqrt{\lambda}} f^x(\lambda)$$
$$+ \frac{\pi}{b \sqrt{\lambda}} \sum_{0 < z_j \leq b} (F_{z_j}(\lambda) - f^x(\lambda))$$
$$+ \frac{\pi}{b \sqrt{\lambda}} \sum_{\sqrt{b} < z_j \leq b} (F_{z_j}(\lambda) - f^x(\lambda))$$
$$= \frac{N^x_b(\lambda) \pi}{b \sqrt{\lambda}} f^x(\lambda)$$
$$+ \frac{N^x_b(\lambda) \pi}{b \sqrt{\lambda}} \mathcal{O} \left( \int_0^\infty |V_1| \, dt + \int_0^\infty dW_2(t) + \int_0^\infty dU_2(t) \right)$$
$$+ \frac{\pi}{b \sqrt{\lambda}} (N^x_b(\lambda) - N^x_{\sqrt{b}}(\lambda)) \mathcal{O} \left( \int_0^\infty |V_1| \, dt + \int_{\sqrt{b}}^\infty dW_2(t) + \int_{\sqrt{b}}^\infty dU_2 \right) \quad (5.17)$$

uniformly for $x \in [0, \pi)$, where we have made use of estimates (3.21) which are also uniform in $x$. The first term converges to $f^x$ by application of Lemma 5.1(ii). Applying Lemma 5.1(ii) to the second and third terms we find they are, respectively, $O(1/ \sqrt{b})$ and $O(\int_0^\infty |V_1| \, dt + \int_{\sqrt{b}}^\infty dW_2 + \int_{\sqrt{b}}^\infty dU_2)$, and so they tend to zero as $b \to \infty$. \hfill \Box
In this paper, we implement the computation of \( f_b^\varphi(\lambda) \) and \( F_b^\varphi(\lambda) \) for large \( b \) in order to estimate \( f^\varphi(\lambda) \) by (5.2), (5.4) and (3.4), (3.18), respectively. We compare convergence rates on several test problems. In addition, we use a numerical quadrature to compute

\[
\rho^\varphi(\lambda) = \int_0^\lambda f^\varphi(\mu) \, d\mu
\]  

(5.18)

over a range of \( \lambda \) points. We compare the efficiency and accuracy of these methods with the Levitan–Levinson method implemented in SLEDGE [25] for the \( \rho(\lambda) \) computation. We note that Lemma 3.2 and Theorem 5.1(ii) apply to long range potentials such as

\[
q(x) = \frac{c}{x^2}, \quad 0 < x \leq 1,
\]

(5.19)

which are not \( L_1(a, \infty) \).

6. Algorithm details

As in SLEDGE we introduce an approximating differential equation to (1.1) with piecewise constant coefficients. If \( \hat{y} \) denotes the solution of the approximating Sturm–Liouville equation defined by the same initial conditions (1.2), then for \( b \) finite, define \( \hat{f}_b \), \( \hat{F}_b \), and \( \hat{\rho}_b \) in analogy to (5.1), (3.3), (3.17), and (5.18) i.e.,

\[
\hat{f}_b(\mu) = \left[ \sum_{a < \hat{z}_j \leq b} \frac{1}{[\hat{y}'(\hat{z}_j, \mu)]^2 + \gamma} \right],
\]  

(6.1)

\[
\hat{F}_b(\mu) = \frac{\sqrt{\mu}}{\pi[\mu(\hat{y}(b, \mu))^2 + (\hat{y}'(b, \mu))^2]}
\]

(6.2)

or

\[
\hat{F}_b(\mu) = \frac{\sqrt{\mu}}{\pi[(\mu - V_2(b))(\hat{y}(b, \mu))^2 + (\hat{y}'(b, \mu))^2]}
\]

(6.3)

and

\[
\hat{\rho}_b(\lambda) = \int_A^\lambda \hat{f}_b(\mu) \, d\mu
\]

(6.4)

or

\[
\hat{\rho}_b(\lambda) = \int_A^\lambda \hat{F}_b(\mu) \, d\mu.
\]

(6.5)

The chief advantage of introducing the approximating problem is that most of the intermediate calculations can be done in closed form.

With any of these formulas, for a given \( b \), we choose a mesh

\[
\{a = x_1 < x_2 < \cdots < x_{N+1} = b\}
\]
for some positive integer $N$. The initial value problem (1.1)–(1.2) for $y(\cdot, \lambda)$ will be associated with the approximating initial value problem

$$-\hat{y}'' + \hat{q}(x)\hat{y} = \lambda\hat{y},$$
(6.6)

$$\begin{bmatrix} \hat{y}(a, \lambda) \\ \hat{y}'(a, \lambda) \end{bmatrix} = \begin{bmatrix} -\sin \alpha \\ \cos \alpha \end{bmatrix},$$
(6.7)

for all $\alpha \in (-\infty, \infty)$, where the function $\hat{q}$ is a step function approximation to $q$, corresponding to the given mesh. The standard choice [21,24,25] is to use midpoint approximation; i.e., with $q_n := q((x_n + x_{n+1})/2)$ let $\hat{q}(x) = q_n$ on $(x_n, x_{n+1})$, for $n = 1, 2, \ldots, N$. Henceforth we let $\hat{y}(\cdot, \lambda)$ denote the unique solution in $C^1[a, \infty)$ of (6.6) defined by these initial conditions. Define

$$\tau_n = \lambda_n - q_n,$$
$$\omega_n = \sqrt{|\tau_n|}$$

and

$$\Phi_n(t) = \begin{cases} \frac{\sin \omega_n t}{\omega_n}, & \tau_n > 0, \\ \frac{\sinh \omega_n t}{\omega_n}, & \tau_n < 0. \end{cases}$$
(6.8)

Then

$$\Phi_n'(t) = \begin{cases} \cos \omega_n t, & \tau_n > 0, \\ \cosh \omega_n t, & \tau_n < 0, \end{cases}$$
(6.9)

and the unique solution $\hat{y}(\cdot, \lambda)$ of the initial value problem (6.6)–(6.7), with $\hat{y}$ and $\hat{y}'$ in $C[a, b]$, can be written as

$$\hat{y}(x) = \hat{y}_n \Phi_n'(x - x_n) + \hat{y}'_n \Phi_n(x - x_n),$$
(6.10)

where $\hat{y}_n := \hat{y}(x_n)$, $\hat{y}'_n := \hat{y}'(x_n)$. Moreover,

$$\hat{y}'(x) = -\tau_n \hat{y}_n \Phi_n(x - x_n) + \hat{y}'_n \Phi_n'(x - x_n).$$
(6.11)

When $\tau_n > 0$, the function $\hat{y}$ can be written in phase-amplitude form, for $x$ in $(x_n, x_{n+1})$, as

$$\hat{y}(x) = A_n \sin[\omega_n (x - x_n) + \delta_n], \quad \tau_n > 0,$$

where

$$A_n = \sqrt{\hat{y}_n^2 + (\hat{y}'_n/\omega_n)^2}$$

and

$$\delta_n = \arctan \left( \frac{\omega_n \hat{y}_n}{\hat{y}'_n} \right).$$
(6.12)

Now $\hat{y}$ vanishes at some $\hat{z}_{jn}$ if and only if $\hat{z}_{jn} = x_n + (j\pi - \delta_n)/\omega_n$ for some integer $j$. Since we seek $\hat{z}_{jn}$ in $[x_n, x_{n+1}]$ this requires

$$0 < (j\pi - \delta_n)/\omega_n < h_n,$$
or that \( j \) is an integer in the interval \((\delta_n/\pi, (\delta_n + h_n\omega_n)/\pi)\). Let \( J_n \) be the smallest such integer and \( J_n \) the largest. Then, if zeros exist, there must be \( J_n = J_n - J_n + 1 \) of them. Consequently,

\[
(\hat{y}'(\hat{z}_n))^2 = (\omega_n A_n \cos(\omega_n (\hat{z}_n - x_n) + \delta_n))^2
= [\omega_n^2 \hat{y}_n^2 + \hat{y}_n^2] \cos^2[\omega_n (\hat{z}_n - x_n) + \delta_n]
= [\omega_n^2 \hat{y}_n^2 + \hat{y}_n^2] \cos^2[j\pi]
= \tau_n \hat{y}_n^2 + (\hat{y}_n')^2.
\]

(6.13)

Here, a key observation is that this value of \( \hat{y}'(\hat{z}_n) \) does not depend on \( j \) or explicit knowledge of \( z_j \); for the calculation of \( f_b(\mu) \) only the number of zeros is needed and this is easy to compute. Consequently, the amount of effort expended is independent of the potentially large value \( J_n \), and is merely a function of the number of mesh subintervals \( N \), a much smaller quantity in practice.

For \( \tau_n < 0 \) the circular trig functions must be replaced by hyperbolic ones. It is easy to see that there can be at most one zero of \( \hat{y} \) in any given piece \((x_n, x_{n+1})\). If \( \hat{y}(x_n)\hat{y}(x_{n+1}) < 0 \) so the zero exists, then it occurs at

\[
\hat{z} = x_n - \frac{\text{arctanh}(\omega_n \hat{y}_n/\hat{y}_n')}{\omega_n}
= x_n - \frac{1}{2\omega_n} \ln \left( \frac{\hat{y}_n' + \omega_n \hat{y}_n}{\hat{y}_n' - \omega_n \hat{y}_n} \right),
\]

and since \( \hat{z} = -\delta_n/\omega_n \), where \( \delta_n \) is the hyperbolic analogue of (6.12), we have

\[
(\hat{y}'(\hat{z}))^2 = \hat{y}_n^2 - \omega_n^2 \hat{y}_n^2
= \hat{y}_n^2 + \tau_n \hat{y}_n^2
\]

the same as in (6.13).

From (6.1), when all \( \tau_n > 0 \), it follows that

\[
\hat{f}_b(\mu) = \left[ \sum_{n=1}^{N} \sum_{j=1}^{J_n} \frac{1}{\tau_n \hat{y}_n^2 + \hat{y}_n'^2} + \gamma \right].
\]

(6.15)

The dependence of \( \hat{f}_b(\mu) \) on \( \mu \) is explicit through \( \tau_n = \mu - q_n \), and is implicit through the initial value problem (6.6, 6.7) on \( \hat{y}_n', \hat{y}_n'' \), and hence \( J_n \).

The computation of the \( \hat{y}_n \) and \( \hat{y}_n' \) values is based on a forward sweep across the mesh; by enforcing continuity on \( \hat{y} \) and \( \hat{y}' \), from (6.10) and (6.11) we have

\[
\hat{y}_{n+1} = \Phi_n(h_n)\hat{y}_n + \Phi_n(h_n)\hat{y}_n',
\]

\[
\hat{y}'_{n+1} = -\tau_n \Phi_n(h_n)\hat{y}_n + \Phi_n'(h_n)\hat{y}_n',
\]

for \( n = 1, 2, \ldots, N \) where \( \hat{y}_1 := -\sin z \) and \( \hat{y}'_1 := \cos z \). It is not hard to show that the amplification matrix for this recursion has spectral radius one when \( \tau_n \) is positive, but is \( \exp(\omega_n h_n) \) when \( \tau_n \) is negative.
To avoid overflows and to help stabilize the recursion, we rescale the dependent variable whenever \( n < 0 \). The procedure is a variation on that used in SLEDGE [25]. For the \( n \)th interval define the scale factor
\[
\sigma_n = \begin{cases} 
\exp(h_n \omega_n), & \tau_n < 0, \\
1, & \tau_n > 0 
\end{cases}
\]
and set \( \Psi_n(t) = \Phi_n(t)/\sigma_n \). Introduce the new independent variables \( \hat{v}_n = \hat{y}_n/[(\sigma_1 \ldots \sigma_{n-1}] \) and \( \hat{v}'_n = \hat{y}'_n/[\sigma_1 \ldots \sigma_{n-1}] \).

The equivalent recursions in the new variables are
\[
\hat{v}_{n+1} = \Psi'_n(h_n)\hat{v}_n + \Psi_n(h_n)\hat{v}'_n
\]
and
\[
\hat{v}'_{n+1} = -\tau_n \Psi_n(h_n)\hat{v}_n + \Psi'_n(h_n)v'_n,
\]
where \( \hat{v}_1 := -\sin z, \hat{v}'_1 := \cos z \). By construction, the amplification matrix now has unit spectral radius for any \( \tau_n \).

The calculation of \( \hat{F}_b(\mu) \) is much simpler to describe: we choose a mesh and solve the approximating problem as above, but no zeros of \( \hat{y} \) need to be counted. We simply have
\[
\hat{F}_b(\mu) = \sqrt{\mu} \pi [\mu \hat{y}_{N+1}^2 + \hat{y}'_{N+1}^2],
\]
for (6.2).

### 7. Algorithm error analysis

Errors in the solutions to approximating differential equations have been studied before in various contexts, e.g., [21] or Pryce [28] for Sturm–Liouville eigenvalues and eigenfunctions, or [22] for two-point boundary value problems for which the theory is general enough to include initial value problems. It can be shown for any finite \( b > a \) that
\[
\|y - \hat{y}\| = O(h^2) \quad (7.1)
\]
and
\[
\|y' - \hat{y}'\| = O(h^2). \quad (7.2)
\]
These approximations require the assumption that \( q \in C^2[a, b] \).

Here, and in what follows, \( \| \cdot \| \) is the uniform norm on \([a, b]\). Eqs. (7.1) and (7.2) hold for any choice of the parameter \( \mu \).

We first analyze the error in \( \hat{f}_b \), and later examine \( \hat{F}_b \).

**Lemma 7.1.** For each \( \mu \), if \( z \) in \((a, b)\) is a zero of \( y(x, \mu) \) then when \( h \) is sufficiently small there exists a zero \( \hat{z} \) of \( \hat{y} \) such that
\[
z - \hat{z} = O(h^2)
\]
as \( h \to 0 \).
Proof. Since the zeros of \( y \) are known to be simple, \( y'(z) \neq 0 \). We will show via a contraction mapping argument that for \( h \) sufficiently small there exists a zero of \( \hat{y}(x, \mu) \) within \( O(h^2) \) of \( z \). Define the set

\[
S = \{ x | x - z | \leq 2 \| y - \hat{y} \| / |y'(z)| \}
\]

and the mapping \( T \) on \( S \) by

\[
T(x) = x - \frac{\hat{y}(x)}{y'(z)}.
\]

Now

\[
|T(x) - z| = \frac{|x - z - \frac{\hat{y}(x)}{y'(z)}|}{|y'(z)|} = \frac{|[\hat{y}(x) - y(x)] + [y(x)] - (x - z)y'(z)|}{|y'(z)|} \leq \frac{||y - \hat{y}|| + ||y(z) + (x - z)y'(z) + (x - z)^2y''(\zeta)/2 - (x - z)y'(z)||}{|y'(z)|} = \frac{||y - \hat{y}|| + 2||y - \hat{y}||^2\|y''\|/|y'(z)|^2}{|y'(z)|} \leq 2||y - \hat{y}||/|y'(z)|,
\]

for \( h \) sufficiently small because of (7.1). Thus, \( T \) is an into mapping for small \( h \). To show that it contracts, we examine \( T'(x) \):

\[
|T'(x)| = \left| 1 - \frac{\hat{y}'(x)}{y'(z)} \right| = \frac{|y'(z) - \hat{y}'(x)|}{|y'(z)|} \leq ||y'(z) - y'(x)|| + ||y'(x) - \hat{y}'(x)||/|y'(z)| \leq ||y''||(|z - x|^2/2 + ||y' - \hat{y}'||)/|y'(z)| \leq ||y''|| \cdot O(h^4) + O(h^2) = O(h^2).
\]

Hence, for sufficiently small \( h \), we have shown that \( T \) is a contraction from \( S \) into \( S \) and therefore has a unique fixed point, call it \( \hat{z} \), in \( S \). Simple algebra leads to \( \hat{y}(\hat{z}) = 0 \). That \( |z - \hat{z}| = O(h^2) \) follows from \( \hat{z} \in S \) and (7.1). \( \square \)

From the form of \( \hat{y} \) given in (6.10) and (6.11), the zeros of \( \hat{y} \) must be simple. As a consequence of the Lemma, for \( h \) sufficiently small, the number of zeros of \( \hat{y} \) in \([a, b]\) is the same as the number of zeros of \( y \) in this interval, so we can label them as

\[
\hat{z}_1 < \hat{z}_2 < \hat{z}_3 < \cdots.
\]
Corollary 7.1. For each \( j \), and \( h \) sufficiently small:
\[
y'(z_j) - \hat{y}'(\hat{z}_j) = O(h^2)
\]
as \( h \to 0 \).

Proof. The conclusion follows from
\[
|y'(z_j) - \hat{y}'(\hat{z}_j)| \leq |y'(z_j) - y'(\hat{z}_j)| + |y'(\hat{z}_j) - \hat{y}'(\hat{z}_j)|.
\]
\( \square \)

The first term is \( O(h^2) \) from the lemma and the Lipschitz continuity of \( y' \); the second is \( O(h^2) \) from (7.1).

Corollary 7.2. Let \( \mu_j \) and \( \hat{\mu}_j \) be the \( j \)th points of discontinuity of \( f_b \) and \( \hat{f}_b \), respectively. Recall that these points are defined implicitly by \( z_j(\mu_j) = b \) and \( \hat{z}_j(\hat{\mu}_j) = b \). For each \( j \), and \( h \) sufficiently small:
\[
\mu_j - \hat{\mu}_j = O(h^2),
\]
as \( h \to 0 \).

Proof. Let
\[
\theta = \arctan \left( \frac{\hat{y}(x, \mu)}{\hat{y}'(x, \mu)} \right),
\]
where \( \hat{y}(x, \mu) \) is the solution of (6.6) fixed by initial conditions at \( x = a \). It follows readily from the Prüfer equation and standard comparison theorems (see [6, p. 212]) that

1. \( \frac{\partial \theta}{\partial \mu}(\hat{z}_j(\mu), \mu) < 0 \),
2. \( \theta(\hat{z}_j(\mu), \mu) = j\pi \), and \( \theta'(\hat{z}_j(\mu), \mu) = 1 \).

Since \( \theta(\hat{z}_j(\mu), \mu) = 0 \) for all \( \mu \in (A, \infty) \), differentiation of this with respect to \( \mu \) gives that \( \hat{z}_j(\mu) \) is a monotone decreasing function of \( \mu \) with a continuous derivative given by
\[
\frac{d\hat{z}_j(\mu)}{d\mu} = -\frac{\partial \theta}{\partial \mu}(\hat{z}_j(\mu), \mu) < 0.
\]
Of course, the same statements also hold for \( z_j(\mu) \) and its derivative. The inverse function, \( \hat{z}_j^{-1} \), also has a continuous derivative on \( (a, \infty) \). Therefore, for some compact interval containing \( b \in (a, \infty) \) we can apply Lipschitz continuity of \( \hat{z}_j^{-1} \) to obtain
\[
|\mu_j - \hat{\mu}_j| = |\hat{z}_j^{-1}(\hat{z}_j(\mu_j)) - \hat{z}_j^{-1}(b)| \leq L|\hat{z}_j(\mu_j) - b|.
\]
The result now follows by application of the lemma. \( \square \)

Theorem 7.1. Assume \( q \in C^2[a, b] \) and assume \( \mu \) is a point of continuity of \( f_b \), then

(i) for \( h \) sufficiently small, \( \mu \) is a point of continuity of each \( \hat{f}_b \), and
(ii) \( f_b(\mu) - \hat{f}_b(\mu) = O(h^2) \) as \( h \to 0 \).
Proof. The first part follows from Corollary 7.2. Restricting to a small neighborhood of \( \mu \) in which both \( f_b \) and \( \hat{f}_b \) are continuous for all \( h \) sufficiently small, it then follows from Corollary 7.1 that

\[
\hat{f}_b(\mu) = \left[ \sum_j \frac{1}{[\hat{y}'(z_j, \mu)]^2} + \gamma \right]
= \left[ \sum_j \frac{1}{[y'(z_j, \mu)]^2} + \gamma \right] + O(h^2)
= f_b(\mu) + O(h^2).
\]

The analysis of the error in \( \hat{F}_b \), is more straightforward.  □

Theorem 7.2. If \( q \in C^2[a, b] \) then \( F_b(\mu) - \hat{F}_b(\mu) = O(h^2) \) as \( h \to 0 \), for both (6.2) and (6.3).

Proof. From the definitions of \( F_b \) and \( \hat{F}_b \), after minor algebra and using (7.1) and (7.2), it follows that

\[
F_b(\mu) - \hat{F}_b(\mu) = \frac{-\sqrt{\mu}(y - \hat{y})(y + \hat{y}) + (y' - \hat{y}')(y'' - \hat{y}'')}{\pi[y'(y(b))^2 + (y'(b))^2][\mu(\hat{y}(b))^2 + (\hat{y}'(b))^2]}
= \frac{-2\sqrt{\mu}}{\pi[y'(y(b))^2 + (y'(b))^2]}
[y(y - \hat{y}) + y'(y' - \hat{y}')] + O(h^4)
= O(h^2). \quad □
\]

There are two other theoretical results that are desirable for implementation purposes. We were able to use Richardson’s \( h^2 \)-extrapolation to great success in SLEDGE to estimate errors and accelerate convergence. This requires knowledge of the nature of the leading terms in the error. In particular, we need to know the behavior of \( H(t, \mu) \) in

\[
F_b(\mu) - \hat{F}_b(\mu) = \sum_j h_j^2 \int_{x_j}^{x_{j+1}} H(t, \mu) \, dt + O(h^4). \quad (7.3)
\]

A careful study of the proof of Theorem 7.2 will give us what we need. First we mention that similar analysis is difficult for \( f_b - \hat{f}_b \) due to the effects of the zeros. We have observed from numerical output that \( h^2 \)-extrapolation is valid for uniform subdivisions of nonuniform meshes, but the analysis is formidable. The case for \( \hat{F}_b \) is much more direct—we follow a development analogous to that found in [21,22]. Let \( v_1 \) and \( v_2 \) be the pair of fundamental solutions for the Sturm–Liouville equation (1.1) satisfying \( v_1(a) = 1 \), \( v_1'(a) = 0 \), \( v_2(a) = 0 \), and \( v_2'(a) = 1 \). Use of a variation of parameters argument (see [23]) leads to

\[
(y - \hat{y})(b) = \int_a^b (-v_1(b)v_2(t) + v_2(b)v_1(t))(q - \hat{q})\hat{y}(t) \, dt
\]
and
\[
(y' - \hat{y}') (b) = \int_a^b (-v_1' (b) v_2 (t) + v_2' (b) v_1 (t)) (q - \hat{q}) \hat{y} (t) \, dt.
\]
The second quantity can be expanded as
\[
y' (b) - \hat{y}' (b) = \sum_{j=1}^N h_j^2 \int_{x_j}^{x_{j+1}} \left[ \frac{1}{8} q' (t) \frac{\partial w}{\partial t} + \frac{1}{16} q'' (t) w (t) \right] \, dt + O (h^4),
\]
where \( w (b, t) = (v_2' (b) v_1 (t) - v_1' (b) v_2 (t)) \hat{y} (t) \). This is in the appropriate form for \( h^2 \)-extrapolation to be justified.

It is important for the efficiency of the implementation to use a mesh that is equidistributed with respect to an appropriate monitor function \([3, 15]\). We have tried several different schemes: overall, the best was to equidistribute \(|q'|\), which arises from the underlying approximation of \( q \) by \( \hat{q} \). This same quantity is part of the SLEDGE heuristic too. The details of the algorithm follow those in \([4, \text{Chapter XII}]\).

8. Numerical examples

In this section we discuss implementation issues and present several numerical examples. Heretofore we have focused on the calculation of \( f_b (t) \) for some sufficiently large \( b \); since \( \rho_b (t) \) is just a quadrature of \( f_b \) the final part seems clear enough (a standard numerical initial value code could be used as well). The integration interval in the definition for \( \rho (\lambda) \) is \((-\infty, \lambda)\) but the continuous spectrum lies only in \((\lambda, \infty)\). Any contribution to \( \rho (\lambda) \) below the cutoff arises from point spectrum and should be computed by another algorithm, for example SLEDGE. Hence, if we wish \( \rho \) approximations at \( \mu_i \) points in \((\lambda, \infty)\) we need to compute (numerically)
\[
\rho (\mu_i) = \rho (A) + \int_A^{\mu_i} f (\mu) \, d\mu.
\]
Of course, for efficiency one should use
\[
\rho (\mu_i) = \rho (\mu_{i-1}) + \int_{\mu_{i-1}}^{\mu_i} f (\mu) \, d\mu,
\]
for each \( i > 1 \). To smooth the typical square-root behavior of the integrand near \( \lambda \), we actually start with
\[
\rho (\mu_1) = \rho (A) + 2 \int_{\sqrt{\lambda}}^{\sqrt{\mu_1}} t f (t^2) \, dt.
\]
Computer codes were written for each of the two characterizations: the one corresponding to (5.1) is referred to as FPP0, while that from (3.3) or (3.17) is called FPP1. We have compared these with the SLEDGE code \([10, 25, 26]\). In the authors’ previous testing it was apparent that for spectral function approximation SLEDGE generally is more successful at modest tolerances, i.e., \(10^{-3} - 10^{-4}\). This is clear from the current output as well. For testing purposes we chose \( \{\mu_i\} = \{0.1, 0.2, 0.4, 1, 2, 4, \ldots, 10, 000\} \). All data were collected on a PC using IEEE arithmetic with an 800 MHz CPU, and a Lahey Fortran
Table 1
Timings and errors on Problem 1

<table>
<thead>
<tr>
<th>Tolerance</th>
<th>Method</th>
<th>$b - a$</th>
<th>$N_x$</th>
<th>Time (s)</th>
<th>Maximum error in $\hat{p}_b$</th>
<th>$\hat{p}'_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu = 0, \pi = 0$ DIRICHLET B.C. at $a = 1$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.(-4)</td>
<td>SLEDGE</td>
<td>171</td>
<td>27</td>
<td>1.21</td>
<td>2.2(-4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>5667</td>
<td>32</td>
<td>0.05</td>
<td>3.0(-5)</td>
<td>8.6(-5)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>36</td>
<td>9</td>
<td>0.01</td>
<td>4.5(-5)</td>
<td>9.2(-5)</td>
</tr>
<tr>
<td>1.(-6)</td>
<td>SLEDGE</td>
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<td>35</td>
<td>23.73</td>
<td>4.4(-6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>578800</td>
<td>156</td>
<td>1.23</td>
<td>6.8(-7)</td>
<td>7.6(-7)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>299</td>
<td>115</td>
<td>0.55</td>
<td>3.4(-7)</td>
<td>9.7(-7)</td>
</tr>
<tr>
<td>$\nu = 3, \pi = \pi/2$ NEUMANN B.C. at $a = 1$</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1.(-4)</td>
<td>SLEDGE</td>
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<td>27</td>
<td>5.71</td>
<td>1.2(-4)</td>
<td></td>
</tr>
<tr>
<td></td>
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<td>100</td>
<td>0.30</td>
<td>8.6(-5)</td>
<td>1.6(-5)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
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<td>37</td>
<td>0.08</td>
<td>8.9(-5)</td>
<td>4.2(-5)</td>
</tr>
<tr>
<td>1.(-6)</td>
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<td>35</td>
<td>507.29</td>
<td>1.5(-6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
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<td>409</td>
<td>12.64</td>
<td>9.6(-7)</td>
<td>1.9(-7)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>394</td>
<td>449</td>
<td>3.33</td>
<td>5.4(-7)</td>
<td>4.6(-7)</td>
</tr>
</tbody>
</table>

90 compiler. For the quadrature we used the code ADAPT taken from [30]. Times are measured in seconds and for the FPP codes are the average of five repetitions. The notation 1.2(-3) means 1.2 $\times$ 10^{-3}.

The first family of test Problems is Problem 1 from Section 2. Here the known solutions for $f^0$ and $f^{\pi/2}$ in (2.10) and (2.11) provide exact results; the exact $\rho$ can then be computed from these to high accuracy by a quadrature. In Table 1 are shown some results for Problem 1 using the three codes. Since exact answers are known for $f(\mu)$ the ‘error in $\hat{p}_b$’ column gives the maximum magnitude difference between $f(\mu)$ and the computed $\hat{f}_b(\mu)$ or $\hat{F}_b$ for the $b$ displayed. When the exact answer exceeds one in magnitude then the relative error was used. For the ‘error in the $\hat{p}_b$’ column we used a high-accuracy quadrature to generate ‘exact’ answers. The displayed ‘Tolerance’ is the tolerance asked of SLEDGE for its global error criterion. The value of $b - a$ displayed is the width of the domain for the final $b$ used by the code. The tabled $N_x$ is the number of points in the initial mesh, before any refinement. For the new codes the values of $b$ and $N_x$ were chosen by experimentation to achieve the same tolerance used for the corresponding SLEDGE run. The actual internal tolerances for extrapolation and for the adaptive quadrature were tighter than this. Work is in progress to automate the choice of $b$, $N_x$ and the internal tolerances, so that user-prescribed tolerance can be achieved. Sometimes SLEDGE halted with an error flag indicating that it was working too hard; this is indicated by a $>$ in the ‘Time’ column. The current implementation of SLEDGE does not return any $\rho'$ values, so the error column for this is left empty.

The potential $q(x)$, boundary condition constants, etc., for nine other problems from our test collection are found in Table 2. In all cases the cutoff $\Lambda = 0$. Table 3 contains numerical results for these test problems using the three codes. High-accuracy values from SLEDGE and/or FPP1 for very tight tolerances were used for the ‘exact’ values in error calculations for these nine problems.
Table 2
Other test problems

<table>
<thead>
<tr>
<th>Problem</th>
<th>( q(x) )</th>
<th>( a )</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( \rho(A) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>( 1/x )</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>( 1/x^{1.25} )</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>( 1/x^{1.5} )</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>( 1/x^{1.75} )</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>( 1/x^3 )</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>( 1/x^4 )</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>( 1/x^6 )</td>
<td>1</td>
<td>3</td>
<td>(-4)</td>
<td>0.0</td>
</tr>
<tr>
<td>9</td>
<td>(-160[\exp(-2x) + 1])</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>131.48962</td>
</tr>
<tr>
<td>10</td>
<td>(-\exp(-x)/x)</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0.30596625</td>
</tr>
</tbody>
</table>

Overall, what is striking is the low times required by the new codes, though one must remember that they have a much narrower scope and do not automatically choose \( b \) as does the software package SLEDGE. Even at the lower tolerances, FPP0 is nearly always faster than SLEDGE and often by ten to twenty times. FPP1 is another two to three times faster, and at tighter tolerances both of the new codes can be hundreds of times faster.

The \( b \) values needed by FPP0 are much larger than those used by SLEDGE; there is a simple explanation for this. As discussed in [26], SLEDGE uses an interpolation scheme to smooth its step function \( \hat{\rho}_b \) approximations to \( \rho \). The observed rate of convergence of these interpolants to \( \rho \) for problems in Liouville normal form is \( O(1/b^2) \). Contrast this with the FPP0 data where generally \( O(1/b) \) convergence is observed. This appears to be as good as can be expected from the bounds (5.10) and (5.12) in Lemma 5.1, since these bounds dominate the error in (5.14) and (5.17). For FPP1 Lemma 3.1(vi) implies the rate of convergence is \( O(|q(b)|) \) as \( b \to \infty \) for all test problems in \( L_1(a, \infty) \), and Lemma 3.2(vi) implies, for test Problem 2 \( (q = V_2 = +1/x) \), the rate of convergence is \( O(1/b) \) (also, see the discussion below and Table 4). This explains the much smaller \( b \) values needed to achieve a given tolerance, and consequent smaller computing times for those problems with rate of convergence faster than \( O(1/b) \).

Data on the convergence rates of \( f_b \) to \( f \) and \( F_b \) to \( f \) as \( b \to \infty \) are displayed in Table 4. The potentials of the example problems have varying decay rates as \( b \to \infty \). The Problem 1 here refers to the case of \( \nu = 0 \) and a Neumann boundary condition at \( x = a \). For this illustration the fixed value of \( \mu = 2 \) was used, although the rates of convergence will generally be independent of \( \mu \). Generally, internal tolerances of \( 10^{-12} \) were used to eliminate mesh effects, i.e., the errors shown are believed to be from \( f_b \) and \( F_b \), not \( \hat{F}_b \) and \( \hat{F}_b \). When necessary even tighter internal tolerances were used. Three different \( b \) values were chosen to examine the convergence rate; the initial width \( w_1 = b_1 - a \) is shown, as well as a constant \( c \). The second width is \( c \) times the first, the third is \( c \) times the second. The quantity labelled \( E_j \) is the computed error \( |f - f_b| \) (FPP0) or \( |f - F_b| \) (FPP1) for the \( j \)th width. The quantity in the last two columns, denoted by \( r_{ij} \), is an estimated rate of convergence in \( b \) of \( f - f_b \) (FPP0) or of \( f - F_b \) (FPP1) from the formula:

\[
\frac{\log[\text{error}(b_i)/\text{error}(b_j)]}{\log[b_j/b_i]}
\]
### Table 3
Timings and errors on Problems 2–10

<table>
<thead>
<tr>
<th>Tolerance</th>
<th>Method</th>
<th>$b - a$</th>
<th>$N_k$</th>
<th>Time (s)</th>
<th>Maximum error in $\hat{\rho}_b$</th>
<th>Maximum error in $\hat{\rho}_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A) Timings and errors on Problem 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. ($-4$)</td>
<td>SLEDGE</td>
<td>171</td>
<td>27</td>
<td>1.26</td>
<td>7.7 ($-5$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>10,800</td>
<td>98</td>
<td>1.25</td>
<td>5.6 ($-5$)</td>
<td>4.9 ($-5$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>6480</td>
<td>249</td>
<td>1.00</td>
<td>2.2 ($-5$)</td>
<td>5.7 ($-5$)</td>
</tr>
<tr>
<td>1. ($-6$)</td>
<td>SLEDGE</td>
<td>2003</td>
<td>45</td>
<td>151.65</td>
<td>1.5 ($-6$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>1,100,000</td>
<td>488</td>
<td>47.27</td>
<td>4.7 ($-7$)</td>
<td>2.6 ($-7$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>587,000</td>
<td>1039</td>
<td>22.52</td>
<td>9.1 ($-7$)</td>
<td>8.1 ($-7$)</td>
</tr>
<tr>
<td>(B) Timings and errors on Problem 3</td>
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<tr>
<td>1. ($-4$)</td>
<td>SLEDGE</td>
<td>171</td>
<td>27</td>
<td>1.48</td>
<td>7.3 ($-5$)</td>
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</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>4590</td>
<td>115</td>
<td>0.33</td>
<td>8.4 ($-5$)</td>
<td>9.8 ($-5$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>238</td>
<td>59</td>
<td>0.10</td>
<td>4.4 ($-5$)</td>
<td>6.6 ($-5$)</td>
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<tr>
<td>1. ($-6$)</td>
<td>SLEDGE</td>
<td>1001</td>
<td>35</td>
<td>138.85</td>
<td>4.0 ($-6$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>474,000</td>
<td>470</td>
<td>29.80</td>
<td>4.7 ($-7$)</td>
<td>9.1 ($-7$)</td>
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<td></td>
<td>FPP1</td>
<td>587,000</td>
<td>845</td>
<td>20.65</td>
<td>1.0 ($-6$)</td>
<td>9.7 ($-7$)</td>
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<td>(C) Timings and errors on Problem 4</td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>SLEDGE</td>
<td>171</td>
<td>27</td>
<td>1.21</td>
<td>1.2 ($-4$)</td>
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</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>4520</td>
<td>87</td>
<td>0.20</td>
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<td>9.4 ($-5$)</td>
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<td>FPP1</td>
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<td>53</td>
<td>0.08</td>
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<td>9.6 ($-5$)</td>
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<tr>
<td>1. ($-6$)</td>
<td>SLEDGE</td>
<td>1001</td>
<td>35</td>
<td>76.85</td>
<td>4.7 ($-6$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>474,000</td>
<td>396</td>
<td>14.70</td>
<td>5.6 ($-7$)</td>
<td>8.5 ($-7$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>1990</td>
<td>796</td>
<td>8.94</td>
<td>6.7 ($-7$)</td>
<td>5.7 ($-7$)</td>
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<td>(D) Timings and errors on Problem 5</td>
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</tr>
<tr>
<td>1. ($-4$)</td>
<td>SLEDGE</td>
<td>171</td>
<td>27</td>
<td>1.32</td>
<td>1.2 ($-4$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>4430</td>
<td>113</td>
<td>0.30</td>
<td>9.7 ($-5$)</td>
<td>8.9 ($-5$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>54</td>
<td>29</td>
<td>0.04</td>
<td>6.6 ($-5$)</td>
<td>1.0 ($-4$)</td>
</tr>
<tr>
<td>1. ($-6$)</td>
<td>SLEDGE</td>
<td>1001</td>
<td>35</td>
<td>70.14</td>
<td>5.3 ($-6$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>453,000</td>
<td>406</td>
<td>3.99</td>
<td>7.1 ($-7$)</td>
<td>7.0 ($-7$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>1093</td>
<td>291</td>
<td>1.85</td>
<td>4.6 ($-7$)</td>
<td>5.2 ($-7$)</td>
</tr>
<tr>
<td>(E) Timings and errors on Problem 6</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. ($-4$)</td>
<td>SLEDGE</td>
<td>172</td>
<td>27</td>
<td>1.32</td>
<td>5.9 ($-5$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FPP0</td>
<td>25700</td>
<td>24</td>
<td>0.04</td>
<td>4.1 ($-5$)</td>
<td>6.1 ($-5$)</td>
</tr>
<tr>
<td></td>
<td>FPP1</td>
<td>25</td>
<td>9</td>
<td>0.01</td>
<td>9.7 ($-5$)</td>
<td>8.2 ($-5$)</td>
</tr>
<tr>
<td>1. ($-6$)</td>
<td>SLEDGE</td>
<td>1002</td>
<td>35</td>
<td>139.95</td>
<td>1.8 ($-6$)</td>
<td></td>
</tr>
</tbody>
</table>
Table 3 (continued)

<table>
<thead>
<tr>
<th>Tolerance</th>
<th>Method</th>
<th>$b - a$</th>
<th>$N_x$</th>
<th>Time (s)</th>
<th>Maximum error in $\hat{\rho}_b$</th>
<th>$\hat{\rho}_b'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FPP0</td>
<td>2,540,000</td>
<td>235</td>
<td>1.71</td>
<td>6.2(-7)</td>
<td>5.4(-7)</td>
<td></td>
</tr>
<tr>
<td>FPP1</td>
<td>225</td>
<td>121</td>
<td>0.42</td>
<td>9.8(-7)</td>
<td>7.2(-7)</td>
<td></td>
</tr>
</tbody>
</table>

(F) timings and errors on Problem 7
1.(-4)
| SLEDGE | 171 | 27 | 1.32 | 6.6(-5) |
| FPP0   | 37700 | 25 | 0.04 | 9.0(-5) |
| FPP1   | 10   | 8  | 0.01 | 5.6(-5) |

1.(-6)
| SLEDGE | 2003 | 45 | 138.14 | 1.9(-6) |
| FPP0   | 3,970,000 | 213 | 2.65 | 2.3(-7) |
| FPP1   | 39   | 95 | 0.50 | 9.9(-7) |

(G) timings and errors on Problem 8
1.(-4)
| SLEDGE | 171 | 27 | 1.53 | 6.4(-5) |
| FPP0   | 27700 | 24 | 0.04 | 7.5(-5) |
| FPP1   | 5    | 5  | 0.01 | 6.1(-5) |

1.(-6)
| SLEDGE | 2003 | 45 | 136.21 | 1.6(-6) |
| FPP0   | 2,660,000 | 157 | 8.71 | 4.1(-7) |
| FPP1   | 9    | 20 | 0.50 | 1.0(-6) |

(H) timings and errors on Problem 9
1.(-4)
| SLEDGE | 170 | 27 | 8.90 | 3.2(-4) |
| FPP0   | 44,200 | 81 | 0.57 | 4.3(-5) |
| FPP1   | 8    | 24 | 0.09 | 1.4(-5) |

1.(-6)
| SLEDGE | 2000 | 45 | >411.28 | |
| FPP0   | 4,580,000 | 228 | 7.44 | 6.3(-8) |
| FPP1   | 10   | 36 | 0.26 | 1.2(-7) |

(I) timings and errors on Problem 10
1.(-4)
| SLEDGE | 171 | 27 | 60.52 | 8.7(-5) |
| FPP0   | 31,200 | 17 | 0.10 | 2.7(-5) |
| FPP1   | 7    | 4  | 0.01 | 9.7(-5) |

1.(-6)
| SLEDGE | 2003 | 45 | >869.42 | |
| FPP0   | 2,960,000 | 119 | 1.75 | 9.2(-7) |
| FPP1   | 11   | 39 | 0.10 | 9.7(-7) |

If $f - f_b$ is directly proportional to $1/b^E$, then this formula would produce $E$ exactly. The last column in Table 4 contains the smallest $E$ for which $q = O(1/b^E)$ as $b \to \infty$. An exception is the final row for which the decay is exponential. It is interesting to note the irregularity of the estimated rates for FPP0, though it is generally around 1.0; also, the large-$b$ behavior of the potential seems to have little affect on this rate. In contrast, the estimated rates of $F_b \to f$ for FPP1 are closer to the theoretical rates of $O(|1/b^E|)$ as $b \to \infty$. 


Theorem 5.1. They significantly reduce the computation time that SLEDGE requires for the same task. As to be determined and this is cheap to compute. In addition, for either \( \hat{E} \) are \( O(h^n) \) methods by Iserles, Norsett, Munthe-Kaas, and Owren et al. [12–14, 18] is certainly germane to our interpolation of Section 6 with Richardson’s extrapolation used for refinement. The recent work on Magnus methods from [13] to produce the fastest methods into SLEDGE.

Table 4

<table>
<thead>
<tr>
<th>Problem</th>
<th>( w_1 )</th>
<th>( c )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( E_3 )</th>
<th>( r_{12} )</th>
<th>( r_{23} )</th>
<th>( E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>FPP0</td>
<td>( f_b = O(1/b^{23}) )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>10,000</td>
<td>10</td>
<td>2.7412(−5)</td>
<td>3.4972(−6)</td>
<td>2.3700(−7)</td>
<td>0.89</td>
<td>1.17</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>8000</td>
<td>10</td>
<td>3.1254(−5)</td>
<td>3.1214(−6)</td>
<td>4.5118(−7)</td>
<td>1.00</td>
<td>0.84</td>
<td>1.25</td>
</tr>
<tr>
<td>4</td>
<td>6000</td>
<td>10</td>
<td>2.4702(−5)</td>
<td>3.7052(−6)</td>
<td>1.7037(−7)</td>
<td>0.82</td>
<td>1.33</td>
<td>1.5</td>
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<tr>
<td>5</td>
<td>6000</td>
<td>10</td>
<td>3.5349(−5)</td>
<td>2.7185(−6)</td>
<td>2.7918(−7)</td>
<td>1.11</td>
<td>0.99</td>
<td>1.75</td>
</tr>
<tr>
<td>6</td>
<td>4000</td>
<td>10</td>
<td>4.1472(−5)</td>
<td>4.1588(−6)</td>
<td>3.4034(−7)</td>
<td>1.00</td>
<td>1.09</td>
<td>2</td>
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<td>7</td>
<td>4000</td>
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<td>5.4980(−5)</td>
<td>4.2962(−6)</td>
<td>3.4054(−7)</td>
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<td>1.10</td>
<td>3</td>
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<td>8</td>
<td>4000</td>
<td>10</td>
<td>5.1244(−5)</td>
<td>4.3449(−6)</td>
<td>3.4837(−7)</td>
<td>1.07</td>
<td>1.09</td>
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</tr>
<tr>
<td>9</td>
<td>4000</td>
<td>10</td>
<td>6.3430(−5)</td>
<td>5.5286(−6)</td>
<td>4.4488(−7)</td>
<td>1.06</td>
<td>1.09</td>
<td>6</td>
</tr>
<tr>
<td>FPP1</td>
<td>( F_b = O(1/b^{23}) )</td>
<td></td>
<td></td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>400</td>
<td>10</td>
<td>1.7952(−4)</td>
<td>1.7929(−5)</td>
<td>1.7309(−6)</td>
<td>1.00</td>
<td>1.02</td>
<td>1</td>
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<tr>
<td>3</td>
<td>400</td>
<td>8</td>
<td>9.2032(−6)</td>
<td>2.6473(−6)</td>
<td>1.7334(−7)</td>
<td>0.60</td>
<td>1.31</td>
<td>1.25</td>
</tr>
<tr>
<td>4</td>
<td>300</td>
<td>6</td>
<td>9.7809(−6)</td>
<td>1.0520(−6)</td>
<td>8.0371(−8)</td>
<td>1.24</td>
<td>1.44</td>
<td>1.5</td>
</tr>
<tr>
<td>5</td>
<td>300</td>
<td>2</td>
<td>3.5961(−6)</td>
<td>1.2175(−6)</td>
<td>3.5398(−7)</td>
<td>1.56</td>
<td>1.78</td>
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<td>6</td>
<td>30</td>
<td>2</td>
<td>1.3739(−5)</td>
<td>3.5153(−6)</td>
<td>8.7678(−7)</td>
<td>1.97</td>
<td>2.00</td>
<td>2</td>
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9. Conclusions

The results obtained on the problems presented here clearly demonstrate the power of the algorithms based on the new characterizations of spectral density functions \( f^2 \) given in Lemmas 3.1 and 3.2, and Theorem 5.1. They significantly reduce the computation time that SLEDGE requires for the same task. As mentioned in Section 6, for \( \hat{f}_b \) this is due to the fact that only the number of zeros, not their location, needs to be determined and this is cheap to compute. In addition, for either \( \hat{f}_b \) or \( \hat{F}_b \), we need only one \( y(b, \mu) \) estimate at each output point \( \mu \), not the large number of eigenfunction norms that SLEDGE requires. We anticipate that further analysis and testing on these codes against SLEDGE will result in the decision to incorporate the fastest methods into SLEDGE.

A referee has suggested alternatives to the use of coefficient approximation, at least to the midpoint interpolation of Section 6 with Richardson’s extrapolation used for refinement. The recent work on Magnus methods by Iserles, Norsett, Munthe-Kaas, and Owren et al. [12–14, 18] is certainly germane to our differential equation (1.1). As is true for coefficient approximation, their methods, arising from a very general framework of Lie group methods or first-order systems of differential equations, have the advantage that the resulting approximate solution can incorporate high-oscillation and/or exponential decay. We have so far succeeded in implementing the MG4 method from [13] to produce \( \hat{F}_b \) approximations which are \( O(h^5) \). It remains to be seen whether this implementation is competitive with the current midpoint interpolation of \( q \) followed by \( O(h^2) \) extrapolation. We hope to report on this in the future, after further testing. Of course, in a final code the ability to effectively estimate global errors and to select a good
initial mesh will be at least as important as the choice of underlying approximations. We thank the referee for bringing the papers on the Magnus methods to our attention.

References