The Computation of Spectral Density Functions for Singular Sturm-Liouville Problems Involving Simple Continuous Spectra

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The software package SLEDGE has as one of its options the estimation of spectral density functions $\rho(t)$ for a wide class of singular Sturm-Liouville problems. In this article the underlying theory and implementation issues are discussed. Several examples exhibiting quite varied asymptotic behavior in ρ are presented.

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1. INTRODUCTION AND MATHEMATICAL THEORY

The software package SLEDGE [Fulton et al. 1999; Pruess and Fulton 1993; Pruess et al. 1991; 1995] is capable of computing eigenvalues,

eigenfunctions, and spectral density functions for regular Sturm-Liouville problems and for a wide class of singular ones; the Fortran code is currently available over NETLIB. In this article we describe the theory and implementation of that part of the SLEDGE package which computes spectral density functions for problems having continuous spectra, and analyze the performance of the code on selected problems. The test problems for this article come from the SLEDGE test set [Pruess et al. 1991] of over 200 problems. The choice of test problems was made to exhibit a wide variety of asymptotic behaviors for the spectral density function near infinity. To provide an independent check on the accuracy we have also restricted the test problems to those for which the spectral density function is known in closed form and therefore independently computable.

We consider the general Sturm-Liouville problem on (a, ∞), assuming that the left endpoint $x = a$ is either (1) regular, or (2) nonoscillatory for all real λ and a regular singular point. We also assume that $x = \infty$ falls in Weyl's limit point case, and generates some continuous spectrum. Under these assumptions the problems considered are

$$-(p(x)u')' + q(x)u = \lambda r(x)u, \ a < x < \infty \qquad (1.1)$$

with the boundary conditions:

(1) When $x = a$ is a regular endpoint,

$$a_1 u(a) - a_2(pu')(a) = \lambda(a_1'u(a) - a_2'(pu')(a)), \qquad (1.2)$$

with either $a_1' = a_2' = 0$, and a_1, a_2 not both zero, or $\alpha = a_1'a_2 - a_2'a_1 > 0$ (λ-dependent boundary condition). In this case we make the standard assumptions that p, q, and r are locally L_1 functions in (a, ∞), $1/p$, q, and r are absolutely integrable near $x = a$ and $p(x) > 0$, $r(x) > 0$ almost everywhere.

(2) When $x = a$ is a singular endpoint and nonoscillatory for all real λ,

$$\lim_{x \to a} p(x)W_x(u(\cdot, \lambda), v) = \lim_{x \to a} p(x)(u(x, \lambda)v'(x) - u'(x, \lambda)v(x)) = 0, \qquad (1.3)$$

where v is the principal solution of Eq. (1.1) for any fixed real value of λ. This is the Friedrichs boundary condition which is automatically satisfied for all real and complex λ by the square integrable solution near $x = a$ in the limit point case, and which fixes the Friedrichs extension in the limit circle case. In this case we make the assumptions that p, q, and r are locally L_1 functions in (a, ∞) and $p(x) > 0$, $r(x) > 0$ almost everywhere.

Here we give a brief description of the standard real variable approach of Levitan [1950] and Levinson [1951], on which SLEDGE is based, in the

case when $x = a$ is regular and $a_1' = a_2' = 0$. To define the singular spectral function associated with the problem (1.1)–(1.2), this approach considers a regular self-adjoint Sturm-Liouville problem on the finite interval $[a,b]$ where $b \in (a,\infty)$, and then passes $b \to \infty$. The current implementation of SLEDGE makes use of the Dirichlet boundary condition

$$u(b) = 0. \tag{1.4}$$

Let $\phi(x,t)$ ($t \equiv \lambda$ in Eq. (1.1)) be the unique solution for all complex t of (1.1) defined by the initial conditions

$$\begin{pmatrix} \phi(a,t) \\ p(a)\phi'(a,t) \end{pmatrix} = \begin{pmatrix} a_2 \\ a_1 \end{pmatrix}. \tag{1.5}$$

Then $\phi(\cdot,t)$ satisfies the boundary condition (1.2) with $a_1' = a_2' = 0$ for all $t = \lambda \in \mathbb{C}$, where $\mathbb{C}$ is the set of complex numbers. Let the eigenvalues and eigenfunctions of the regular problem (1.1)–(1.2), (1.4) be denoted by $\lambda_{n,b}$ and $\phi(x,\lambda_{n,b})$, $n = 0,1,2, \ldots$, where the eigenvalues are ordered by

$$\lambda_{0,b} < \lambda_{1,b} < \lambda_{2,b} < \cdots.$$

Here $\lambda_{n,b}$ is characterized as the nth real solution of the equation $\phi(b,\lambda) = 0$. Let $H_1 = L_2((a,b);r)$ denote the Hilbert space with norm

$$\|f\|^2 = \int_a^b |f|^2 r(x)\, dx,$$

where $r(x)$ is the weight function from (1.1). Each $f \in H$ has an expansion in eigenfunctions of the regular problem (1.1)–(1.2), (1.4) of the form

$$f(x) = \sum_{n=0}^{\infty} c_n \phi(x,\lambda_{n,b}), \tag{1.6}$$

where

$$c_n = \frac{\displaystyle\int_a^b f(x)\phi(x,\lambda_{n,b})r(x)\, dx}{\|\phi(\cdot,\lambda_{n,b})\|^2},$$

and convergence is in the norm of the Hilbert space. This expansion may also be written in the equivalent form of a Riemann-Stieltjes integral,

$$f = \int_{-\infty}^{\infty} T_b(f)(t)\phi(x,t)\, d\rho_b(t), \tag{1.7}$$

where

$$T_b(f) = \int_a^b f(x)\phi(x,t)r(x) \; dx,$$

and $\rho_b(t)$ is the step function integrator defined for all real t by

$$\rho_b(t) = \sum_{\lambda_{n,b}\leq t} r_{n,b} = \sum_{\lambda_{n,b}\leq t} ||\phi(\cdot\, ,\lambda_{n,b})||^{-2}. \tag{1.8}$$

The step spectral function $\rho_b(\cdot)$ for the finite interval problem on $[a,b]$ is monotone increasing and right-continuous at the eigenvalues. It is clear that the magnitude of the jumps in ρ_b at the eigenvalues is fixed by the normalization of ϕ from the initial conditions (1.5) at $x = a$; multiplying a_1 and a_2 by a positive constant, for example, results in a division of $\rho_b(\cdot)$ by the square of the constant. The normalizations of $\phi(\cdot\,,t)$ and $\rho_b(t)$ are thus interconnected in such a way that the right-hand side of (1.7) is unaffected by a change of normalization.

  To write the eigenfunction expansion for the singular problem (1.1)–(1.2) on the half line $[a,\infty)$ assuming that the limit point case occurs at ∞, we first define the singular spectral density function as the pointwise limit

$$\rho(t) = \lim_{b\to\infty}\rho_b(t) \tag{1.9}$$

for all t where $\rho(t)$ is continuous, and at points of discontinuity so as to make ρ right-continuous. The eigenfunction expansion associated with the singular Sturm-Liouville problem (1.1)–(1.2) on the half line $[a,\infty)$ may be derived from Eq. (1.7) by letting $b \to \infty$. Without going into the detail of the associated real variable theory, the end result is the expansion

$$f = \int_{-\infty}^{\infty} T(f)(t)\phi(x,t) \; d\rho(t), \tag{1.10}$$

where

$$T(f) = \int_a^{\infty} f(x)\phi(x,t)r(x) \; dx,$$

and $\rho(t)$ is the singular spectral function defined in (1.9). This expansion is valid in the usual sense of norm convergence for all functions f in the Hilbert space $H_2 = L_2((a,\infty);r)$ with norm

$$||f||^2 = \int_a^{\infty} |f|^2 r(x) \; dx.$$

When the eigenfunction expansion (1.10) (or (1.7)) is written using the solution ϕ defined by the initial conditions (1.5) we say that the corresponding spectral function ρ (or ρ_b) is normalized relative to ϕ. The normalizations of ϕ and ρ are necessarily interconnected; some observations on this matter have been given in Fulton [1980, pp. 28–30].

The above analysis was generalized to the problem when λ is in the boundary condition at the left endpoint in Fulton [1980]. In this case the Hilbert space for the finite interval problem (1.1)–(1.2), (1.4) is

$$H_3 = \left\{ F = \begin{pmatrix} f_1(x) \\ f_2 \end{pmatrix} \middle| f_1 \in L_2((a,b);r), f_2 \in \mathbb{C} \right\}$$

with inner product

$$(F, G) = \int_a^b f_1 \, \bar{g}_1 r(x) \, dx + \frac{1}{\alpha} f_2 \, \bar{g}_2$$

where $\alpha = a_1' a_2 - a_1 a_2' > 0$. Similarly, the Hilbert space for the half line $[a, \infty)$ is

$$H_4 = \left\{ F = \begin{pmatrix} f_1(x) \\ f_2 \end{pmatrix} \middle| f_1 \in L_2((a,\infty);r), f_2 \in \mathbb{C} \right\}$$

with inner product

$$(F, G) = \int_a^\infty f_1 \, \bar{g}_1 r(x) \, dx + \frac{1}{\alpha} f_2 \, \bar{g}_2.$$

For problems with eigenparameter in the boundary conditions, the solution ϕ used in the associated eigenfunction expansion is normalized by the initial conditions

$$\begin{pmatrix} \phi(a,t) \\ p(a)\phi'(a,t) \end{pmatrix} = \begin{pmatrix} a_2 - a_2't \\ a_1 - a_1't \end{pmatrix}, \tag{1.11}$$

and the associated step spectral function for the regular problem (1.1)–(1.2), (1.4) is defined by

$$\rho_b(t) = \sum_{\lambda_{n,b} \leq t} r_{n,b} = \sum_{\lambda_{n,b} \leq t} \left\| \begin{pmatrix} \phi(\cdot, \lambda_{n,b}) \\ \alpha \end{pmatrix} \right\|^{-2}. \tag{1.12}$$

Using this step spectral function, the singular spectral density function, $\rho(\cdot)$, for the singular problem on the half line $[a, \infty)$ is defined as before in (1.9). The associated eigenfunction expansion for an arbitrary $F \in H_4$ using this singular ρ has two components and is given in Fulton [1980, Eq. (6.16)

with regular left endpoint]. The spectral functions ρ_b and ρ have (in contrast to the case $a_1' = a_2' = 0$) total variation (for all b) over $(-\infty,\infty)$ equal to $1/\alpha$. For further details see Fulton [1980].

The above analysis also generalizes to the case when $x = a$ is a singular endpoint which is nonoscillatory for all real λ. If the boundary condition (1.3) is imposed at $x = a$ in the case of the doubly singular interval (a,∞), then one has to select a solution ϕ of the Eq. (1.1) which satisfies the following requirements:

(1) $\phi(\cdot ,t)$ satisfies the Friedrichs boundary condition (1.3) for all $t \in \mathbb{C}$.

(2) $\phi(x,t)$ and $\phi'(x,t)$ are continuous for $(x,t) \in (a,\infty) \times \mathbb{C}$ and entire in t for each $x \in (a,\infty)$.

If $x = a$ is in the limit circle case then this is possible by transforming Eq. (1.1) to a first-order system and letting $\phi(\cdot ,t)$ be defined by "end conditions" as in Fulton [1977, Eq. (2.5)]. For example, taking in (1.3) v to be a principal solution for $t = \lambda = 0$ and choosing w to be any nonprincipal solution for $t = 0$ with $p(x)W_x(w,v) = 1$, a solution $\phi(\cdot ,t)$ satisfying (1.3) which has the properties (1) and (2) is defined for all $t \in \mathbb{C}$ by

$$\lim_{x \to a} \left(\begin{array}{c} p(x)W_x(\phi(\cdot ,t), v) \\ -p(x)W_x(\phi(\cdot ,t), w) \end{array} \right) = \left(\begin{array}{c} 0 \\ 1 \end{array} \right).$$

The solution $\phi(\cdot ,t)$ so defined is a principal solution for all real values of t, and its normalization is fixed by the choice of w. In the limit circle case the fact that the self-adjoint operator T on (a,∞) associated with (1.1) and the boundary condition (1.3) has spectral multiplicity one follows from Dunford and Schwartz [1963, Theorem 4 and Corollary 5, pp. 1336–1337]; a solution $\phi(\cdot ,t)$ satisfying (1.3) for all $t \in \mathbb{C}$ and normalized so as to satisfy the above requirements (1) and (2) serves, in this case, as a "determining set for the operator T on $t \in (-\infty,\infty)$" in the sense of Dunford and Schwartz [1963, p. 1374]. If $x = a$ is in the limit point case and nonoscillatory for all real t, then near $x = a$ there exists a solution $\phi(\cdot ,t) \in L_2((a,a + \epsilon);r)$, $\epsilon > 0$, for all real and complex t, and it can be normalized to satisfy the above properties (1) and (2); moreover, it is necessarily the principal solution for all real values of t. Letting ϕ be a solution normalized to satisfy properties (1) and (2) in both the limit circle and limit point cases, the discrete eigenfunction expansion for the problem (1.1), (1.3)–(1.4) on $(a,b]$ may be written in the form (1.7) using this "singular" choice of ϕ, where ρ_b is defined as in (1.8). Here $\lambda_{n,b}$, $n = 0,1,2, \ldots$, are the eigenvalues of the singular (limit circle or limit point) problem on $(a,b]$ (known to be bounded below by the nonoscillatory assumption) and $r_{n,b}$ are the squares of the norm reciprocals of the eigenfunctions $\phi(\cdot ,\lambda_{n,b})$. Letting $b \to \infty$ then yields the singular eigenfunction expansion for the problem (1.1), (1.3) on (a,∞) in

the form (1.10) where the singular spectral density function is defined as in (1.9). For the doubly singular interval (a, ∞) the normalizations of ϕ and ρ are, as before, interdependent, and we say that ρ is normalized relative to ϕ. When the left endpoint is singular the initial-value problem for (1.1) is not well posed at $x = a$, so the choice of normalization of ϕ is more problematic, and one can expect a wider variety of admissible normalizations depending on what assumptions are placed on the coefficient functions.

In addition to the mathematical problem of defining a suitable normalization of ϕ under assumptions which guarantee that (1.1) is nonoscillatory at $x = a$ for all real λ, there is the very real practical problem of implementing a given normalization numerically. Currently SLEDGE is only capable of handling the special case when $x = a$ is a regular singular point of (1.1) which is nonoscillatory for all real λ. In this case (which may be limit circle or limit point) a solution ϕ which satisfies the above two properties may be uniquely defined for all $t \in \mathbb{C}$ by requiring the normalization

$$\phi(x,t) = (x - a)^{r_1}(1 + c_1(x - a) + \cdots), \qquad (1.13)$$

where r_1 is the largest real root of the indicial equation (the indicial roots necessarily being real by the nonoscillatory assumption) in the Frobenius theory. The normalization can be implemented numerically (see Section 3), since the Frobenius exponent is computable.

In general, when $x = a$ is not a regular singular point but satisfies the requirement of being nonoscillatory for all real λ, a normalization of the principal solution ϕ which can be easily implemented numerically is not known. In a special case which is nonoscillatory and limit circle with $p = r = 1$ and with further assumptions on q, it is shown in Atkinson and Fulton [1999] that there is a principal solution which satisfies $\phi(x,t) = x \cdot (1 + o(1))$, as $x \to 0$ for all real t. It may be possible to extend the definition of this solution to complex t in such a way that the requirements (1) and (2) are met. But it remains to devise a numerical implementation of such a normalization. In general, problems with two singular endpoints and simple spectrum remain a challenge both mathematically and numerically. The interdependence of the normalizations of ϕ and ρ is more dramatic when $x = a$ is a singular endpoint, and there is still much work to be done to establish mathematical theorems for normalizations of the principal solution ϕ under various assumptions on the coefficient functions, and to find numerical implementations of them. As we shall see in the case of Bessel's equation of order ν (Example 3) the above choice of normalization (1.13) for ϕ allows a wide range of possible asymptotic behaviors for the singular spectral function ρ defined by (1.9).

In the remainder of this article we shall adopt the endpoint classification terminology of Fulton et al. [1999] (see also Pryce [1993]). It is well known

that for each singular endpoint $x = e$ of Eq. (1.1) one and only one of the following cases occurs:

(1) (OSC) Eq. (1.1) is oscillatory at $x = e$ for all real λ.

(2) (NONOSC) Eq. (1.1) is nonoscillatory at $x = e$ for all real λ.

(3) (O-NO) There exists a real number Λ such that (1.1) is nonoscillatory at $x = e$ for all $\lambda \in (-\infty, \Lambda)$ and oscillatory at $x = e$ for $\lambda \in (\Lambda, \infty)$. The cutoff value Λ may be either oscillatory or nonoscillatory.

This classification is mutually exclusive and depends only on the coefficient functions p, q, and r. Accordingly we shall call a singular endpoint OSC, NONOSC, or "O-NO with cutoff Λ," according as it belongs to the above cases (1), (2), or (3). All possible combinations of the LP/LC and OSC/ NONOSC/O-NO classifications can occur at a singular endpoint except that it is not possible to be both LC and "O-NO with cutoff Λ." The five mutually exclusive classifications which may occur at a singular endpoint are therefore LP/OSC, LP/NONOSC, LP/O-NO, LC/OSC, and LC/NONOSC. In the present article we assume that the endpoint $x = a$ is either LP/NONOSC or LC/NONOSC (cases which do not generate any continuous spectrum) and that the endpoint $x = \infty$ is LP/O-NO, which ensures that the problem has some continuous spectrum in the interval (Λ, ∞) and has spectrum bounded below.

The numerical computation of $\rho(t)$ at user selected points $\{t_i\}$ using SLEDGE is based on the definition (1.8) (and (1.12) when $\alpha > 0$), and approximating $\rho_b(t_i)$ for sufficiently large b. A justification for using (1.9) computationally is the following theorem which establishes that the convergence in (1.9) is not just pointwise, but uniform on compact t-intervals on which $\rho(t)$ is continuous.

THEOREM 1. *Assume (1) the endpoint $x = a$ is regular with boundary condition (1.2) or it is a singular endpoint of NONOSC type with Friedrichs boundary condition (1.3), and (2) $\rho(t)$ is continuous in $[T_0, T_1]$. Then the convergence of ρ_b to ρ in (1.9) is uniform over $[T_0, T_1]$.*

PROOF. For any $\epsilon > 0$, since $\rho(t)$ is uniformly continuous on $[T_0, T_1]$, there exists $\delta > 0$ such that for all $t, t' \in [T_0, T_1]$

$$|t - t'| < \delta \text{ implies } |\rho(t) - \rho(t')| < \epsilon/2.$$

The set of open sets

$$S = \{I_t | I_t = (t - \delta/2, t + \delta/2)\}$$

is an open covering of $[T_0, T_1]$, so compactness implies there exists a finite subcover $\{I_{t_i} | i = 1, \ldots, n\}$ such that

$$[T_0, T_1] \subset \cup_{i=1}^n (t_i - \delta/2, t_i + \delta/2),$$

where $T_0 \leq t_1 < t_2 < \cdots < t_n \leq T_1$. It follows that $0 < t_i - t_{i-1} < \delta$ for all i, and therefore, by the uniform continuity of $\rho(t)$,

$$0 \leq \rho(t_i) - \rho(t_{i-1}) < \epsilon/2 \text{ for all } i = 1, \ldots, n. \tag{1.14}$$

By the pointwise convergence at t_i in (1.9) we have existence, for each i, of $b_i > 0$ such that $|\rho_b(t_i) - \rho(t_i)| < \epsilon/2$ whenever $b \geq b_i$. Taking $B = \max_i b_i$ we have

$$-\epsilon/2 < \rho_b(t_i) - \rho(t_i) < \epsilon/2 \text{ for all } i = 1, \ldots, n \tag{1.15}$$

whenever $b > B$. We can now make use of (1.14) and (1.15) and the monotonicity of ρ_b and ρ to complete the proof. Let $t \in [T_0, T_1]$ be a fixed generic point, and let i be the unique index for which $t_{i-1} \leq t < t_i$. Then from (1.14) we have

$$\rho(t_{i-1}) \leq \rho(t) \leq \rho(t_i) < \rho(t_{i-1}) + \epsilon/2$$

and

$$-\rho(t_{i-1}) \geq -\rho(t) \geq -\rho(t_i) \geq -\rho(t_i) - \epsilon/2,$$

while from (1.15) we have

$$\rho(t_{i-1}) - \epsilon/2 < \rho_b(t_{i-1}) \leq \rho_b(t) \leq \rho_b(t_i) < \rho(t_i) + \epsilon/2.$$

Combining these inequalities readily yields

$$-\epsilon < \rho_b(t) - \rho(t) < \epsilon$$

whenever $b > B$. $\quad \square$

For the case of the problem (1.1) and (1.2) with λ in the boundary condition and $\alpha > 0$, the spectral functions ρ_b and ρ are both of bounded variation over the whole real t-axis with the same total variation; it therefore becomes possible to extend the theorem to an infinite or semi-infinite interval. In this case we have the following theorem:

THEOREM 2. *For the problems (1.1) and (1.2) on $[a, \infty)$ assume $\alpha = a_1' a_2 - a_1 a_2' > 0$. If $\rho(t)$ is continuous in $(-\infty, \infty)$, or $[T_0, \infty)$, then the convergence of ρ_b to ρ in (1.9) is uniform over $(-\infty, \infty)$, or $[T_0, \infty)$, respectively.*

The proof follows by taking advantage of the fact that $\rho_b(-\infty) = \rho(-\infty) = 0$, and $\rho_b(+\infty) = \rho(+\infty) = 1/\alpha$ [Fulton 1980, Eq. (5.12)] for all $b \in (a, \infty)$ to truncate the interval near the infinite endpoints, and then applying the same argument as in Theorem 1.

In view of the fact that the underlying assumptions for the present article arise partly from mathematical considerations and partly from software considerations, a few remarks may help to set the perspective. It is not always the case that one attempts to run a software package like SLEDGE only on those problems for which the p, q, and r functions satisfy every assumption of every theorem that was employed in deriving the methods of approximation on which the code is based; for it is often the case that at run time when certain tests are not passed, the code automatically elects not to implement a given method and to use instead a backup method which may not require the same assumptions on p, q, and r. Also, the mathematical theory associated with eigenfunction expansions generally holds under much weaker conditions than the code can handle. A few remarks along these lines are in order:

(1) The underlying method of approximation in SLEDGE replaces the coefficient functions p, q, and r by piecewise constant step functions $\hat{p}$, $\hat{q}$, $\hat{r}$ on each mesh interval, and performs repeated bisections of the initial mesh, to generate a sequence of numerical approximations to the eigenvalues, the eigenfunction norm reciprocals, and the step spectral function $\rho_b(t_i)$ at the desired output points t_i. Sufficient conditions for the second-order convergence of these step spectral functions over the sequence of meshes (needed for the application of a Richardson's extrapolation) are p, q, r $\in C^4[a,b]$. For more details see Pruess and Fulton [1996]. When the numerics do not justify the use of the Richardson's extrapolation the code employs Aitken extrapolation as a backup method.

(2) When $x = a$ is a singular endpoint, the assumption that it is also a regular singular point is needed to implement the normalization (1.13), so it suffices to assume that p, q, and r satisfy the assumptions for a RSP in a small neighborhood of $x = a$.

(3) When $x = a$ is a regular endpoint SLEDGE automatically switches to the use of asymptotic formulas for $\lambda_{n,b}$ and $r_{n,b}$ for use in the formulas for ρ_b in (1.8) and (1.12) when n is large. Sufficient conditions for the validity of the asymptotic formulas utilized are that Eq. (1.1) should be convertible to Liouville Normal Form and that the LNF potential Q should be of bounded variation over $[a,b]$. See Fulton and Pruess [1994, Eq. (2.9) and Theorem 2]. However, in case the computed values of $\lambda_{n,b}$ and $r_{n,b}$ do not come close enough to the asymptotic formulas as n increases, the code does not make use of the asymptotics.

(4) The numerical scheme used in SLEDGE to automatically generate output for the LP/LC and OSC/NONOSC/O-NO classifications and the heuristics for selecting the initial mesh require that the coefficient

functions p, q, and r must behave like powers of x near the singular endpoints. For further details see Fulton et al. [1999]. When the code is run on problems not satisfying these assumptions it generally returns an error flag to indicate no decision on these classifications; in such cases the user must obtain the classification information from known mathematical theory.

2. IMPLEMENTATION OF THE SPECTRAL FUNCTION CALCULATION

The code SLEDGE requires the user to specify a finite set $\{t_i\}_{i=1}^{NUMT}$ of points where output for $\rho(t_i)$ is desired, and a tolerance TOL for the desired accuracy. The routine then chooses a b-value and estimates the eigenvalues $\lambda_{n,b}$, and reciprocals of the eigenfunction norms $r_{n,b}$, for $0 \leq n \leq MAXNEV$, where $\lambda_{MAXNEV,b} > t_{NUMT}$ so that (1.8), or (1.12), can be used to compute ρ_b at the given t-values. For details on the algorithm for computing the eigenvalues and eigenfunctions see Pruess and Fulton [1993] and Pruess et al. [1995]. Given $t_i > \Lambda$, let k be the eigenvalue index for which $\lambda_{k-1,b} \leq t_i < \lambda_{k,b}$; then linear interpolation between the midpoints of successive steps is given by

$$\bar{\rho}_b(t) := \rho_b(\lambda_{k,b}) + \left(\frac{\rho_b(\lambda_{k+1,b}) - \rho_b(\lambda_{k,b})}{\zeta_{k+1} - \zeta_k} \right)(t - \zeta_k) \qquad (2.1)$$

for $t \in [\zeta_k, \zeta_{k+1}]$ where $\zeta_k = (\lambda_{k,b} + \lambda_{k+1,b})/2$.

Consider the example $-u'' = \lambda u, u'(0) = 0$, on $[0,\infty)$ which gives rise to the Fourier cosine integral with spectral function $\rho(t) = 2\sqrt{t/\pi}$. When the approximating regular problem on $[0,b]$ has the Neumann boundary condition at $x = b$, $u'(b) = 0$, the associated regular eigenvalues are $(n\pi/b)^2$, the eigenfunction norm reciprocals are $2/b$ for all n, and the expansion on $[0,b]$ is the Fourier Cos Series. It is clear from the graphs of ρ and ρ_b that

$$\max_{t \in [0,\infty)} |\rho(t) - \rho_b(t)| \leq 2/b \qquad (2.2)$$

and that the bound is sharp. Thus, with no interpolation, a tolerance request of 10^{-3} would require $b = 2000$, 10^{-4} would require $b = 20,000$, etc., hence, the need for interpolation. Unfortunately, sharp mathematical error bounds of the form

$$\max_{t \in [0,t_{NUMT}]} |\bar{\rho}_b(t) - \rho(t)| < \epsilon(b) \qquad (2.3)$$

are not, in general, known. Of course we may expect Theorem 1 to hold with ρ_b replaced by $\bar{\rho}_b$ in (1.9), but this supplies no information on the size of $\epsilon(b)$. Our experience with SLEDGE over a wide variety of test problems

is that $\epsilon(b)$ is significantly smaller than the $2/b$ bound in (2.2). This is due to the smoothing effect of the interpolation. In the simplest case of $-u'' = \lambda u$ there are explicit formulas for $\lambda_{n,b}$ and $r_{n,b}$, and it is possible to obtain an analytic bound of the form $\epsilon(b) = 0(1/b^2)$. For this analysis and a discussion of alternative interpolation schemes we refer to Pruess and Fulton [1996].

SLEDGE makes use of heuristics based on available information, particularly the coefficient functions p, q, and r, and the requested tolerances, to generate a sequence of increasing b-values for which $\bar{\rho}_b$ is believed to converge to ρ at a reasonable rate. The initial b-value depends on (1) the asymptotic behavior of the coefficient functions (see Fulton et al. [1999]) and (2) the user's requested tolerance. This classification information also determines the number and distribution of mesh points used throughout the computation. Subsequent values of b are functions of the density of eigenvalues (number per unit t of $\rho_b(t)$) for the previous choice of b. Too low a density means that ρ_b is likely to be a poor approximation to ρ so the next b must be much greater. Too high a density means the code is working too hard, so b should be increased only modestly. Based on these decisions the code either takes $b_n = 2b_{n-1}$ or $b_n = (1.4)b_{n-1}$ as the next increment for b. The exit criterion is that the difference of output $\bar{\rho}_b$-approximations for two successive choices of b-values must be within the user's requested tolerance over the finite set of output points, t_i, that is,

$$\max_{1 \leq i \leq NUMT} |\bar{\rho}_{b_n}(t_i) - \bar{\rho}_{b_{n-1}}(t_i)| \leq TOL, \qquad (2.4)$$

where TOL is the user-requested accuracy. This is a very crude measure, but the current state of theoretical knowledge concerning the behavior of $\rho(t) - \bar{\rho}_b(t)$ precludes anything more sophisticated. There is a maximum limit (determined by internal heuristics) to the number of b-values attempted; when the number of b-values permitted by SLEDGE is exceeded without achieving user-requested accuracy SLEDGE exits with IFLAG $= -3$.

3. IMPLEMENTATION OF THE ϕ-NORMALIZATION

The routines which compute estimates for the eigenfunctions automatically normalize any eigenfunction U to have unit L_2 norm, i.e.,

$$\int_a^b U^2(x, \lambda_{n,b}) r(x) \, dx = 1. \qquad (3.1)$$

At a regular endpoint, instead of (1.5), the normalization actually chosen by SLEDGE is

$$\begin{pmatrix} \phi(a,t) \\ p(a)\phi'(a,t) \end{pmatrix} = \begin{pmatrix} a_2/\sqrt{a_1^2 + a_2^2} \\ a_1/\sqrt{a_1^2 + a_2^2} \end{pmatrix} \tag{3.2}$$

when $a'_1 = a'_2 = 0$, and instead of (1.11)

$$\begin{pmatrix} \phi(a,t) \\ p(a)\phi'(a,t) \end{pmatrix} = \begin{pmatrix} (a_2 - a'_2 t)/\sqrt{\alpha} \\ (a_1 - a'_1 t)/\sqrt{\alpha} \end{pmatrix} \tag{3.3}$$

when $\alpha > 0$. The first normalization corresponds to the manner in which Titchmarsh [1962] normalizes $\phi(x,t)$. The second, for problems with λ in the boundary condition, renormalizes α in the theory given by Fulton [1980]; consequently, SLEDGE renormalizes the boundary condition constants in (1.2) and (1.11) to make $\alpha = 1$.

Since $U(x,\lambda_{n,b})$ and $\phi(x,\lambda_{n,b})$ differ only by a constant multiple, say $U(x,\lambda_{n,b}) = K\phi(x,\lambda_{n,b})$, it follows that

$$K = \frac{1}{\|\phi\|_2} = \frac{U(a)}{\phi(a)} = \frac{p(a)U'(a)}{p(a)\phi'(a)}$$

$$= \frac{\sqrt{a_1^2 + a_2^2}}{|a_2|}|U(a)| = \frac{\sqrt{a_1^2 + a_2^2}}{|a_1|}|p(a)U'(a)|. \tag{3.4}$$

Since $U(a)$ and $p(a)U'(a)$ are computable quantities, (3.4) provides two formulas for computing the norm reciprocals in (1.8); the actual choice depends on whether $a_2 \neq 0$ or $a_1 \neq 0$. Similar formulas apply to the implementation of the normalization (3.3) for problems with λ in the boundary condition.

To implement the normalization (1.13) at a regular singular point is more difficult, and we must be content with an approximate normalization based on asymptotics. If SLEDGE's eigenfunction approximation $U(x,\lambda_{n,b})$ satisfies (3.1), and the desired eigenfunction $\phi(x,\lambda_{n,b})$ satisfies the normalization (1.13), then as for the regular case, $U(x) = K\phi(x)$ for some constant K. Moreover,

$$K = \frac{1}{\|\phi\|_2} = \frac{U(a + \epsilon)}{\phi(a + \epsilon)} = \frac{p(a + \epsilon)U'(a + \epsilon)}{p(a + \epsilon)\phi'(a + \epsilon)} \text{ for any } 0 < \epsilon < b - a.$$

From the approximations (1.13) near the regular singular point we have that

$$\phi(x) = (x - a)^{r_1}(1 + O(x - a))$$

and

$$\phi'(x) = r_1(x - a)^{r_1 - 1}(1 + O(x - a)).$$

From the assumed power behavior of $p(x)$ near $x = a$ we also have that

$$p(x) = c_p(x - a)^{E_p}(1 + O((x - a)^{\bar{p}})), \text{ for some } \bar{p} > 0.$$

Two versions for the scaling factor K are therefore

$$K = \frac{1}{\|\phi(x)\|_2} = \frac{U(a + \epsilon)}{\epsilon^{r_1}(1 + O(\epsilon^{r_1+1}))} \approx \frac{U(a + \epsilon)}{\epsilon^{r_1}} \tag{3.5}$$

and

$$K = \frac{1}{\|\phi(x)\|_2} = \frac{(pU')(a + \epsilon)}{c_p r_1 \epsilon^{E_p+r_1-1}(1 + O(\epsilon^{r_1+1}) + O(\epsilon^{\bar{p}}))} \approx \frac{(pU')(a + \epsilon)}{c_p r_1 \epsilon^{E_p+r_1-1}}. \tag{3.6}$$

In these formulas SLEDGE takes ϵ to be the length of the first mesh interval in the initial mesh. In theory either of (3.5) or (3.6) can be used; in practice, the code selects (3.5) whenever $|U(a + \epsilon)| \geq |(pU')(a + \epsilon)|$; otherwise (3.6) is used. Exceptions occur when $r_1 = 0$ or $E_p + r_1 - 1 = 0$ in which case the code reverts to using one of the formulas in (3.4).

4. THE TEST EXAMPLES

Example 1 (Bessel Equation of Order Zero on $[1,\infty)$ with Dirichlet Boundary Condition at the Regular Endpoint). The general Fourier-Bessel Integral on $[a,\infty)$, $a > 0$, associated with the Bessel equation of order 0 in Liouville Normal Form,

$$-u'' - \frac{1}{4x^2} u = tu \qquad a \leq x < \infty \tag{4.1}$$

with Dirichlet boundary condition $u(a) = 0$, is given by Titchmarsh [1962, Eq. (4.10.3)]. For $a = 1$, imposing the normalization (1.5) with $a_1 = 1$ and $a_2 = 0$ gives the eigenfunction expansion in the form (1.10) where

$$\phi(x,t) = \frac{\pi}{2}\sqrt{x}[-J_0(x\sqrt{t})Y_0(\sqrt{t}) + Y_0(x\sqrt{t})J_0(\sqrt{t})],$$

$$\rho(t) = \begin{cases} 0, & t \leq 0 \\ \displaystyle\int_0^t \frac{1}{\pi\sigma_1(\xi)}d\xi, & t > 0, \end{cases}$$

and

$$\sigma_1(\xi) = \frac{\pi}{2}[J_0^2(\sqrt{\xi}) + Y_0^2(\sqrt{\xi})].$$

Example 2 (Bessel Equation of Order Zero with λ in the Boundary Conditions).　If we impose the λ-dependent boundary condition

$$-u'(a) = tu(a)$$

at $a = 1$, the solution of the Bessel equation (4.1) normalized by (1.11) is

$$\phi(x,t) = \frac{\pi}{2}\left(t + \frac{1}{2}\right)\sqrt{x}[J_0(x\sqrt{t})Y_0(a\sqrt{t}) - Y_0(x\sqrt{t})J_0(a\sqrt{t})]$$

$$+ \frac{\pi}{2}\sqrt{tx}[J_1(a\sqrt{t})Y_0(x\sqrt{t}) - Y_1(a\sqrt{t})J_0(x\sqrt{t})].$$

For this example there is one eigenvalue λ_0 below the cutoff $\Lambda = 0$,

$$\rho(t) = \begin{cases} 0 & t < \lambda_0 \\[2ex] r_0 = 1/\left(\int_1^\infty |\phi(x,\lambda_0)|^2\,dx + 1\right) & \lambda_0 < t < 0 \\[3ex] r_0 + \int_0^t \frac{1}{\pi\sigma_3(\xi)}d\xi & 0 < t < \infty, \end{cases}$$

$\lambda_0 = -s_0^2$ where s_0 is the positive zero of the equation

$$(-s^2 + 1/2)K_0(s) - sK_1(s) = 0,$$

$$r_0 = \frac{-K_0(s_0)}{-\frac{3}{4}K_0(s_0) - \frac{1}{s_0}\left(-\frac{s_0^2}{2} + \frac{3}{4}\right)K_1(s_0) + \frac{1}{4}K_2(s_0)},$$

and

$$\sigma_3(\xi) = \frac{\pi}{2}\left[\left((\xi + 1/2)J_0(\sqrt{\xi}) - \sqrt{\xi}J_1(\sqrt{\xi})\right)^2 + \left((\xi + 1/2)Y_0(\sqrt{\xi}) - \sqrt{\xi}Y_1(\sqrt{\xi})\right)^2\right].$$

For Examples 1 and 2, the continuous part of the $\rho(t)$ function over $t \in (0,\infty)$ was obtained by two different methods: (1) the "$m(\lambda)$-function" approach of Weyl [1910] and Titchmarsh [1962] and (2) the real variable method of Atkinson [1985].

Example 3 (Fourier Bessel Integral of Order ν on (0,∞)). This differential equation in Liouville normal form is

$$-u'' + \frac{\nu^2 - 1/4}{x^2}u = tu \quad 0 < x < \infty, \quad 0 \leq \nu < \infty. \tag{4.2}$$

Imposing the normalization (1.13) (via SLEDGE's approximate formulas (3.5) or (3.6)), the ordinary Fourier Bessel integral of order ν on (0,∞) [Titchmarsh 1962, p. 88] can be written in the form (1.10) where

$$\phi(x,t) = t^{-\nu/2}2^\nu\Gamma(\nu + 1)\sqrt{x}J_\nu(x\sqrt{t})$$

$$= x^\nu + O(x^{\nu+2}) \text{ for all } t \in \mathbb{C}$$

and

$$\rho(t) = \begin{cases} 0, & t < 0 \\ \dfrac{1}{2^{2\nu+1}\Gamma^2(\nu + 1)}\left(\dfrac{t^{\nu+1}}{\nu + 1}\right), & t \geq 0. \end{cases} \tag{4.3}$$

This problem is singular and NONOSC at the endpoint $x = 0$; it is limit point for $\nu \in [1,\infty)$ and limit circle for $\nu \in [0,1)$. The Friedrichs boundary condition (1.3) selects the above principal solution ϕ for all real t and all $\nu \in [0,\infty)$; other requirements on u, which also select this same solution, may be regarded as equivalent to the limiting wronskian form (1.3) of the Friedrichs boundary condition. In particular, SLEDGE automatically generates a regular boundary condition at an LC/NONOSC or LP/NONOSC endpoint, which selects the principal solution (necessarily the L_2 solution for real λ at an LP/NONOSC endpoint). For Example 3, SLEDGE's output for this "regular" characterization of the Friedrichs boundary condition is $u(0) = 0$ for all $\nu \in [0,\infty)$. The cutoff is $\Lambda = 0$, and there are no eigenvalues below Λ.

Using

$$||\phi(x,\lambda_{nb})||^2 = \lambda_{nb}^{-\nu}2^{2\nu}\Gamma^2(\nu + 1)b^2J_{\nu+1}^2(\alpha_{\nu n})/2, \tag{4.4}$$

where λ_{nb} are the eigenvalues of (4.2), (1.3), (1.4), and standard asymptotic expansions for J_ν and its nth zero, $\alpha_{\nu n}$, we have the asymptotics for Example 3 on $(0,b]$, for $n = 1,2, \ldots$,

$$\lambda_{n-1,b} = \frac{1}{b^2}\left\{\left[\left(n + \frac{\nu}{2} - \frac{1}{4}\right)\pi\right]^2 - \frac{4\nu^2 - 1}{4}\right\} + O\left(\frac{1}{n^2}\right), \tag{4.5}$$

and

$$r_{n-1,b} = \frac{\pi\left[\left(n + \frac{\nu}{2} - \frac{1}{4}\right)\pi\right]^{2\nu+1}}{2^{2\nu}\Gamma^2(\nu + 1)b^{2\nu+2}}\left\{1 + O\!\left(\frac{1}{n^2}\right)\right\}. \tag{4.6}$$

Example 4 (Coulomb Potential for the Hydrogen Atom with Zero Angular Momentum).   The differential equation in Liouville normal form is

$$-u'' - \frac{1}{x}u = tu, \ \ 0 < x < \infty. \tag{4.7}$$

The endpoint $x = 0$ is singular, limit circle, and NONOSC. SLEDGE output for the "regular" form of the Friedrichs boundary condition is $u(0) = 0$. Imposing the normalization (1.13) via SLEDGE's approximate formulas (3.5) or (3.6) the eigenfunction expansion may be written in the form (1.10) where

$$\begin{aligned}\phi(x,t) \ \ &= \frac{-1}{2i\sqrt{t}}M_{\beta,1/2}(-2ix\sqrt{t}), \qquad \beta = \frac{i}{2\sqrt{t}}\\ &= x + O(x^2) \text{ for all } t \in \mathbb{C},\end{aligned}$$

where $M_{\beta,1/2}$ is the first Frobenius solution of the Whittaker equation, and where

$$\rho(t) = \begin{cases} \displaystyle\sum_{\lambda_n<t}\frac{1}{2(n + 1)^3}, & t \leq 0 \\[2ex] \displaystyle\frac{1}{2}\zeta(3) = 0.6010284516, & t = 0 \\[2ex] \displaystyle\rho(0) + \int_0^t \frac{1}{1 - \exp(-\pi/\sqrt{s})}ds, & t > 0. \end{cases} \tag{4.8}$$

Here ζ is the Riemann zeta function. Compare Titchmarsh [1962, Section 4.17].

5. PERFORMANCE OF SLEDGE

SLEDGE was used to estimate the spectral density at various t points for each of the examples in the previous section. For the first two, which are regular at $x = a$, we sought 27 $\rho(t)$ values for $t \in [0,50000]$ with requested tolerances (TOL) varying from 10^{-3} down to 10^{-5} (the 27 t-values used were the same as in Table V). Statistics for these runs are given in Table I. The code returned IFLAG equal zero in all cases. The third column of the table lists the maximum b-value chosen by SLEDGE; the fourth column is the number of b-values tried. The next column contains the total

Table I. SLEDGE Performance Statistics for Problems Regular at $x = a$

Example	TOL	Last b	Number of b's	Number of λ_{nb}	Time (in seconds)	Inaccurate at $t =$	Max Error	IFLAG
1	10^{-3}	42	2	13026	1.76	none	0.001	0
1	10^{-4}	172	2	54663	17.59	10	0.0002	0
1	10^{-5}	482	2	153954	124.48	5	0.00002	0
2	10^{-3}	84	3	13035	4.32	none	0.001	0
2	10^{-4}	172	2	54669	106.61	none	0.0005	0
2	10^{-5}	482	2	205280	1914.56	none	0.00001	0

number of λ_{nb} and r_{nb} computed by the code for all the b-values. The computer times in Table I were measured in seconds on a Cray Y/MP; the timing data given are averages for three separate runs at each tolerance. The third column from the right lists those t-values, out of the set of 27, where the code failed to achieve the requested tolerance (by greater than a factor of 1.9). The column labeled "max error" lists the maximum over the 27 points of

$$\max\{\text{absolute error}, \rho(t) * \text{relative error}\}.$$

Note that even when SLEDGE's output had errors exceeding the requested tolerance, it was still within a factor of 2 of TOL.

Inspection of the data in Table I shows that the computing time per eigenvalue and eigenfunction norm is remarkably low. This is due mainly to that fact that SLEDGE makes use of known asymptotic formulas whenever possible. These formulas, from Fulton and Pruess [1994, Eqs. $(4.11)_2$, $(4.13)_2$, $(4.15)_2$, $(4.18)_2$, $(6.8)_2$–$(6.11)_2$] and Fulton [1982, Eq. $(2.4)_2$], require only a few flops for each $\{\lambda_{n,b}; r_{n,b}\}$ pair and are used as soon as they are as accurate as those produced by the usual numerical method. In particular, for Example 1 when TOL $= 10^{-3}$ the standard shooting algorithm was used for only 19 eigenvalues at the first b and 34 at the second. The remaining 12,973 were found by the asymptotic formulas. Similarly, the shooting algorithm was used for 138 eigenfunction norms at the first b and 289 at the second, while the remaining 12,599 were found by asymptotic formulas. For the same example when TOL $= 10^{-5}$, all but 934 of the 153,954 eigenvalues were found using asymptotic formulas. In contrast, 40,126 of the $r_{n,b}$ had to be computed by the much slower shooting algorithm, and only the remaining 113,828 were found with the asymptotic formulas. Generally, the switchover to the asymptotic eigenvalue formulas occurs much sooner than the switchover to the asymptotic $r_{n,b}$ formulas.

For problems with $x = a$ regular and $r = p = 1$, standard asymptotic formulas for $\rho(t)$ as $t \to \infty$ are well known (see Levitan [1952; 1953; 1955] or Atkinson [1982], and for Example 1 under the normalization (3.2) we have

Table II. Asymptotic Approximation of the Spectral Function for Example 1

t	Exact $\rho(t)$	$\rho(t) = 2t^{3/2}/3\pi$	Relative Error
50.0	0.75481080E+2	0.75026360E+2	0.006024
100.0	0.21288959E+3	0.21220659E+3	0.003208
200.0	0.60121999E+3	0.60021088E+3	0.001678
500.0	0.23742018E+4	0.23725418E+4	0.000699
1000.0	0.67129570E+4	0.67105616E+4	0.000356
2000.0	0.18983771E+5	0.18980334E+5	0.000181
5000.0	0.75031863E+5	0.75026360E+5	0.000073
10000.0	0.21221442E+6	0.21220659E+6	0.000037
50000.0	0.23725595E+7	0.23725418E+7	0.000007

$$\rho(t) = \frac{2t^{3/2}}{3\pi} + o(1).$$

The utility of ρ-asymptotics is, however, limited. As an illustration, we have listed in Table II the asymptotic approximation $2t^{3/2}/3\pi$ for Example 1 together with the exact $\rho(t)$ values, and the relative error in this asymptotic approximation. As is seen the latter is less than 10^{-3} starting at $t = 500$, less than 10^{-4} starting at $t = 5,000$, and less than 10^{-5} starting at $t = 50,000$. If the ρ-asymptotics were stronger, say with higher-order terms in descending powers of $1/\sqrt{t}$, they might make a switchover to asymptotics for ρ worthwhile; but the above ρ-formula is clearly too weak to be worthwhile. Some results in this direction have been obtained by Harris [1985, Theorem 1] and Harris [1987, Theorem 3]. These theorems apply only for the case of the Neumann boundary condition at $x = 0$ when $r = p = 1$, but an extension to the Dirichlet boundary condition may be possible and could be useful for Example 1. Further testing on ρ-asymptotics of this type would be desirable. We also mention that a number of asymptotic results for ρ and the Weyl-Titchmarsh m-function in special cases (and not necessarily in Liouville Normal Form) are given by Bennewitz [1989].

Examples 3 and 4 are singular at the left endpoint $x = a$. For these cases asymptotic formulas λ_{nb} and r_{nb} are not known in any generality so SLEDGE has to work much harder, expecially for large t-values requiring large numbers of eigenvalues and eigenfunction norms. We requested accuracies of 10^{-3} and 10^{-4} over 18 t-points in [0,20]. The output is summarized in Table III; the computer times were measured in seconds on a CRAY Y/MP, and the data given are averages over three separate runs at each tolerance.

The warning flag of 2 on Example 3 when $\nu = 1$ indicates that SLEDGE was unsure of the classifications for this problem (since it is on the borderline between LP and LC at $x = 0$).

When SLEDGE was asked to return estimates for $\rho(t)$ for larger t-values, it did not perform as well. As an illustration, in Table IV is displayed the

Table III. SLEDGE Performance Statistics for Problems Singular at $x = a$

Example	TOL	Last b	Number of b's	Number of λ_{nb}	Time (in seconds)	Inaccurate at $t =$	Max Error	IFLAG
3($\nu = 1$)	10^{-3}	40	2	340	3.51	none	0.0007	2
3($\nu = 1$)	10^{-4}	128	2	1510	28.20	10	0.0002	2
3($\nu = 4$)	10^{-3}	40	2	410	6.26	none	0.0006	0
3($\nu = 4$)	10^{-4}	127.5	2	1794	51.39	none	0.00001	0
4	10^{-3}	160	4	354	3.87	none	0.001	0
4	10^{-4}	286.875	4	1084	12.54	0.1,0.2,0.3	0.0002	0

Table IV. Behavior of Example 3 ($\nu = 1$ and $b = 160$) without Asymptotics

t	Exact $\rho(t)$	SLEDGE Estimate	Relative Error
50.0	0.15625000E+3	0.15567413E+3	0.00369
100.0	0.62500000E+3	0.62029617E+3	0.00753
200.0	0.25000000E+4	0.24621913E+4	0.01512
500.0	0.15625000E+5	0.15033952E+5	0.03783
1000.0	0.62500000E+5	0.57834473E+5	0.07465
2000.0	0.25000000E+6	0.21381308E+6	0.14475
5000.0	0.15625000E+7	0.10478064E+7	0.32940
10000.0	0.62500000E+7	0.27293153E+7	0.56331
50000.0	0.15625000E+9	0.17922281E+8	0.88530

output for Example 3 ($\nu = 1$) with TOL $= 0.001$ at larger t-values. While SLEDGE only needed two b-values to produce the data in Table III (out to $t = 20$), it required four values of b to get to $t = 50000$. The data shown in the Table IV came from the last b-value, $b = 160$, and had IFLAG equal to -3, indicating that SLEDGE performed the four iterations allowed without satisfying the exit criterion (2.4).

By way of comparison, Example 3 ($\nu = 1$) was run with use of the explicit asymptotic formulas (4.5) and (4.6) in place of the usual asymptotic routines. In Table V is displayed the output with TOL $= 0.001$ for all 27 output points in [0,50000]. The "error" listed in the third column is absolute when "exact" $\rho < 1$, and relative otherwise. The error was well below the tolerance level at all 27 points, and the exit criterion was satisfied after three values of b. The data shown in the table came from $b = 80$. In Table VI is displayed performance statistics for the Example 3 ($\nu = 1$) similar to those in Table I for the problems with regular left endpoint. This data clearly demonstrates that when good asymptotic formulas are available, the code can achieve user-requested accuracy over a large range of t-values; in fact, the accuracy gets better for larger t because of the switchovers to the asymptotic formulas. For the Bessel equation the asymptotic formula (4.5) is close enough to the actual eigenvalues that the code switches to the asymptotic eigenvalue formula for $n = 1$ or 2 at almost every level of every iteration. Most of the time is spent computing the r_{nb} until the switchover to the asymptotic r_{nb} occurs. For tolerance 10^{-3}

Table V. Behavior of Example 3 ($\nu = 1$) with Asymptotics

t	Exact $\rho(t)$	SLEDGE Estimate	Error
0.0	0.00000000E+00	0.00000000E+00	+0.00E+00
0.1	0.62500000E-03	0.62485176E-03	-0.15E-06
0.2	0.25000000E-02	0.25012566E-02	+0.13E-05
0.3	0.56250000E-02	0.56186354E-02	-0.64E-05
0.4	0.10000000E-01	0.10002562E–01	+0.26E-05
0.5	0.15625000E-01	0.15620775E-01	-0.42E-05
0.6	0.22500000E-01	0.22457294E-01	-0.43E-04
0.7	0.30625000E-01	0.30634228E-01	+0.92E-05
0.8	0.40000000E-01	0.39941439E-01	-0.59E-04
0.9	0.50625000E-01	0.50635190E-01	+0.10E-04
1.0	0.62500000E-01	0.62496618E-01	-0.34E-05
1.1	0.75625000E-01	0.75553094E-01	-0.72E-04
1.2	0.90000000E-01	0.89958926E-01	-0.41E-04
1.5	0.14062500E+00	0.14064468E+00	+0.20E-04
2.0	0.25000000E+00	0.24998581E+00	-0.14E-04
5.0	0.15625000E+01	0.15623888E+01	-0.71E-04
10.0	0.62500000E+01	0.62498511E+01	-0.24E-04
20.0	0.25000000E+02	0.24999247E+02	-0.30E-04
50.0	0.15625000E+03	0.15625006E+03	+0.39E-06
100.0	0.62500000E+03	0.62499537E+03	-0.74E-05
200.0	0.25000000E+04	0.25000018E+04	+0.70E-06
500.0	0.15625000E+05	0.15625002E+05	+0.15E-06
1000.0	0.62500000E+05	0.62500015E+05	+0.23E-06
2000.0	0.25000000E+06	0.24999989E+06	-0.45E-06
5000.0	0.15625000E+07	0.15624998E+07	-0.13E-06
10000.0	0.62500000E+07	0.62499999E+07	-0.89E-08
50000.0	0.15625000E+09	0.15625000E+09	+0.19E-08

Table VI. SLEDGE Performance Statistics for Example 3 ($\nu = 1$) with Asymptotics

Example	TOL	Last b	Number of b's	Number of λ_{nb}	Time (in seconds)	Inaccurate at $t =$	Max Error	IFLAG
3	10^{-3}	80	3	38432	29.49	none	0.00007	2
3	10^{-4}	340	3	157300	274.24	none	0.000003	2
3	10^{-5}	480	3	187902	104.62	none	0.000004	2

at the deepest level of the third iteration, 5694 eigenvalue/eigenfunction norm pairs were required, all of which were computed by the asymptotic formulas except for 2 eigenvalues and 4 r_{nb}'s; the same was true at the tolerance levels 10^{-4} and 10^{-5} where, respectively, 24,200 and 34,164 eigenvalues were required in the last iteration.

6. CONCLUSIONS

For spectral function computations, SLEDGE generally performs better with respect to both accuracy and timing on problems with $x = a$ regular than when $x = a$ is singular. This is due to the incorporation of asymptotic formulas for the eigenvalues and eigenfunction norm reciprocals. The

asymptotic formulas become more accurate approximations the larger n is; this is the main reason why the errors in Tables I, V, and VI remain small for large t while those in Table IV become worse with increasing t. Accordingly, further work would be desirable on asymptotics for eigenvalues and eigenfunction norm reciprocals on $(0,b]$ when $x = 0$ is singular and NONOSC, for various classes of coefficient functions. This is a difficult area where little work has been done. For a special case which is LC and NONOSC at $x = 0$, Atkinson and Fulton [1984] have given eigenvalue asymptotics depending on q when $r = p = 1$; but no eigenfunction or eigenfunction norm asymptotics are available. Until such time that more general asymptotic formulas are available, further numerical work on the tolerance testing and heuristics for the λ_{nb}, r_{nb}, and $\bar{\rho}(t)$-approximations for large t will be required. To this end further theoretical work on the interpolation error in (2.3) would be desirable.

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