Approximation of eigenvalues of Sturm-Liouville differential equations by the sinc-collocation method
by Mary Katherine Jarratt

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematics
Montana State University

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A collocation method with sinc function basis elements is developed to approximate the eigenvalues of regular and singular Sturm-Liouville boundary value problems. The method generates a matrix system Ax = &lamba;Bx with A and B both symmetric and positive definite matrices. In the case of singular problems, the matrix norm of B-1 is unbounded; however, the error in the eigenvalue approximation is shown to converge at a fate of exp(-a√N) for a positive and 2N + 1 basis elements for both regular and singular problems. This is done by circumventing the standard error analysis which typically involves ||B-1||.

Test examples of the Sturm-Liouville differential equations given on finite and infinite intervals are included to illustrate the accuracy and implementation of the method. Several of the test examples are used to compare the performance of the sinc-collocation method to other numerical methods.

APPROXIMATION OF EIGENVALUES OF STURM-LIOUVILLE DIFFERENTIAL EQUATIONS BY THE SINC-COLLOCATION METHOD

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APPROVAL

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ABSTRACT

A collocation method with sinc function basis elements is developed to approximate the eigenvalues of regular and singular Sturm-Liouville boundary value problems. The method generates a matrix system $Ax = \lambda Bx$ with A and B both symmetric and positive definite matrices. In the case of singular problems, the matrix norm of B^{-1} is unbounded; however, the error in the eigenvalue approximation is shown to converge at a rate of $\exp(-a\sqrt{N})$ for a positive and $2N + 1$ basis elements for both regular and singular problems. This is done by circumventing the standard error analysis which typically involves $\|B^{-1}\|$.

Test examples of the Sturm-Liouville differential equations given on finite and infinite intervals are included to illustrate the accuracy and implementation of the method. Several of the test examples are used to compare the performance of the sinc-collocation method to other numerical methods.

CHAPTER 1

INTRODUCTION

The Sturm-Liouville equation is a second order linear differential equation of the form

$$(1.1) \qquad \frac{d}{dx}\left[p(x)\frac{du}{dx}\right] + (\lambda\rho(x) - g(x))u = 0$$

where λ is a parameter and p, ρ, and g are real with p and ρ strictly positive.

The Sturm-Liouville equation, along with appropriate boundary conditions, describes many physical phenomena typically connected with vibration problems in continuum mechanics, that is, boundary value problems corresponding to simple harmonic standing waves. Several phenomena described in some detail in Birkoff and Rota [1] are the vibrating string where the eigenvalues are proportional to the squared frequency, the longitudinal vibrations of the elastic bar, and the vibrating membrane.

The Sturm-Liouville equation can be written in several forms. The form given in (1.1) is called the self-adjoint form for real λ. Assuming g and ρ are continuous and p is continuously differentiable, solutions to (1.1) exist.

The Liouville normal form of the Sturm-Liouville equation will be the form used throughout Chapters 2-5.

Any differential equation (1.1) with $p, \rho \in C^2$ and $g \in C$ can be rewritten in normal form

$$(1.2) \qquad \frac{d^2\omega}{dt^2} + [\lambda - \hat{g}(t)]\omega = 0$$

where $\hat{g} = g/\rho + (p\rho)^{-1/4} \frac{d^2}{dt^2} [(p\rho)^{1/4}]$. This is accomplished by the change of variable

$$u = \omega(t)/(p(x)\rho(x))^{1/4} \quad \text{and} \quad t = \int \frac{\rho(x)}{p(x)}^{1/2} dx.$$

This transformation is discussed in Birkoff and Rota [1].

The Sturm-Liouville equation in standard form is given by

$$(1.3) \qquad y'' + P(x)y' + Q(x)y = \lambda R(x)y \ .$$

By the change of variable

$$y(x) = u(x)v(x) \quad \text{for} \quad v(x) = \exp\left(-\tfrac{1}{2}\int P dx\right) ,$$

(1.3) can be rewritten in normal form

$$(1.4) \qquad u'' + q(x)u = \lambda r(x)u$$

where $q(x) = Q(x) - \frac{1}{4}(P(x))^2 - \frac{1}{2}P'(x)$. Simmons [2] discusses at length the theory dealing with (1.3) and (1.4). Each of the forms (1.2), (1.3), and (1.4) are equivalent up to transformations and play different roles in the numerical approximation of their eigenvalues. This will be discussed in more detail in Chapter 5.

The Sturm-Liouville equation (1.1) can be posed on a finite, semi-infinite, or infinite interval. In the case

that (1.1) is on a closed, finite interval [a,b], p and ρ are strictly positive on [a,b], and p, ρ, and g are bounded in the interval, (1.1) is called a regular Sturm-Liouville equation. A regular Sturm-Liouville system is defined to be a regular Sturm-Liouville equation on the finite interval [a,b] with two separated endpoint conditions

$$\alpha u(a) + \alpha' u'(a) = 0$$

and

$$\beta u(b) + \beta' u'(b) = 0$$

for α, α', β, and β' real constants. The following theorem, stated with proof in Birkoff and Rota [1], gives information concerning the eigenfunctions of a regular Sturm-Liouville system.

Theorem 1.5: Eigenfunctions of a regular Sturm-Liouville system having different eigenvalues are orthogonal with respect to the weight ρ; that is, if u, λ and v, μ are eigenpairs and $\lambda \neq \mu$,

$$\int_a^b \rho(x)u(x)v(x)\,dx = 0 .$$

The transformation of (1.1) to normal form (1.2) takes a regular Sturm-Liouville system to a regular Sturm-Liouville system, does not change the eigenvalues, and takes functions orthogonal with respect to the weight ρ to functions orthogonal with respect to the weight 1.

There are Sturm-Liouville systems of interest that are not regular. That is, the function h (h = p, ρ, and/or g) is singular at one or both endpoints of the interval on which the problem is posed or one or both endpoints is infinite. If either or both of the preceeding situations occur, (1.1) is called a singular Sturm-Liouville equation. Comparable to Theorem 1.5 is

Theorem 1.6: Eigenfunctions u and v, with different eigenvalues, of a singular Sturm-Liouville system are orthogonal with respect to the weight ρ whenever

$$\lim_{\alpha \to a^+,\ \beta \to b^-} p(x)[u(x)v'(x) - v(x)u'(x)] \Big|_{x=\alpha}^{\beta} = 0$$

where b can be infinite (Birkoff [1]).

Many differential equations that arise in physical problems have singular points, that is, points at which P and/or Q are not analytic in (1.3). As Simmons [2] describes, choosing the most physically appropriate solution is many times determined by the behavior of the solution at a singular point.

The two types of singular points are regular and irregular. A singular point x_0 is called regular, if $(x - x_0)P(x)$ and $(x - x_0)^2Q(x)$ are analytic at x_0. If these two conditions are not satisfied, x_0 is called an irregular singular point. In terms of the normal form

(1.4), z_0 is a regular singular point if q has at worst a pole of order two at z_0.

Several numerical approaches are used to solve for the eigenvalues of Sturm-Liouville systems. They include finite differences [3], [4], [5], [6], [7], finite elements [5], [6], [8], [9], [10], [11], Galerkin [4], [5], [8], [9], [10], [11], the tau method [4], [12], [13], and collocation [4], [12], [13].

The finite difference method is straightforward for problems posed on a finite interval. It yields a matrix system $A\vec{x} = \lambda B\vec{x}$ which is symmetric [3].

The Rayleigh-Ritz approximation method described in Examples 5.1, 5.2, and 5.3 is a Galerkin method using polynomials or piecewise polynomials as basis functions [8], [10]. The tau method, using Chebyshev basis functions [4], is demonstrated in Example 5.4.

The sinc-collocation method defines an approximate solution to the Sturm-Liouville system at a finite set of nodes using sinc functions as basis functions. Before the complete description of the method is given in Chapter 4, Chapters 2 and 3 discuss some preliminary ideas. Chapter 2 introduces some general mathematical notions which form part of the basis for the analysis and implementation of the sinc-collocation method. Basic information on the sinc function and various properties of it are found in Chapter 3. Chapter 5 gives specific examples of Sturm-Liouville

systems using the sinc-collocation method and compares these results with results of other methods mentioned earlier.

CHAPTER 2

PRELIMINARY RESULTS

For the formulation and implementation of the sinc-collocation method, several general mathematical notions need to be considered. This chapter gives a general discussion of the WKB approximation to solutions of particular differential equations, indicial equations related to the solution of differential equations, and the method of solving a generalized eigenvalue problem. Two theorems concerning eigenvalues will be included for completeness. Concluding the chapter is a general discussion of the Rayleigh-Ritz method of solving boundary value problems.

The following discussion of the WKB approximation is due to Olver [14]. Suppose $\omega(x)$ is a function satisfying

$$\frac{d^2\omega}{dx^2} = f(x)\omega(x) \tag{2.1}$$

for x real or complex and f some given positive function. To approximate the solution ω of (2.1), let $\eta(x)$ be three times differentiable and

$$W(x) = \{\eta'(x)\}^{\frac{1}{2}}\omega(x) .$$

A new differential equation in W is

$$(2.2) \qquad \frac{d^2W}{d\eta^2} = \{(\ddot{x})^2 f(x) + (\ddot{x})^{1/2} \frac{d^2}{d\eta^2} ((\ddot{x})^{-1/2})\}W$$

where dots represent differentiation with respect to η. This is called the Liouville transformation. Without loss of generality, $\eta(x)$ can be chosen so that $(\dot{x})^2 f(x) = 1$; hence,

$$\eta(x) = \int (f(x))^{1/2}\, dx \quad .$$

Given that f is twice differentiable, (2.2) can be written

$$(2.3) \qquad \frac{d^2W}{d\eta^2} = (1 + \phi(x))W$$

where

$$\phi = -f^{-3/4} \frac{d^2}{dx^2}(f^{-1/4}) \quad .$$

If ϕ is neglected, (2.3) is a separable differential equation and the two independent solutions are $e^{\pm\eta}$. Noting that

$$\eta'(x) = (f(x))^{1/2}$$

and using the original variables, an approximation to ω of (2.1) is given by

$$(2.4) \qquad \omega \simeq Af^{-1/4}\exp\left(\int f^{1/2}dx\right) + Bf^{-1/4}\exp\left(-\int f^{1/2}dx\right)$$

where A and B are arbitrary constants. This approximation is called the WKB (in recognition of the works of Wentzel, Kramers, and Brillouin) approximation or Liouville-Green approximation. The functions

$$f^{-1/4}\exp\left(\int f^{1/2}dx\right)$$

and

$$f^{-1/4}\exp\left(-\int f^{1/2}dx\right)$$

are called LG (Liouville-Green) functions.

The accuracy of the approximation, of course, depends on the magnitude of ϕ. One obvious case where the approximation fails is when zeros of f lie in the interval over which the differential equation is posed.

This approximation will be used in the example section in Chapter 5 when considering the asymptotic behavior of the solution of a differential equation at infinity for the problems posed on the infinite interval $(0,\infty)$.

The indicial equation of a differential equation, also used in Chapter 5, will give, from the method of Frobenius, a series solution at singular points. The singular points of interest are $x = 0$ in the examples posed on $(0,\infty)$ and $x = a$ and $x = b$ on the interval (a,b).

Simmons [2] has the following discussion. Given the differential equation

$$-u''(x) + (g(x) - \lambda\rho(x))u(x) = 0 \quad , \tag{2.5}$$

the method of Frobenius gives, for a singular point at $x = a$,

$$u(x) = (x - a)^s \sum_{j=0}^{\infty} \gamma_j (x - a)^j \quad . \tag{2.6}$$

An assumption made is that $\gamma_0 \neq 0$ since another power of $x - a$ could have been incorporated in $(x - a)^s$ if $\gamma_0 = 0$.

Computing u" from (2.6), substituting that and (2.6) into (2.5), combining corresponding powers of $(x - a)$, and equating those to zero yields a system of equations, the first of which is

$$\gamma_0[s(s - 1) - (g_a - \lambda\rho_a)] = 0 \tag{2.7}$$

where

$$\begin{cases} g_a = \lim_{x\to a}(x - a)^2 g(x) \\ \\ \rho_a = \lim_{x\to a}(x - a)^2 \rho(x) \ . \end{cases} \tag{2.8}$$

The indicial equation is the bracketed piece of (2.7), that is,

$$s(s - 1) - (g_a - \lambda\rho_a) = 0 \ . \tag{2.9}$$

Once s has been calculated, (2.6) is the series solution of $u(x)$ near the singularity $x = a$.

Solving for the eigenvalues of Sturm-Liouville differential equations by the sinc-collocation method will be done by solving a generalized eigenvalue problem, that is,

$$A\vec{x} = \lambda B\vec{x} \tag{2.10}$$

where λ and $\vec{x} \neq \vec{0}$ are the eigenpair of A and B which are real, square matrices. This means that there exists a nonzero vector $\vec{x}$ if and only if there exists a number λ satisfying

(2.11) $\det[A - \lambda B] = 0$.

Hohn discusses this problem in [15] and included here are some ideas important to the development of this thesis.

Consider the case where A is a symmetric matrix and B is both symmetric and positive definite (these assumptions hold for all Sturm-Liouville problems in normal form for which the sinc-collocation method is applied). In this case, the generalized eigenvalue problem is equivalent to a regular eigenvalue problem. That is, there is a matrix W so that when

$$\det[W - \lambda I] = 0$$

is solved for λ, the same λ's will solve (2.10). These eigenvalues will all be real, since W is a symmetric matrix.

The details of the preceeding paragraph follow. Because B is symmetric, there exists an orthogonal matrix U such that

$$U^T B U = D(\mu)$$

where $D(\mu)$ is a diagonal matrix with diagonal elements μ_i, the eigenvalues of B. Since B is positive definite, $\mu_i > 0$ for all i. Put $R = D(\mu^{-\frac{1}{2}})$. Then

$$R^T(U^T B U)R = R^T D(\mu) R$$
$$= I .$$

Set S = UR. S is nonsingular since

$$\det S = \det(UR)$$

$$= \det U \cdot \det R$$

$$= \det U \left(\prod_{i=1}^{n} \mu_i^{-\frac{1}{2}} \right) \neq 0 \ .$$

This is nonzero because U is orthogonal ($U^T U = I$ implies $\det U^T \cdot \det U = 1$) and $\mu_i > 0$ for all i. Also

$$S^T B S = R^T (U^T B U) R$$

$$= I \ .$$

Because S is nonsingular, solving the generalized eigenvalue problem $\det[A - \lambda B] = 0$ is equivalent to $\det S^T[A - \lambda B]S = 0$. Then

$$\det[S^T A S - \lambda S^T B S]$$

$$= \det[W - \lambda I] = 0 \tag{2.12}$$

which is a regular eigenvalue problem with $W = S^T A S$.

To see that the eigenvalues of (2.12) are real, note that

$$(S^T A S)^T = S^T A^T (S^T)^T$$

$$= S^T A S$$

by the symmetry of A; hence, W is symmetric. Since $S^T A S$ is symmetric there exists an orthogonal matrix Q so that

$$Q^T (S^T A S) Q = D(\lambda)$$

where λ is in the spectrum of $S^T A S$, that is, $\lambda \in \sigma(S^T A S)$ and, equivalently, $\lambda \in \sigma(A)$.

$$(SQ)^T A (SQ) = D(\lambda)$$

and

$$(SQ)^T B (SQ) = Q^T (S^T B S) Q$$

$$= Q^T (I) Q = I \ .$$

Hence, there exists a matrix V = SQ that simultaneously diagonalizes A and B relative to conjugacy. That is,

(2.13) $V^T A V = D(\lambda)$

with the eigenvalues of A making up the matrix $D(\lambda)$ and

(2.14) $V^T B V = I$.

Finally, two theorems will be stated here, without proof, that will be needed later in the paper. They can be found in Parlett [16]. The Monotonicity Theorem gives bounds on the eigenvalues of the sum of two matrices.

Theorem 2.15: Monotonicity Theorem.
Let W = A + Y where W, A, and Y are all square, real, symmetric matrices. Let $\omega_i \in \sigma(W)$, $\alpha_i \in \sigma(A)$, and $y_i \in \sigma(Y)$ so that the eigenvalues are ordered, that is, for $i < j$, $\beta_i \leq \beta_j$ for $\beta = \omega, \alpha$, and y. Then

$$\alpha_1 + y_j \leq \omega_j \leq y_j + \alpha_n$$

and

$$y_1 + \alpha_j \leq \omega_j \leq \alpha_j + y_n \ .$$

The Courant-Fischer Max-Min Theorem gives the eigenvalues of the matrix A via the Rayleigh quotient.

Theorem 2.16: Courant-Fischer Max-Min Theorem
Let A be a symmetric, n x n matrix and $\alpha_i \in \sigma(A)$ such that for $i < j$, $\alpha_i \leq \alpha_j$. Then for $\vec{x} \neq \vec{0}$

$$\alpha_n = \max_{\vec{x}\in R^n} \frac{\vec{x}^T A\vec{x}}{\vec{x}^T\vec{x}} ,$$

$$\alpha_1 = \min_{\vec{x}\in R^n} \frac{\vec{x}^T A\vec{x}}{\vec{x}^T\vec{x}} ,$$

and

$$\alpha_k = \max_{R^{k-1}} \min_{\vec{x}\in R^{k-1}} \frac{\vec{x}^T A\vec{x}}{\vec{x}^T\vec{x}}$$

where R^{k-1} ranges over all (k - 1)-dimensional subspaces of R^n.

Many boundary value problems that describe physical phenomena satisfy a variational property. That is, a differential equation Au = f with specified boundary conditions can be solved by minimizing a functional of the form

$$F(u) = (Au,u) - 2(u,f)$$

where $(\cdot,\cdot)$ denotes an inner product. The variational property is fundamental to the Rayleigh-Ritz method of solving boundary value problems.

To carry out the Rayleigh-Ritz method, it is necessary to find the stationary values, or critical points, of the functional R[v]. The Rayleigh quotient is given by

$$(2.17) \qquad R[v] = \frac{a[v]}{b[v]} = \frac{\int_a^b \{(v')^2 + gv^2\}dx}{\lambda\int_a^b \rho v^2 dx}$$

for a differential equation of the form

$$-v'' + gv = \lambda\rho v$$

with appropriate boundary conditions. The stationary

values occur where the gradient of R vanishes. A suitable set of basis functions is chosen to approximate v in (2.17) and the result forms the approximate to the eigenvalue λ.

Equivalently, by the variational property, the differential equation can be solved. Minimize the Galerkin form

$$(2.18) \qquad \int_a^b [(v')^2 + gv^2]dx = \lambda \int_a^b \rho v^2 dx$$

with respect to a set of basis functions where an approximation to v is given by

$$(2.19) \qquad \tau(x) = \sum_{i=1}^{n} c_i \tau_i(x)$$

with $\{\tau_i\}_{i=1}^n$ the set of basis functions.

Both approaches, for the same choice of basis functions, yield the same matrix system $A\vec{x} = \lambda B\vec{x}$. They also involve integrations that usually require a numerical quadrature. When the differential equation is posed on an infinite interval the problem in general requires the truncation of the interval. For example, in the minimization of the Galerkin form for a problem on the interval $(0,\infty)$, the elements a_{ij} of A are

$$(2.20) \qquad a_{ij} = \int_0^K [c_i \tau_i'(x)\tau_j'(x) + g(x)c_i\tau_i(x)\tau_j(x)]dx$$

and the elements b_{ij} of B are

$$(2.21) \qquad b_{ij} = \int_0^K \rho(x) c_i \tau_i(x) \tau_j(x) dx$$

for fixed $K \in (0,\infty)$. For each particular $g(x)$ and $\rho(x)$ the truncation point K needs to be determined, and the numerical integrations need to be carried out. In the case where $g(x)$ and/or $\rho(x)$ are singular, a_{ij} and/or b_{ij} are singular integrals. This requires more computational work in constructing the entries of the matrices A and B.

CHAPTER 3

SINC-COLLOCATION METHOD

The sinc-collocation method applied to the calculation of eigenvalues of Sturm-Liouville problems depends on several aspects of the theory of sinc functions [17]. The development of the method begins with the sinc approximating formulas -- an interpolation formula and a quadrature rule for the entire real line. From these the method of conformal mappings allows a Sturm-Liouville problem on an arbitrary interval to be solved by the same basic method. From this development come the matrices of the sinc-collocation method.

The sinc function is defined by

$$\operatorname{sinc}(x) = \frac{\sin(\pi x)}{\pi x} \quad .$$

If f is defined over the whole real line, then for $h > 0$,

$$(3.1) \qquad C(f,h)(x) = \sum_{k=-\infty}^{\infty} f(kh)\operatorname{sinc}\left(\frac{x - kh}{h}\right)$$

is called the Whittaker cardinal expansion for f whenever the series converges. The properties of this expansion have been studied extensively by Stenger [17]. To use (3.1) as an approximation on $\mathbb{R}^1$, define

$$C_{M,N}(f,h)(x) = \sum_{k=-M}^{N} f(kh)\,\mathrm{sinc}\left(\frac{x - kh}{h}\right) .$$

The following definition and theorem are found in [17].

Definition 3.2: For $d > 0$, let $B(S)$ be the family of functions f that are analytic in the infinite strip $S = \{z \in C \mid |Imz| < d\}$ and satisfy

$$\int_{-d}^{d} |f(t + is)|\, ds \to 0 \quad \text{as} \quad t \to \pm\infty$$

and

$$N(f) = \lim_{s \to d^-} \int_{-\infty}^{\infty} (|f(t + is)|^2 + |f(t - is)|^2)dt < \infty .$$

Theorem 3.3: Assume $f \in B(S)$. If $h > 0$ and $\pi d/h > 1$, then

$$\left\| \frac{d^2 f}{dt^2} - \frac{d^2}{dt^2} C(f,h) \right\|_2 \leq \left(\frac{\pi}{h}\right)^2 \frac{N(f)}{\sinh(\pi d/h)} .$$

Since $$\frac{d^2}{dt^2}(C_{M,N}(f,h)(t)) = \sum_{k=-M}^{N} f(kh)\, \frac{d^2}{dt^2}\, \mathrm{sinc}\left(\frac{t - kh}{h}\right)$$

and if there exist positive constants C, α, and β so that

$$(3.4) \qquad |f(t)| \leq C \begin{cases} e^{\alpha t}, & t \in (-\infty, 0] \\ e^{-\beta t}, & t \in (0, \infty) \end{cases}$$

then

(3.5)

$$\left\| \frac{d^2 f}{dt^2} - \frac{d^2}{dt^2} C_{M,N}(f,h) \right\|_2 \leq \left(\frac{\pi}{h}\right)^2 \left\{ \frac{N(f)}{\sinh(\pi d/h)} + \frac{C}{5h}\left(\frac{e^{-\alpha h}}{\alpha} + \frac{e^{-\beta h}}{\beta}\right)\right\}.$$

For the selections $h = \left(\frac{\pi d}{\alpha M}\right)^{1/2}$ and $N = \left[\left[(\alpha/\beta)M\right]\right]$,

(3.6) $$\left\| \frac{d^2 f}{dt^2} - \frac{d^2}{dt^2} C_{M,N}(f,h) \right\|_2 \leq KM^{5/4} \exp(-(\pi d \alpha M)^{1/2})$$

where K depends on f and d.

Error bound theorems involving $C_{M,N}$ and $\frac{d}{dt}C_{M,N}$ also appear in [17]. However, for the method of this paper, those bounds are not necessary.

Many important examples are not posed on the whole real line. The following definition will allow a problem posed on an arbitrary interval in the complex plane to be mapped to the infinite strip S of Definition 3.2, thus allowing Theorem 3.3 to be used.

Definition 3.7: Let D be a simply-connected domain in the complex plane with boundary points a and b. For a given $d > 0$, let $\phi(z)$ be a conformal mapping of D onto S such that $\phi(a) = -\infty$ and $\phi(b) = \infty$. Define $\Gamma = \{\psi(\eta) : \eta \in R, -\infty < \eta < \infty\}$ where $\psi = \phi^{-1}$, $z_k = \psi(kh)$ for $k = 0, \pm 1, \pm 2, \ldots$, and $h > 0$. See Figure 1.

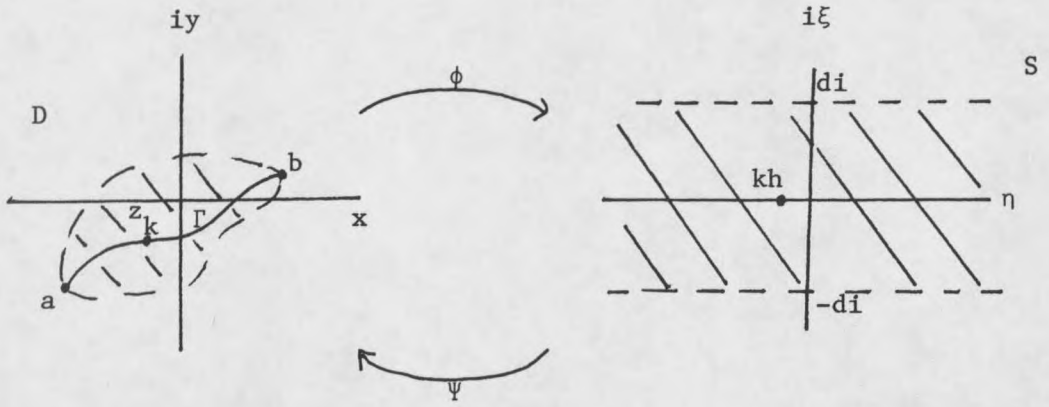

Figure 1: The Domain D and Strip S

The particular intervals of interest here are subsets of the real line. For the finite interval $(a,b) \subset \mathbb{R}$ an appropriate mapping ϕ is

$$\phi_1(x) = \text{An}\left(\frac{x - a}{b - x}\right) .$$

For the semi-infinite interval two maps will be considered. They are

$$\phi_2(x) = \text{An}(x)$$

and

$$\phi_3(x) = \text{An}\left(\sinh(x)\right) .$$

Figure 2 shows the domains mapped by these to the infinite strip.

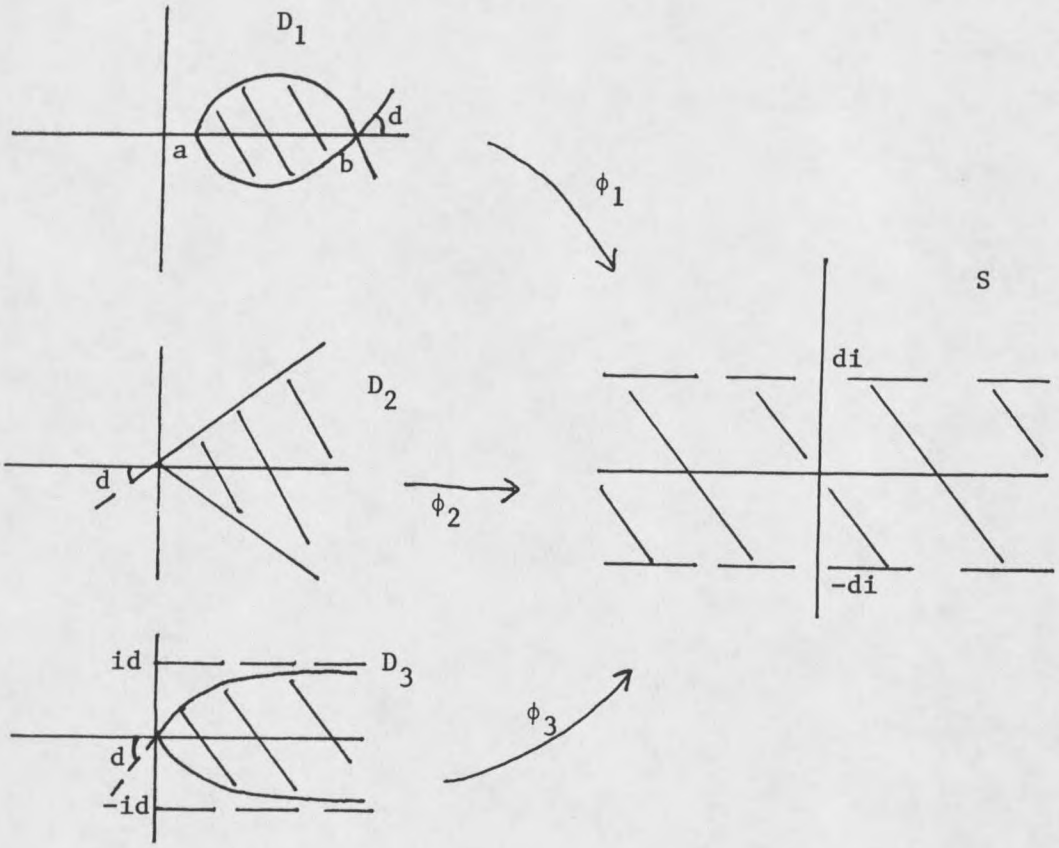

Figure 2: The Mappings ϕ_i and Their Domains

The procedure for choosing ϕ_2 or ϕ_3 is somewhat problem dependent and will be discussed in greater detail in Chapter 5.

It will be convenient to note here that for ϕ_1

$$z_k = \phi_1^{-1}(kh) = \frac{be^{kh} + a}{e^{kh} + 1},$$

for ϕ_2

$$z_k = \phi_2^{-1}(kh) = e^{kh},$$

and for ϕ_3

$$z_k = \phi_3^{-1}(kh) = \ln\left[e^{kh} + \sqrt{e^{2kh} + 1}\right].$$

Definition 3.8: Let d, ϕ, and ψ be as in Definition 3.7. Let B(D) denote the family of functions f that are analytic in D, a simply-connected domain in the complex plane, that satisfy

$$\int_{\psi(\eta+L)} |f(z)dz| \to 0 \quad \text{as} \quad \eta \to \pm\infty$$

where $L = \{i\xi \mid |\xi| < d\}$ and

$$N(f) \equiv \lim_{C\to\partial D} \inf_{C\subset D} \int_C |f(z)dz| < \infty . \tag{3.9}$$

The following theorem [17] gives a quadrature rule with error for functions which are elements of B(D).

Theorem 3.10: For $f \in B(D)$

$$\int_\Gamma f(z)dz - h \sum_{p=-\infty}^{\infty} \frac{f(z_p)}{\phi'(z_p)} = (i/2) \int_{\partial D} \frac{f(z)K(\phi,h)(z)}{\sin(\pi\phi(z)/h)}\, dz \tag{3.11}$$

where $K(\phi,h)(z) = \exp[(i\pi\phi(z))\,\mathrm{sgn}\,\mathrm{Im}(\phi(z))/h]$. Note that

$$|K(\phi,h)(z)| = \exp(-\pi d/h) \text{ for } z \in \partial D. \tag{3.12}$$

The quadrature rule given in Theorem 3.10 will be used in approximating inner products defined by

$$(r,s) = \int_\Gamma r(z)s(z)w(z)dz$$

where w(z) is a weight function and Γ is the curve given in Definition 3.7. The two specific inner products of interest here are $(u'', S_k \circ \phi)$ and $(gu, S_k \circ \phi)$ where

$$S_k \circ \phi(z) = \operatorname{sinc}\left[\frac{\phi(z) - kh}{h}\right] ,$$

with $\phi(z)$ being the conformal map in Definition 3.7 and g a function defined on Γ. Then, by two integrations by parts,

$$(u'', S_k \circ \phi) = \int_\Gamma u''(z) S_k \circ \phi(z) w(z) dz$$

$$= u'(z)[S_k \circ \phi(z)w(z)]\Big|_a^b - \int_\Gamma u'(z)[S_k \circ \phi(z)w(z)]' dz$$

$$= -u(z)[S_k \circ \phi(z)w(z)]'\Big|_a^b + u'(z)[S_k \circ \phi(z)w(z)]\Big|_a^b$$

$$+ \int_\Gamma u(z)[S_k \circ \phi(z)w(z)]'' dz$$

$$\equiv B_T + \int_\Gamma u(z)[S_k \circ \phi(z)w(z)]'' dz .$$

Note that if

$$u^{(1-j)}(z)[S_k \circ \phi(z)w(z)]^{(j)}\Big|_a^b = 0 \quad \text{for } j = 0,1,$$

then $B_T = 0$ and using (3.11)

$$(u'', S_k \circ \phi) = \int_\Gamma u(z)[S_k \circ \phi(z)w(z)]'' dz$$

$$= h \sum_{p=-\infty}^{\infty} \frac{u(z_p)[S_k \circ \phi(z)w(z)]''\Big|_{z=z_p}}{\phi'(z_p)} + E_1(u)$$

where

$$(3.13)\qquad E_1 = \left(i/2\right)\int_{\partial D} \frac{K(\phi,h)(z)u(z)[S_k \circ \phi(z)w(z)]''}{\sin(\pi\phi(z)/h)}\,dz\ .$$

The weight $w(z)$ must be chosen to force $B_T = 0$ and to bound $|E_1|$. Consider then the term $[S_k \circ \phi(z)w(z)]''$ in E_1.

$$\begin{aligned}[S_k \circ \phi(z)w(z)]'' &= [S_k \circ \phi(z)w'(z) + w(z)S_k' \circ \phi(z)\phi'(z)]' \\ &= S_k'' \circ \phi(z)(\phi'(z))^2 w(z) + S_k \circ \phi(z)w''(z) \\ &\quad + S_k' \circ \phi(z)(\phi'(z)w'(z) + (w(z)\phi'(z))')\ .\end{aligned}$$

For $w(z) = (\phi'(z))^{-1/2}$, the coefficient of $S_k' \circ \phi(z)$ is zero. As will be shown later, this choice of $w(z)$ will satisfy all the necessary properties, including $B_T = 0$. It also simplifies the inner product

$$\begin{aligned}(u'', S_k \circ \phi) &= h\sum_{p=-\infty}^{\infty} \frac{u(z_p)\left[S_k \circ \phi(z)(\phi'(z))^{-1/2}\right]''\Big|_{z=z_p}}{\phi'(z_p)} + E_1(u) \\ &= h\sum_{p=-\infty}^{\infty} u(z_p)\Big\{S_k'' \circ \phi(z_p)(\phi'(z_p))^{1/2} \\ &\quad + S_k \circ \phi(z_p)\frac{1}{\phi'(z_p)}\left((\phi'(z))^{-1/2}\right)''\Big|_{z=z_p}\Big\} + E_1(u) \\ &= \frac{1}{h}\sum_{p=-\infty}^{\infty} u(z_p)\delta_{kp}^{(2)}(\phi'(z_p))^{1/2} \\ &\quad + hu(z_k)\frac{1}{\phi'(z_k)}\left((\phi'(z))^{-1/2}\right)''\Big|_{z=z_k} + E_1(u)\end{aligned} \qquad (3.14)$$

where

$$(3.15)\qquad h^2 \frac{d^2}{d\phi^2}(S_k \circ \phi(z))\Big|_{z=z_p} = \delta_{kp}^{(2)} = \begin{cases} -\pi^2/3 & , \ p = k \\ \dfrac{-2(-1)^{p-k}}{(p-k)^2} & , \ p \neq k \end{cases}$$

and

$$(3.16)\qquad S_k \circ \phi(z_p) = \delta_{kp}^{(0)} = \begin{cases} 1 & , \ p = k \\ 0 & , \ p \neq k \end{cases}$$

by Stenger [17].

To bound the modulus of E_1, the following inequalities are needed:

$$\tfrac{1}{2}\left\| \left| \frac{\frac{d^2}{d\phi^2}(S_k \circ \phi(z))}{\sin(\pi\phi(z)/h)} \right| \right\|_{z\in\partial D} \leq \frac{\pi d + h \tanh\left(\frac{\pi d}{h}\right)}{\pi d^3 \tanh\left(\frac{\pi d}{h}\right)} + \frac{\pi}{2hd}$$

$$\equiv C_2(h,d)$$

and

$$(3.17)\qquad \tfrac{1}{2}\left\| \left| \frac{S_k \circ \phi(z)}{\sin(\pi\phi(z)/h)} \right| \right\|_{z\in\partial D} \leq \frac{h}{2\pi d} \equiv C_0(h,d)$$

also from Stenger [17]. Now consider

$$|E_1(u)| =$$

$$\frac{i}{2}\int_{\partial D} \frac{K(\phi,h)(z)u(z)\left\{S_k'' \circ \phi(z)(\phi'(z))^{3/2} + \dfrac{S_k \circ \phi(z)}{((\phi'(z))^{1/2})''}\right\}}{\sin(\pi\phi(z)/h)} dz$$

$$\leq e^{-\pi d/h}\left\{C_2(h,d)N(u(\phi')^{3/2}) + C_0(h,d)N\left(u\left((\phi')^{-1/2}\right)''\right)\right\}$$

where $N(f)$ is as in (3.9) and the bound on $K(\phi,h)$ is as in (3.12).

For the other inner product of interest, with $w(z) = (\phi'(z))^{-1/2}$,

$$(gu,\ S_k \circ \phi) = h \sum_{p=-\infty}^{\infty} \frac{g(z_p)u(z_p)S_k \circ \phi(z_p)}{(\phi'(z_p))^{3/2}} + E_2(gu)$$

(3.18)

$$= h\, \frac{g(z_k)u(z_k)}{(\phi'(z_k))^{3/2}} + E_2(gu)$$

by (3.11) and (3.16) where

(3.19)

$$E_2(gu) = \frac{i}{2} \int_{\partial D} \frac{g(z)u(z)K(\phi,h)(z)S_k \circ \phi(z)(\phi'(z))^{-1/2}}{\sin(\pi\phi(z)/h)}\, dz\ .$$

Bounding the modulus of E_2 gives

(3.20) $\quad |E_2| \le e^{-\pi d/h}\, C_0(h,d)N(gu(\phi')^{-1/2})$

by (3.9), (3.12), and (3.17).

Truncating the sum in (3.14) leads to the matrices of the method. Bounding the error, denoted here by T, caused by this truncation will be discussed in Chapter 4. Letting $p = -M, \ldots, N$ (3.14) becomes

$$(u'',\ S_k \circ \phi) = \frac{1}{h} \sum_{p=-M}^{N} u(z_p)\delta_{kp}^{(2)}(\phi'(z_p))^{1/2}$$

$$+ h\, u(z_k)\, \frac{1}{\phi'(z_k)}\, ((\phi'(z))^{-1/2})'' \Big|_{z = z_k}$$

$$+ E_1(u) + T.$$

Letting k run from -M to N and ignoring the errors, the inner product becomes, in matrix form,

$$\left\{\frac{1}{h}\, I^{(2)}\, D(\sqrt{\phi'}) + hD\left(\frac{1}{\phi'}\left((\phi')^{-1/2}\right)''\right)\right\}\vec{u}$$

where D(r) denotes a diagonal matrix of dimension m x m where $m = M + N + 1$ with the (i,i)-th element given by $r(z_i)$. The matrix $\vec{u}$ is of dimension m x 1 with ith element $u(z_i)$. Finally, the matrix $I^{(2)}$ has the same dimension as the diagonal matrix with the (k,p)-th element given by $\delta_{kp}^{(2)}$ in (3.15). Explicitly this is

$$I^{(2)} = \begin{bmatrix} \pi^2/3 & \frac{-2}{1^2} & \frac{2}{2^2} & \cdots & (-1)^{m-1}\frac{2}{(m-1)^2} \\ \frac{-2}{1^2} & \pi^2/3 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & \frac{-2}{1^2} \\ (-1)^{m-1}\frac{2}{(m-1)^2} & & & \frac{-2}{1^2} & \pi^2/3 \end{bmatrix}.$$

This matrix is symmetric, negative definite, with all its eigenvalues lying in the open interval $(-\pi^2,0)$ [17]. It is also a Toeplitz matrix, that is, a matrix with all diagonals constant.

The matrix describing $(gu, S_k \circ \phi)$ in (3.18) is a diagonal matrix of dimension m x m given by $hD\left(\frac{gu}{(\phi')^{3/2}}\right)$. Notice that with (3.16) no truncation error is incurred in this inner product.

CHAPTER 4

ERROR OF SINC-COLLOCATION METHOD

Most numerical methods used to approximate the eigenvalues of Sturm-Liouville problems lead to a discrete system $A\vec{u} = \lambda B\vec{u}$. The same is true for the sinc-collocation method. This section carries out the convergence analysis for the sinc-collocation method of the eigenvalue approximation. A standard proof of convergence for other numerical methods, in particular, finite differences [3], involves $\|B^{-1}\|$ and the norm of the local truncation error. The method often cannot be applied when the original problem is singular and $\|B^{-1}\|$ is not uniformly bounded. The analysis for the sinc-collocation method is valid whether the Sturm-Liouville problem is regular or singular.

The form of the differential equation considered here is the normal form given by

$$(4.1) \qquad \begin{cases} -u''(x) + g(x)u(x) = \lambda\rho(x)u(x) \\ u(a) = u(b) = 0 \end{cases}$$

It will be convenient to transform (4.1) to a differential equation on the whole real line by using the change of variable

$$\omega(t) = (u\sqrt{\phi'}) \circ \psi(t)$$

where ϕ and ψ are as described in Definition 3.7. To

simplify the transformation several steps will be used. Let

$$u(x) = \omega(x)(\phi'(x))^{-\frac{1}{2}} \quad (4.2)$$

Then

$$u'(x) = \omega'(x)(\phi'(x))^{-\frac{1}{2}} + \omega(x)((\phi'(x))^{-\frac{1}{2}})'$$

and

$$u''(x) = \omega''(x)(\phi'(x))^{-\frac{1}{2}} + 2\omega'(x)\left((\phi'(x))^{-\frac{1}{2}}\right)' + \omega(x)\left((\phi'(x))^{-\frac{1}{2}}\right)'' .$$

Replacing the above statements in (4.1) yields

$$-\omega''(x) - 2\omega'(x)(\phi'(x))^{\frac{1}{2}}\left((\phi'(x))^{-\frac{1}{2}}\right)' + \omega(x)\left\{ g(x) - (\phi'(x))^{\frac{1}{2}}\left((\phi'(x))^{-\frac{1}{2}}\right)''\right\} = \lambda\rho(x)\omega(x) . \quad (4.3)$$

Given $\omega \in B(S)$ in Definition 3.2, let ω satisfy the bounds in (3.4). Using the change of variable (4.2) in the form $\omega(x) = u(x)\sqrt{\phi'(x)}$, (3.4) takes the form

$$|\omega(x)| = |u(x)\sqrt{\phi'(x)}| \le C \begin{cases} e^{-\alpha|\phi(x)|} & x \in \Gamma_a \\ e^{-\beta|\phi(x)|} & x \in \Gamma_b \end{cases} \quad (4.4)$$

where $\Gamma_a = \{\psi(t): \ t \in (-\infty, 0]\}$

and $\Gamma_b = \{\psi(t): \ t \in (0, \infty)\}$.

Hence the boundary conditions in (4.1) can be seen to be

$$\lim_{t\to\pm\infty} \omega(t) = 0 . \quad (4.5)$$

Let $x = \psi(t)$ which implies $t = \phi(x)$. Then

$$\frac{d\omega}{dx} = \frac{d\omega}{dt}\frac{dt}{dx} = \omega'(t)\phi'(x)$$

and

$$\frac{d^2\omega}{dx^2} = \frac{d}{dx}\,(\omega'(t)\phi'(x))$$

$$= \omega'(t)\phi''(x) + \omega''(t)(\phi'(x))^2 \ .$$

Now (4.3) becomes

$$(4.6)\qquad -\omega''(t) - \omega'(t)\left\{\frac{\phi''(x)}{(\phi'(x))^2} + 2(\phi'(x))^{-1/2}\left((\phi'(x))^{-1/2}\right)'\right\}$$

$$+ \omega(t)\left\{\frac{g(x)}{(\phi'(x))^2} - (\phi'(x))^{-3/2}\left((\phi'(x))^{-1/2}\right)''\right\}$$

$$= \lambda\,\frac{\rho(\psi(t))}{(\phi'(x))^2}\,\omega(t) \ .$$

A short computation shows that the coefficient of $\omega'(t)$ is zero. Using the fact that

$$\phi'(x) = \frac{1}{\psi'(\phi(x))} = \frac{1}{\psi'(t)}$$

in (4.6) yields

$$(4.7)\qquad L\omega = -\omega''(t) + \omega(t)\gamma_g(t) = \lambda\rho(\psi(t))(\psi'(t))^2\omega(t)$$

for

$$(4.8)\qquad \gamma_g(t) = g(\psi(t))(\psi'(t))^2 - (\psi'(t))^{3/2}\left(\sqrt{\psi'(t)}\right)'' \ .$$

Define an approximation to $\omega(t)$ by

$$(4.9)\qquad C_M(\omega,h)(t) \equiv C_{M,M}(\omega,h)(t) = \sum_{k=-M}^{M} \omega(kh)S_k(t) \ .$$

It is not necessary to define the approximation to be a centered sum, that is, a sum which goes from -M to M. In fact, the computations of Chapter 5 will show that noncentered sums can give the accuracy desired with less

summands. It is for simplicity of notation that centered sums are used in the present section.

Substituting (4.9) into (4.7) yields

$$LC_M(\omega,h)(jh) = -\sum_{k=-M}^{M} \frac{1}{h^2}\,\delta_{jk}^{(2)}\omega(kh) + \gamma_g(jh)\omega(jh)$$

$$= \lambda\rho(\psi(jh))(\psi'(jh))^2\omega(jh)$$

for $j = -M, \ldots, M$ and $\delta_{jk}^{(2)}$ as in (3.15). The matrix form for the sinc-collocation method is then given by

(4.10) $$L\vec{C}_M(\omega,h) = A\vec{\omega} = \lambda B\vec{\omega}$$

where $$A = -\frac{1}{h^2}\,I^{(2)} + D(\gamma_g)\ ,$$

$$B = D(\rho(\psi')^2)\ ,$$

and $$\vec{\omega} = [\omega(-Mh),\ \omega((-M+1)h),\ \ldots,\ \omega(Mh)]^T\ .$$

The diagonal matrices and $I^{(2)}$ are as described in Chapter 3, and all are of dimension $2M + 1$ by $2M + 1$.

The equation in (4.10) gives the method of computing the eigenvalues of the Sturm-Liouville problem described by (4.7) and (4.5). Even though the problem has been translated, the eigenvalues computed are the same as in the original problem (4.1).

To develop the error in using (4.10) to approximate the eigenvalues, assume for given ψ and g

(4.11) $$\gamma_g(t) \geq (\delta(g,\psi,h))^{-1} \equiv \delta^{-1} > 0 \quad \text{for } t \in (-\infty,\infty)\ .$$

The example section, Chapter 5, will say more about this assumption; but, in particular, on a finite interval, (4.11) holds for $g(x) > 0$ on the interval. Using the fact

that $-I^{(2)}$ is symmetric, $D(\gamma_g)$ is diagonal, and Theorem 2.15

$$\begin{aligned} a_m &\equiv \min_{a_j \in \sigma(A)} \{a_j\} \\ &\geq \min_{p_j \in \sigma((-1/h^2)I^{(2)})} \{p_j\} + \min_{d_j \in \sigma(D(\gamma_g))} \{d_j\} \\ &\geq 0 + \delta^{-1} = \delta^{-1} \end{aligned} \tag{4.12}$$

Assume, also, that λ_0 and ω_0 are an eigenpair to (4.7) with ω_0 normalized by

$$\int_{-\infty}^{\infty} \omega_0^2(t)\rho(\psi(t))(\psi'(t))^2 dt = 1 \tag{4.13}$$

which is equivalent to

$$\int_a^b u_0^2(x)\rho(x)dx = 1 \tag{4.14}$$

for u_0 a solution to (4.1). This is possible since by Sturm-Liouville theory the eigenfunctions are orthogonal with respect to ρ. This normalization of the eigenfunction will be used, for convenience, for the remainder of the section.

Substitute ω_0 into (4.7) and evaluate at $t = jh$ for $j = -M, \ldots, M$, to get

$$L\vec{\omega}_0 = \lambda_0 D(\rho(\psi(jh))(\psi'(jh))^2)\vec{\omega}_0 .$$

Subtracting the above equation from (4.10) yields

$$\begin{aligned} \Delta\vec{\omega}_0 \equiv L\vec{C}_M(\omega_0,h) - L\vec{\omega}_0 &= A\vec{\omega}_0 - \lambda_0 \mathcal{D}^2\vec{\omega}_0 \\ &= (A - \lambda_0 \mathcal{D}^2)\vec{\omega}_0 \end{aligned}$$

where $\mathcal{D} = D(\sqrt{\rho}\psi')$. By the assumption (4.11), (4.12)

guarantees that A is positive definite and by observation $\mathcal{D}^2$ is positive definite. Hence by (2.13) and (2.14) there exist vectors $\vec{z}_i$ and positive eigenvalues $\mu_i \le \mu_j$ for $-M \le i \le j \le M$ so that

$$Z^T A Z = D(\mu) \tag{4.15}$$

and

$$Z^T \mathcal{D}^2 Z = I \tag{4.16}$$

for $Z = [\vec{z}_{-M}\ \vec{z}_{-M+1} \cdots \vec{z}_M]$,

and

$$A\vec{z}_i = \mu_i \mathcal{D}^2 \vec{z}_i \quad \text{for } i = -M, \ldots, M . \tag{4.17}$$

Since $(\vec{z}_i)_{i=-M}^{M}$ are linearly independent, there are constants β_i so that

$$\vec{\omega}_0 = \sum_{i=-M}^{M} \beta_i \vec{z}_i \tag{4.18}$$

which implies

$$\Delta\vec{\omega}_0 = (A - \lambda_0 \mathcal{D}^2) \sum_{j=-M}^{M} \beta_j \vec{z}_j$$

$$= \sum_{j=-M}^{M} \beta_j A\vec{z}_j - \sum_{j=-M}^{M} \lambda_0 \beta_j \mathcal{D}^2 \vec{z}_j$$

$$= \sum_{j=-M}^{M} \beta_j \mu_j \mathcal{D}^2 \vec{z}_j - \sum_{j=-M}^{M} \lambda_0 \beta_j \mathcal{D}^2 \vec{z}_j \quad \text{by (4.17)}$$

$$= \sum_{j=-M}^{M} \beta_j (\mu_j - \lambda_0) \mathcal{D}^2 \vec{z}_j .$$

Then

$$(4.19) \qquad \vec{z}_i^T \Delta\vec{\omega}_0 = \beta_i(\mu_i - \lambda_0)\vec{z}_i^T \mathcal{D}^2 \vec{z}_i$$
$$= \beta_i(\mu_i - \lambda_0) \qquad \text{by (4.16)} .$$

The following lemmas are needed.

Lemma 4.20: Assume $\omega_0^2 \rho(\psi')^2 \in B(S)$. Then for

$$h = \left(\frac{\pi d}{\alpha M}\right)^{1/2} ,$$

$$|\beta_p| \equiv \max_{-M \le i \le M} |\beta_i| \ge (2(2M + 1)h)^{-1/2} .$$

Proof: Apply $\mathcal{D}^2$ to both sides of (4.18) yielding

$$\mathcal{D}^2\vec{\omega}_0 = \sum_{i=-M}^{M} \beta_i \mathcal{D}^2 \vec{z}_i .$$

Then

$$\|\mathcal{D}\vec{\omega}_0\|_2^2 = \mathcal{D}\vec{\omega}_0 \cdot \mathcal{D}\vec{\omega}_0$$
$$= \vec{\omega}_0 \cdot \mathcal{D}^T\mathcal{D}\vec{\omega}_0$$
$$= \vec{\omega}_0 \cdot \mathcal{D}^2\vec{\omega}_0$$
$$= \sum_{j=-M}^{M} \sum_{i=-M}^{M} \beta_j \vec{z}_j^T(\beta_i \mathcal{D}^2 \vec{z}_i) \qquad \text{(using 4.18)}$$
$$= \sum_{j=-M}^{M} \beta_j^2 \qquad \text{by (4.16)}$$
$$\le (2M + 1)\beta_p^2$$

where $|\beta_p| \equiv \max_{-M \le i \le M} |\beta_i| .$

Applying (3.11) to (4.14) gives

$$(4.21)\qquad 1 = h \sum_{p=-\infty}^{\infty} \frac{u_0^2(z_p)\rho(z_p)}{\phi'(z_p)}$$

$$+ \frac{i}{2} \int_{\partial D} \frac{u_0^2(z)\rho(z)K(\phi,h)(z)}{\sin(\pi\phi(z)/h)}\, dz$$

$$= h \sum_{p=-M}^{M} \frac{u_0^2(z_p)\rho(z_p)}{\phi'(z_p)} + TE + IE$$

where TE is the error created when truncating the sum and IE is the integral error.

Using the variable change $\omega_0 = (u_0\sqrt{\phi'}) \circ \psi$, by hypothesis $u_0^2\rho \in B(D)$. Then in an argument analogous to (3.19) and (3.20), $|IE| = O(e^{-2\pi d/h})$. Hence, as M gets larger IE goes to zero, and necessarily TE must also go to zero since the right-hand side of (4.21) is equal to 1. Therefore, letting $\varepsilon = TE + IE$, $\varepsilon \to 0$ as $M \to \infty$.

Now use the variable change to rewrite (4.21) as

$$1 = h \sum_{p=-M}^{M} \frac{u_0^2(z_p)\rho(z_p)}{\phi'(z_p)} + \varepsilon$$

$$= h \sum_{p=-M}^{M} \omega_0^2(t_p)\rho(\psi(t_p))(\psi'(t_p))^2 + \varepsilon$$

$$= h\|\mathcal{D}\vec{\omega}_0\|_2^2 + \varepsilon$$

$$\leq h\|\mathcal{D}\vec{\omega}_0\|_2^2 + \tfrac{1}{2}$$

for M sufficiently large. Then

$$(4.22)\qquad \|\mathcal{D}\vec{\omega}_0\|_2^2 \geq 1/h - 1/2h = 1/2h$$

Finally,

$$1/2h \le \|\mathcal{D}\vec{\omega}_0\|_2^2 \le (2M + 1)\beta_p^2$$

and $$|\beta_p| \ge (2(2M + 1)h)^{-\frac{1}{2}} .$$

Lemma 4.23: Let $\mu_j > 0$ and $\vec{z}_j$ for $j = -M, \ldots, M$ be from (4.16). If $\gamma_g(t) \ge \delta^{-1} > 0$, then for all $j = -M, \ldots, M$

$$\|\vec{z}_j\|_2^2 \le \delta\mu_j .$$

Proof: Using (4.12), (4.15), and Theorem 2.16

$$\delta^{-1} \le \min_{a_j \in \sigma(A)} \{a_j\}$$

$$= \min_{\vec{x} \in R^{2M+1}} \frac{\vec{x}^T A\vec{x}}{\vec{x}^T\vec{x}}$$

$$\le \frac{\vec{z}_j{}^T A\vec{z}_j}{\vec{z}_j{}^T\vec{z}_j} = \frac{\vec{z}_j{}^T A\vec{z}_j}{\|\vec{z}_j\|_2^2} = \frac{\mu_j}{\|\vec{z}_j\|_2^2} .$$

Then $$\|\vec{z}_j\|_2^2 \le \delta\mu_j \quad \text{for each } j = -M, \ldots, M.$$

The following theorem gives the error in approximating the eigenvalues of (4.7).

Theorem 4.24: Assume λ_0 and ω_0 is an eigenpair of $A\vec{\omega} = \lambda B\vec{\omega}$, $\omega_0 \in B(s)$, ω_0 satisfies (3.4), and μ_p is the pth eigenvalue of (4.17). If $|\beta_p| = \max_{-M \le i \le M} |\beta_i|$, $|\mu_p - \lambda_0| \le \lambda_0$, and $h = (\pi d/\alpha M)^{\frac{1}{2}}$, then

$$|\mu_p - \lambda_0| \le 2\{((2M + 1)h)^{\frac{1}{2}}|\cos\theta_p|\}\sqrt{\delta\lambda_0}\,\|\Delta\vec{\omega}_0\|^2$$

with θ_p the angle between $\vec{z}_p$ and $\Delta\vec{\omega}_0$.

Proof: From (4.19)

$$|\vec{z}_p{}^T \Delta\vec{\omega}_0| = |\beta_p||\mu_p - \lambda_0|$$

and $$|\vec{z}_p{}^T \Delta\vec{\omega}_0| = |\Delta\vec{\omega}_0 \cdot \vec{z}_p|$$

$$= \|\Delta\vec{\omega}_0\|_2 \, \|\vec{z}_p\|_2 \, |\cos\theta_p| \ .$$

This implies

$$|\mu_p - \lambda_0| = \frac{\|\Delta\vec{\omega}_0\|_2 \, \|\vec{z}_p\|_2 \, |\cos\theta_p|}{|\beta_p|} \ .$$

Now $\mu_p = \mu_p - \lambda_0 + \lambda_0 \leq |\mu_p - \lambda_0| + \lambda_0 \leq 2\lambda_0$, then $\|\vec{z}_p\|_2^2 \leq \delta\mu_p \leq 2\delta\lambda_0$ by Lemma 4.23.

Finally,

$$|\mu_p - \lambda_0| \leq \frac{\|\Delta\vec{\omega}_0\|_2 \sqrt{2\delta\lambda_0} \, |\cos\theta_p|}{|\beta_p|}$$

$$\leq 2\{((2M + 1)h)^{1/2}|\cos\theta_p|\}\sqrt{\delta\lambda_0} \, \|\Delta\vec{\omega}_0\|_2 \ .$$

Corollary 4.25: Assume ω_0 satisfies the hypotheses of Theorem 3.3. If $|\beta_p| = \max_{-M\leq i\leq M} |\beta_i|$ and $|\mu_p - \lambda_0| \leq \lambda_0$, then $|\mu_p - \lambda_0| \leq K\sqrt{\delta\lambda_0} \ M^{3/2} \exp(-(\pi d\alpha M)^{1/2})$ where K depends on ω_0 and d.

Proof: Using

$$\Delta\vec{\omega}_0 = L\vec{C}_M(\omega_0,h) - L\vec{\omega}_0 \text{ and } S_k(jh) = \delta_{jk}^{(0)} \ ,$$

$$|\Delta\vec{\omega}_0| = |L\vec{C}_M(\omega_0,h) - L\vec{\omega}_0|$$

$$= |-\frac{1}{h^2} \sum_{k=-M}^{M} \delta_{jk}^{(2)}\omega_0(kh) + \gamma_g(jh)\omega_0(jh)$$

(4.26) $$+ \omega_0''(jh) - \gamma_g(jh)\omega_0(jh)|$$

$$= \left| - \frac{d^2}{dt^2} C_M(\omega_0,h)(jh) + \omega_0''(jh) \right|$$

$$= \left| \frac{d^2}{dt^2} C_M(\omega_0,h)(t) - \frac{d^2}{dt^2} \omega_0(t) \right|_{t=jh} .$$

Letting $h = (\pi d/\alpha M)^{1/2}$, (3.6) and (4.26) yield

(4.27) $\quad \|\Delta\vec{\omega}_0\|_2 \leq K'M^{5/4} \exp(-(\pi d\alpha M)^{1/2})$.

Replacing h by $(\pi d/\alpha M)^{1/2}$, $|\cos\theta_p|$ by 1, and $\|\Delta\vec{\omega}_0\|_2$ by (4.27), the conclusion of Theorem 4.24 gives

$$|\mu_p - \lambda_0| \leq 2\{(2M+1)^{1/2}(\pi d/\alpha M)^{1/4}\}\sqrt{\delta\lambda_0}\, K'M^{5/4} \exp(-(\pi d\alpha M)^{1/2})$$

$$\leq 2\{\sqrt{3}\, M^{1/2}(\pi d/\alpha M)^{1/4}\}\sqrt{\delta\lambda_0}\, K'M^{5/4} \exp(-(\pi d\alpha M)^{1/2})$$

$$\leq KM^{3/2} \sqrt{\delta\lambda_0} \exp(-(\pi d\alpha M)^{1/2}) .$$

It should be noted that if $|\mu_p - \lambda_0| > \lambda_0$, then

$$\mu_p = \mu_p - \lambda_0 + \lambda_0 \leq |\mu_p - \lambda_0| + \lambda_0$$

$$\leq 2|\mu_p - \lambda_0|$$

and $\quad \|\vec{z}_p\|_2^2 \leq 2\delta|\mu_p - \lambda_0|$ $\quad$ in Theorem 4.24.

This leads to

(4.28) $\quad |\mu_p - \lambda_0| \leq KM^{3/2} \sqrt{\delta|\mu_p - \lambda_0|} \exp(-(\pi d\alpha M)^{1/2})$

as the conclusion of Corollary 4.25. As $M \to \infty$, $|\mu_p - \lambda_0| \to 0$; so for M sufficiently large, Corollary 4.25 is applicable. As it turns out, for the examples which follow, M = 2 is sufficiently large.

Note that in the conclusion to Corollary 4.25, the eigenvalue itself is part of the error bound. This indicates that as the eigenvalues get larger, the accuracy

of the method decreases. This can be seen in the examples in Chapter 5.

The above discussion contained in this chapter developed the sinc-collocation method. It is a consequence of the inner product approximation that the preceeding method is equivalent to the sinc-collocation method for calculating the eigenvalues of (4.1).

To see this equivalency, consider orthogonalizing the residual

$$
\begin{aligned}
0 &= (Lu - \lambda\rho u,\ S_k \circ \phi) \\
&= -(u'',\ S_k \circ \phi) + (gu,\ S_k \circ \phi) - (\lambda\rho u,\ S_k \circ \phi) \\
&= -\frac{1}{h} \sum_{p=-M}^{M} u(z_p)\delta_{kp}^{(2)}(\phi'(z_p))^{1/2} \qquad (4.29) \\
&\quad - hu(z_k)\ \frac{1}{\phi'(z_k)}\left((\phi'(z))^{-1/2}\right)''\Big|_{z=z_k} \\
&\quad + h\ \frac{g(z_k)u(z_k)}{(\phi'(z_k))^{3/2}} - \lambda h\ \frac{\rho(z_k)u(z_k)}{(\phi'(z_k))^{3/2}} \\
&\quad + E_1(u) + E_2(gu) + E_3(\lambda\rho u) + T
\end{aligned}
$$

from (3.14) and (3.18). Dropping the error terms and identifying the matrix system yields

$$
\left\{ -\frac{1}{h}\, I^{(2)} D((\phi')^{1/2}) - hD\left(\frac{1}{\phi'}\ ((\phi')^{-1/2})''\right) \right\} \vec{u} + hD\left(\frac{g}{(\phi')^{3/2}}\right)\vec{u}
$$

$$
= \lambda hD\left(\frac{\rho}{(\phi')^{3/2}}\right)\vec{u}\ .
$$

Consolidating terms and factoring out $D((\phi')^{1/2})$, yields

$$\left\{ -\frac{1}{h} I^{(2)} + hD\left(\frac{g}{(\phi')^2} - \frac{1}{(\phi')^{3/2}} \left((\phi')^{-1/2} \right)'' \right) \right\} D((\phi')^{1/2})\vec{u}$$

$$= \lambda hD\left(\frac{\rho}{(\phi')^2} \right) D((\phi')^{1/2})\vec{u} \ ,$$

the same system as given in (4.10). The error terms of (4.29) will be used in Chapter 5 to choose the parameters in the implementation of the method.

CHAPTER 5

NUMERICAL RESULTS AND COMPARISONS

The construction of the sinc-collocation system in (4.10) depends on the selection of the parameters h, M, N, and the conformal map ϕ_i, i = 1,2,3, from Figure 1. The map ϕ_i is determined by the interval on which the problem is posed. In problems posed on the semi-infinite interval $(0,\infty)$, there is a choice of whether to use ϕ_2 or ϕ_3 depending on the asymptotic behavior of the solution of the differential equation. The parameters h, M, and N are constants determined by the α and β in (4.4). In particular the exact form of (4.4) is exhibited for each mapping ϕ_i. Combining the appropriate form of (4.4) with (2.9) allows, in general, the choices of h, M, and N to be made so that the error terms of (4.29) are asymptotically balanced.

Following these general considerations the numerical performance of the method will be discussed with a number of examples. These examples have been selected for several reasons. Foremost, the accuracy and simplicity of the discrete system (4.10) for a given problem is shown. Looking at Examples 5.1-5.6, one can see that in passing from one Sturm-Liouville problem to another, the only

changes in the discrete system are two diagonal matrices. Moreover, these changes require no quadratures. They are based solely on a change of nodes (due to an interval change) and different point evaluations (for a function change). Algorithmically, this is a great beauty of the method when several Sturm-Liouville problems are to be considered. This can be clearly seen when contrasting the sinc-collocation method to the Rayleigh-Ritz method discussed in Chapter 2. The intimate connection between the Galerkin and collocation methods using the sinc basis, as described in Chapter 4, indicates that greater accuracy (typically associated with the Galerkin approach) is not sacrificed for simplicity (commonly found with collocation). Figure 3 is included to show the pieces necessary to implement the method for the mappings ϕ_i, $i = 1,2,3$.

A second criteria by which the examples were chosen is to highlight and extend the implementation of (4.10) and illustrate a possible way to make the error bound of Theorem 4.24 sharper. Several assumptions are made in the groundwork of Theorem 4.24. The function g(x) is assumed to be nonnegative, but the Chebyshev Example 5.5 will show in detail that on a finite interval this assumption can be modified and Theorem 4.24 is still applicable. Bessel's equation in Example 5.4 describes the procedure in finding the parameters h, M, and N by referring to the actual error

terms of the method in (4.29). Example 5.2, the Wood-Saxon potential, shows as a consequence of numerical experimentation a case where more accurate results were achieved when the error terms of (4.29) were not asymptotically balanced.

For each of the Examples 5.1-5.6 the asymptotic error rate AER = $\exp(-(\pi d\alpha M)^{1/2})$ is exhibited. In passing from Theorem 4.24 to Corollary 4.25, $|\cos\theta_p|$ was bounded by 1 (recall that θ_p is the angle between $\vec{z}_p$ and $\Delta\vec{\omega}_p$). That this angle may aid in convergence is demonstrated in Tables 1 and 18. To illustrate this idea, Table 18 will include the asymptotic error bound as well as the error bound that results when $|\cos\theta_p|$ is not replaced by 1. However, when considering Table 10, the asymptotic error rate seems to be a fairly "sharp" bound. There has been no success in determining the behavior of θ_p in general. Consequently, without further assumptions, the asymptotic error rate cannot be improved in Corollary 4.25.

The third criteria for choosing particular examples is incorporated into the third section of Chapter 5. This section compares the results of this thesis on several examples with that of other authors who used well-known methods such as finite elements and spectral methods. Comparisons will be made on the size of systems needed to attain comparable accuracy and the amount of work necessary to build the matrix systems. The harmonic oscillator and

Wood-Saxon potentials will be compared with the Rayleigh-Ritz method of Botha and Schoombie [10]. Birkoff, DeBoor, Swartz, and Wendroff [8] apply the Rayleigh-Ritz method to Mathieu's equation. The tau method of Gottlieb and Orszag [4] will be used to do a comparison with Bessel's equation. Although the sinc-collocation method did not always "beat" the compared methods, the sinc method was applicable to the differential equation (4.1) independent of singularities of the solution and the interval on which it was posed. This is another beauty of the sinc-collocation method. Other methods cannot always be used in their standard form and need to be revised to be applied to singular problems and/or problems on an infinite interval to maintain their "nice" qualities.

$$A = -\frac{1}{h^2} I^{(2)} + D\left(\frac{-1}{(\phi')^{3/2}}\left(\frac{1}{\sqrt{\phi'}}\right)'' + \frac{g}{(\phi')^2}\right)$$

$$A\bar{z} = \mu \mathcal{D}^2 \bar{z} \ , \quad \mathcal{D} = D(\sqrt{\rho}/\phi')$$

Interval	ϕ	$(\phi')^{-1}$	$-(\phi')^{-3/2}((\phi')^{-1/2})''$	x_k
(a,b)	$\phi_1(x) = \log\left(\frac{x-a}{b-x}\right)$	$\frac{(x-a)(b-x)}{b-a}$	$\frac{1}{4}$	$\frac{be^{kh}+a}{e^{kh}+1}$
$(0,\infty)$	$\phi_2(x) = \log(x)$	x	$\frac{1}{4}$	e^{kh}
$(0,\infty)$	$\phi_3(x) = \log(\sinh(x))$	$\tanh(x)$	$\frac{4\cosh^2 x - 3}{4\cosh^4 x}$	$\log[e^{kh}+\sqrt{e^{2kh}+1}]$

Figure 3: Discrete System Used to Compute the Approximate Eigenvalues for (4.1)

Numerical Implementation

The parameter selections given just before (3.6), that is

$$h = (\pi d/(\alpha M))^{1/2} \tag{5.1}$$

and

$$N = \left[\left[\left(\alpha/\beta\right) M\right]\right], \tag{5.2}$$

are, in general, used for the construction of the matrix system of the transformed problem (4.3). In calculating α, and for other considerations, it is convenient to rewrite (4.4) for the particular mappings ϕ_1, ϕ_2, and ϕ_3 given in Figure 1.

For the finite interval (a,b) and $\phi_1(x) = \ln\left(\frac{x-a}{b-x}\right)$, consider for $x \in \Gamma_a$

$$\frac{1}{\sqrt{\phi'(x)}}\, e^{-\alpha|\phi(x)|} = \left[\frac{(x-a)(b-x)}{b-a}\right]^{1/2} e^{-\alpha\left|\ln\left(\frac{x-a}{b-x}\right)\right|}$$

$$= \left[\frac{(x-a)(b-x)}{b-a}\right]^{1/2} e^{\alpha\ln\left(\frac{x-a}{b-x}\right)}$$

$$= \left[\frac{(x-a)(b-x)}{b-a}\right]^{1/2} \left(\frac{x-a}{b-x}\right)^{\alpha}$$

$$= (x-a)^{\alpha+1/2}\,(b-x)^{1/2-\alpha}\,(b-a)^{-1/2}$$

$$\leq \begin{cases} (x-a)^{\alpha+1/2}\,(b-a)^{-\alpha} & \text{for } \alpha < 1/2 \\ (x-a)^{\alpha+1/2}\,(b-a)^{-1/2} & \text{for } \alpha \geq 1/2 \end{cases}$$

$$\leq \tilde{C}_1\,(x-a)^{\alpha+1/2}$$

where $\tilde{C}_1 \equiv \max\{(b-a)^{-\alpha},\ (b-a)^{-1/2}\}$.

A similar computation for $x \in \Gamma_b$ yields

$$\frac{1}{\sqrt{\phi'(x)}}\, e^{-\beta|\phi(x)|} \le \tilde{C}_2\, (b - x)^{\beta+\frac{1}{2}}$$

so that (4.4) becomes

$$(5.4) \qquad |u(x)| \le C_1 \begin{cases} (x - a)^{\alpha+\frac{1}{2}} & x \in \Gamma_a \\ (b - x)^{\beta+\frac{1}{2}} & x \in \Gamma_b \end{cases}$$

for $\Gamma_a = \left(a, \frac{a+b}{2}\right]$, $\Gamma_b = \left(\frac{a+b}{2}, b\right)$, and $C_1 = \max\{\tilde{C}_1, \tilde{C}_2\}$.

When (4.1) is posed on the infinite interval $(0,\infty)$, there are two choices for ϕ as suggested in Chapter 3, $\phi_2(x) = \ln(x)$ and $\phi_3(x) = \ln(\sinh(x))$. For $\phi_2(x)$, the computation leading to the bound

$$(5.5) \qquad |u(x)| \le C \begin{cases} x^{\alpha+\frac{1}{2}} & x \in \Gamma_0 = (0,1] \\ x^{-\beta+\frac{1}{2}} & x \in \Gamma_\infty = (1,\infty) \end{cases}$$

is straightforward. When $\phi_3(x) = \ln(\sinh(x))$ is used, consider for $x \in \Gamma_0 = (0, \ln(1 + \sqrt{2})]$

$$\frac{1}{\sqrt{\phi'(x)}}\, e^{-\alpha|\phi(x)|} = \left(\frac{\sinh x}{\cosh x}\right)^{\frac{1}{2}} e^{\alpha \ln(\sinh(x))}$$

$$= \left(\frac{\sinh x}{\cosh x}\right)^{\frac{1}{2}} (\sinh x)^{\alpha}$$

$$= (\sinh x)^{\alpha+\frac{1}{2}}\, (\cosh x)^{-\frac{1}{2}}$$

$$\le (\sinh x)^{\alpha+\frac{1}{2}}$$

$$\le \left(x + (\cosh\xi)\left(\frac{x^3}{3!}\right)\right)^{\alpha+\frac{1}{2}} \quad \text{for } \xi \text{ between 0 and } x$$

$$= x^{\alpha+\frac{1}{2}} \left(1 + (\cosh\xi)\left(\frac{x^2}{3!}\right)\right)^{\alpha+\frac{1}{2}}$$

$$\leq x^{\alpha+\frac{1}{2}} \left\{ (1 + \cosh(\ln(1+\sqrt{2})) \frac{(\ln(1+\sqrt{2}))^2}{3!} \right\}^{\alpha+\frac{1}{2}}$$

$$\equiv K_1 \, x^{\alpha+\frac{1}{2}} \, .$$

For $x \in \Gamma_\infty = (\ln(1 + \sqrt{2}), \infty)$, consider

$$\frac{1}{\sqrt{\phi'(x)}} \, e^{-\beta|\phi(x)|} = \left(\frac{\sinh x}{\cosh x}\right)^{\frac{1}{2}} e^{-\beta \ln(\sinh(x))}$$

$$\leq (\sinh x)^{-\beta}$$

$$= \frac{2^\beta}{(e^x - e^{-x})^\beta}$$

$$= \frac{2^\beta}{e^{\beta x}(1 - e^{-2x})^\beta}$$

$$= e^{-\beta x}\left(\frac{2}{1 - e^{-2x}}\right)^\beta$$

$$\leq e^{-\beta x}\left(\frac{2}{1 - e^{-2\ln(1+\sqrt{2})}}\right)^\beta$$

$$\equiv K_2 \, e^{-\beta x} \, .$$

Hence,

$$(5.6) \qquad |u(x)| \leq C_2 \begin{cases} x^{\alpha+\frac{1}{2}} & x \in \Gamma_0 = (0, \ln(1 + \sqrt{2})] \\ e^{-\beta x} & x \in \Gamma_\infty = (\ln(1 + \sqrt{2}), \infty) \end{cases}$$

for $\phi_3(x) = \ln(\sinh(x))$ and $C_3 \equiv \max\{K_1, K_2\}$.

By comparing (5.4), (5.5), and (5.6) with the Frobenius form of the solution u(x) in (2.6) and assuming (4.1) has at worst a regular singular point at x = a (a = 0 in the $(0,\infty)$ cases), let $s = \alpha + \frac{1}{2}$ in (2.6). With regard to balancing the error terms of (4.29), this is the optimal choice of α. By doing this and using (2.9) to find s, α can be calculated easily just by using information acquired from the original differential equation. Note that $g_a - \lambda\rho_a$ (found using (2.8)) is positive in most physical cases; consequently, the indicial equation (2.9) has one positive root and one negative root, denoted by s_+ and s_-, respectively. Since u(a) = 0 in (4.1), by considering (2.6) s_- is eliminated as a choice for the solution s. Therefore

(5.7) $$\alpha = s_+ - \tfrac{1}{2} .$$

Recalling that (4.4) is a bound on the transformed problem, subtracting the $\frac{1}{2}$ puts α into the context of the original problem in terms of u(x). Intuitively, the $-\frac{1}{2}$ comes from the fact that $u(x) = \omega(x)(\phi'(x))^{-\frac{1}{2}}$.

If b is finite in the interval (a,b), then β can be calculated in the same manner as described above for α. For the infinite interval case, it is convenient to use the WKB approximation of u as given in Chapter 2 to find the β that satisfies the appropriate piece of (5.5) or (5.6).

Two criteria will be used in deciding whether to use ϕ_2 or ϕ_3 for the infinite interval problem. The first

deals with the bounds given in (5.5) and (5.6). If (4.1) has exponentially decaying eigensolutions, that is, $u(x) \sim Ke^{-\gamma x}$ as $x \to \infty$ and $\gamma > 0$, then the second inequality in both (5.5) and (5.6) is satisfied. It has been shown by Lund [18] that since algebraic decay is all that is required in (5.5), when choosing ϕ_2, the selection of N in (5.2) can be replaced by

$$N = \left[\left[\frac{1}{h} \text{An}\left(\frac{\alpha}{\gamma} Mh\right) + 1\right]\right]$$

in order to asymptotically balance the error terms in (4.29). This selection reduces the dimension of the matrix system with no loss of accuracy. Both maps can be used and will give equivalent accuracy. The difference will simply be that the size of the system will be smaller when choosing ϕ_2.

The second criterion deals with the behavior of the solution u in the right-half plane. If g(x) and $\rho(x)$ in (4.1) are analytic in the right-half plane, then the solution u is analytic there also [14] and $\phi_2(x) = \text{An}(x)$ is generally used (all other things being equal) because of its simplicity. If analyticity of the solution cannot be shown in a sector or if the solution has singularities near the positive half-line, then $\phi_3(x) = \text{An}(\sinh(x))$ is used. This last case is described in more detail in Example 5.2, the Wood-Saxon potential of the Schrödinger equation.

Examples Computed by Sinc-Collocation Method

Each of the examples in this section has been calculated by the sinc-collocation method that has given rise to a discrete system $A\vec{x} = \lambda B\vec{x}$. The IMSL [19] routine EIGZS, which uses the symmetry of A and B and the positive-definiteness of B, is called to solve the system.

The tables accompanying the examples include either the error in the calculated eigenvalue (for those examples where the true eigenvalues are known) or the eigenvalues computed (where the true eigenvalues are unknown). The dimension of the system is given in terms of M for M = 4, 8, 16, and 24. The asymptotic error rate, AER = $\exp(-(\pi d\alpha M)^{1/2})$, is given for each M for all examples. The notation in the tables given by .ccc - K is .ccc x 10^{-K}. As noted earlier in conjunction with Corollary 4.25, the larger eigenvalues are not approximated with as much accuracy as the smaller eigenvalues. The blanks present in the tables indicate data that was computed but with accuracy not good enough to be noted.

Example 5.1: Harmonic Oscillator

$$(5.8)\quad \begin{cases} -u''(x) + (x^2 + 2/x^2)u(x) = \lambda u(x) \\ u(0) = u(\infty) = 0 \end{cases}$$

To calculate α, note that $g(x) = x^2 + 2/x^2$ and $\rho(x) = 1$. Then from (2.8) $g_0 = 2$ and $\rho_0 = 0$. And from (2.9), $s_+ = 2$; therefore, $\alpha = 3/2$ from (5.7).

In deciding whether to choose ϕ_2 or ϕ_3 for this problem, it is helpful to calculate the asymptotic behavior of the solution to (5.8) by using the WKB method in (2.4). Note that for λ fixed, $2/x^2 \to 0$ as $x \to \infty$. Thus the dominant function for large x is x^2. Hence,

$$u_\lambda(x) \sim B(x^2)^{-1/4} \exp(-\int (x^2)^{1/2} dx)$$

(5.9)

$$= Bx^{-1/2} \exp(-x^2/2) \ , \ x \to \infty \ ,$$

where B is an arbitrary constant. To satisfy the zero boundary conditions, the constant A in (2.4) necessarily is zero.

Since g and ρ are both analytic in the right-half plane, either ϕ_2 or ϕ_3 may be chosen as the mapping. However, ϕ_3 is preferred due to the following discussion.

Recall from (3.9) that N(f) was required to be finite. Consider

$$I = \int_{\partial D_2} |u_\lambda(z)dz|$$

for D_2 the domain in Figure 1. Now

$$I = \int_0^\infty |u_\lambda(re^{is})ire^{is}|dr + \int_0^\infty |u_\lambda(re^{-is})ire^{-is}|dr$$

(5.10)

$$= \int_0^K |u_\lambda(re^{is})ire^{is}|dr + \int_K^\infty |u_\lambda(re^{is})ire^{is}|dr$$

$$+ \int_0^\infty |u_\lambda(re^{-is})ire^{-is}|dr \ .$$

Because of zero boundary conditions of u_λ and its analyticity in D_2, the first integral is finite. Note that the asymptotic behavior of u given in (5.9) is for x on the real line. From Olver [14], this behavior extends to a sector in the right-half plane. Then for K large enough, the second integral can be rewritten using (5.9) as

$$\int_K^\infty |u_\lambda(re^{is})ire^{is}|dr \sim B \int_K^\infty |r^{-\frac{1}{2}}e^{-is/2}e^{-\frac{1}{2}(re^{is})^2}ire^{is}|dr$$

$$= B \int_K^\infty r^{\frac{1}{2}}e^{-\frac{1}{2}r^2}(\cos 2s + i\sin 2s)|dr$$

$$= B \int_K^\infty |r^{\frac{1}{2}}e^{-\frac{1}{2}r^2}\cos 2s|dr$$

which will be finite if $\cos 2s > 0$. This implies $0 < 2s < \pi/2$ or $0 < s < \pi/4$. Hence, the largest d in Definition 3.2 can be is $\pi/4$. A similar argument shows that the third integral in (5.10) is finite also for $d \in (0, \pi/4)$.

The same procedure can be considered for ϕ_3 and D_3 in Figure 1. The characterization of $N(u_\lambda)$ is a bit more complicated to write down; let $z \in \partial D_3$. Then

$$(5.11) \qquad \int_{\partial D_3} |u_\lambda(z)dz| = \int_0^K |u_\lambda(z)dz| + \int_0^K |u_\lambda(\bar{z})d\bar{z}|$$

$$+ \int_K^\infty |u_\lambda(z)dz| + \int_K^\infty |u_\lambda(\bar{z})d\bar{z}| \ .$$

The first two integrals are finite because of the zero boundary conditions of u_λ and its analyticity in D_3. For K large enough, u_λ can be replaced by (5.9), and since $\partial D_3 \subseteq \{z: \ \mathrm{Im}\ z \le d, \ \mathrm{Re}\ z > 0\}$

$$\int_K^\infty |u_\lambda(z)dz| \le \int_K^\infty |u_\lambda(t + id)|dt$$

$$\tilde{=} \ B \int_K^\infty |(t + id)^{-\frac{1}{2}} e^{-\frac{1}{2}(t + id)^2}|dt$$

$$= B \int_K^\infty |(t + id)^{-\frac{1}{2}} e^{-\frac{1}{2}(t^2 - d^2 + i2dt)}|dt$$

$$= B \int_K^\infty |(t + id)^{-\frac{1}{2}}| e^{-\frac{1}{2}(t^2 - d^2)} dt \ .$$

This final integral will be finite, since for K large enough $t > \pi/2 > d$. Similarly, the fourth integral in (5.11) can be shown to be finite. Therefore, no further restrictions are necessary on d and it can be taken to be its largest possible value, $\pi/2$.

Even though ϕ_3 is preferred over ϕ_2, with regard to convergence rate, note that ϕ_2 can still be used. The matrix system for ϕ_2 will be larger than what is necessary when compared to the matrix system of ϕ_3 (in this example) to achieve the same accuracy.

Because of the speed with which u_λ goes to zero as $x \to \infty$ as shown in (5.9), it is advantageous to go directly to the error statement in (4.29) and consider the truncation error term to find an appropriate N. This procedure will give a smaller N than given by $N = \left[\left[(\alpha/\beta)M\right]\right]$, thus giving a smaller matrix system for the accuracy desired.

The truncation error pieces to be considered are

$$\sum_{p=N+1}^{\infty} u(x_p)\delta_{kp}^{(2)}(\phi'(x_p))^{1/2} \quad \text{and} \quad \sum_{p=-\infty}^{-(M+1)} u(x_p)\delta_{kp}^{(2)}(\phi'(x_p))^{1/2} .$$

By (5.9), as $x \to \infty$ $u(x) = 0(e^{-x^2/2})$. For the map $\phi_3(x) = \text{Ln}(\sinh(x))$, $x_k = \text{Ln}(e^{kh} + \sqrt{e^{2kh} + 1})$; so $x_k = 0(kh)$ as $k \to \infty$. Now consider

$$(\phi_3'(x))^{1/2} = (\coth x)^{1/2} = \left(\frac{e^x + e^{-x}}{e^x - e^{-x}}\right)^{1/2} . \tag{5.12}$$

Hence, as $x \to \infty$, $(\phi_3'(x))^{1/2} \to 1$. Finally, as $x_p \to \infty$ $|u(x_p)\delta_{kp}^{(2)}(\phi_3'(x_p))^{1/2}| = 0\left(e^{-x_p^2/2}\right)$. This implies there exist constants $\tilde{K}_1$ and K_1 so that

$$\begin{aligned}\sum_{p=N+1}^{\infty} |u(x_p)\delta_{kp}^{(2)}(\phi_3'(x_p))^{1/2}| &\le K_1 \sum_{p=N+1}^{\infty} e^{-p^2h^2/2} \\ &= K_1\, e^{-(N+1)^2h^2/2} + e^{-(N+2)^2h^2/2} + \ldots \\ &\le \tilde{K}_1 e^{-(N+1)^2h^2/2}\left(1 + 0\left(e^{-(N+2)^2h^2/2}\right)\right)\end{aligned} \tag{5.13}$$

$$\leq \tilde{K}_1 e^{-N^2h^2/2}\left(1 + O\left(e^{-(N+2)^2h^2/2}\right)\right)$$

$$= O\left(e^{-N^2h^2/2}\right).$$

Similarly, by (5.9) as $x \to 0^+$, $u(x) = O(x^\alpha)$ where $\alpha = 3/2$ as shown earlier. Notice then that $\lim_{x\to 0^+} x^{3/2}(\phi_3'(x))^{1/2} = 0$. Hence, $|u(x_p)\delta_{kp}^{(2)}(\phi_3'(x_p))^{1/2}| = O(x_p^{3/2})$ as $x_p \to 0^+$. For $x_p = \ln(e^{ph} + \sqrt{e^{2ph} + 1})$, use the binomial series expansion

$$\sqrt{1 + e^{2ph}} = 1 + \tfrac{1}{2}e^{2ph} + \frac{1}{8}e^{4ph} + \ldots .$$

This implies that as $p \to -\infty$, $\ln(e^{ph} + \sqrt{e^{2ph} + 1})$ is of order $\ln(e^{ph} + 1)$. Writing the series expansion of the natural logarithm yields

$$\ln(e^{ph} + 1) = e^{ph} - \tfrac{1}{2}e^{2ph} + \frac{1}{3}e^{3ph} - \ldots$$

which implies $\ln(e^{ph} + 1)$ is $O(e^{ph})$ as $p \to -\infty$. Finally then x_p is $O(e^{ph})$ as $p \to -\infty$. So there exist constants K_2, K_3, and $\tilde{K}_3$ so that

$$\sum_{p=-\infty}^{-(M+1)} |u(x_p)\delta_{kp}^{(2)}(\phi_3'(x_p))^{1/2}| \leq K_2 \sum_{p=-\infty}^{-(M+1)} x_p^{3/2}$$

$$\leq K_3 \sum_{p=-\infty}^{-(M+1)} e^{(3/2)ph}$$

$$\leq K_3 \sum_{p=M+1}^{\infty} e^{(-3/2)ph}$$

(5.14)

$$= K_3 \frac{e^{(-3/2)h(M+1)}}{1 - e^{(-3/2)h}}$$

$$\leq K_3 \frac{e^{(-3/2)hM}}{(3/2)h}$$

$$= O(e^{-3M\,h/2}) \ .$$

Now equating (5.13) and (5.14) to balance out the error terms yields

$$\frac{3}{2} Mh = \frac{N^2h^2}{2}$$

which implies $N = \left(\frac{3M}{h}\right)^{1/2}$. As before $h = \left(\frac{\pi d}{\alpha M}\right)^{1/2} = \frac{\pi}{(M)^{1/2}}$.

The matrix system for the harmonic oscillator and map ϕ_3 is

$$\left\{ -\frac{1}{h^2} I^{(2)} + D\left(\frac{4\cosh^2 x_k - 3}{4\cosh^4 x_k} + \left(x_k^2 + \frac{2}{x_k^2}\right)(\tanh^2 x_k)\right)\right\}\vec{z}$$

$$= \lambda D(\tanh^2 x_k)\vec{z}$$

with $x_k = \ln(e^{kh} + \sqrt{e^{2kh} + 1})$. The following table exhibits the calculations of the sinc-collocation method using this system.

Table 1. Harmonic Oscillator.

True Eigenvalues	4	8	16	24	= M
λ_p	.433-2	.454-3	.188-4	.163-5	= AER
		$\lvert\mu_p - \lambda_p\rvert$			
5	.831-2	.513-4	.321-6	.304-8	
9	------	.168-2	.607-6	.194-7	
12	------	------	.177-4	.496-7	
16	------	------	------	.331-5	

Example 5.2: Wood-Saxon

$$(5.15)\quad \begin{cases} -u''(x) + u(x) = \lambda(1 + e^{(x-r)/\varepsilon})^{-1}u(x) \\ u(0) = u(\infty) = 0 \\ r = 5.086855\ ,\ \varepsilon = .929853 \end{cases}$$

For $g(x) = 1$ and $\rho(x) = (1 + e^{(x-r)/\varepsilon})^{-1}$, from (2.8) $g_0 = 0$ and $\rho_0 = 0$; hence, $\alpha = \frac{1}{2}$ from (2.9) and (5.7).

The map ϕ_3 is preferred over ϕ_2 for this example because of the pole of $\rho(x)$ at $r + \varepsilon\pi i$. As can be seen from Figure 4, this pole determines that the largest sector for ϕ_2 in which the solution is guaranteed to be analytic is with $d = \mathrm{Tan}^{-1}\left(\frac{\varepsilon\pi}{r}\right) \approx \pi/6$.

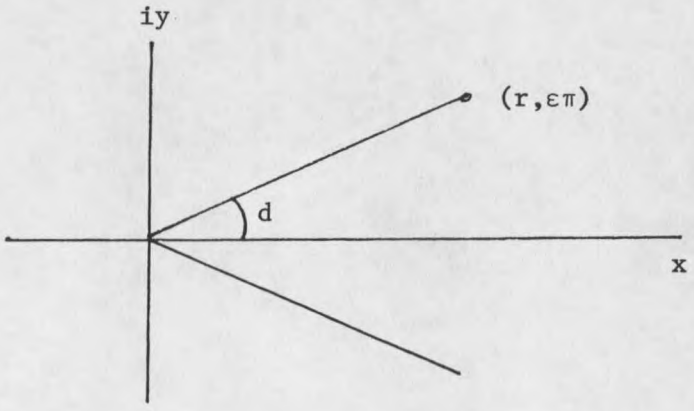

Figure 4: The Sector of Analyticity for Wood-Saxon

The domain of ϕ_3 does not contain the pole; hence, d can be chosen as large as possible; i.e. $d = \pi/2$. Note that ϕ_2 could have been chosen; however, a larger matrix system would have been required for the same amount of accuracy as when using ϕ_3.

The asymptotic behavior of the solution to (5.15) is given by Flugge [20]

$$u_\lambda(x) \sim K\exp[-(x - r)/\varepsilon]$$

which implies from (5.6) that $\beta = 1$.

The matrix system for the Wood-Saxon potential and ϕ_3 is

$$\left\{ -\frac{1}{h^2} I^{(2)} + D\left(\frac{4\cosh^2 x_k - 3}{4\cosh^4 x_k} + \tanh^2 x_k\right)\right\}\vec{z}$$

$$= \lambda D\left(\frac{\tanh^2 x_k}{1 + e^{(x_k - r)/\varepsilon}}\right)\vec{z}$$

with $x_k = \ln(e^{kh} + \sqrt{e^{2kh} + 1})$.

Notice that the matrix systems for the harmonic oscillator and the Wood-Saxon potentials differ only in the two diagonal matrices and to change them only means evaluating two known functions at x_k.

To implement this method for $\alpha = \frac{1}{2}$ and $\beta = 1$, the parameters M, N, and h in (5.1) and (5.2) are $N = \frac{1}{2}M$ and $h = \pi/\sqrt{M}$. In the process of developing the method some very interesting things happened with respect to the computations of this example. The first eigenvalue for the Wood-Saxon potential that will be used for comparison

purposes is 1.424333 which was computed by Mayers [21] by an iterative matching method.

For $\alpha = \frac{1}{2}$ and $N = \frac{1}{2}M$, the error terms of (4.29) are balanced and give the asymptotic error rate, AER, for the first eigenvalue. The first two columns of Table II give AER and the computed error for M = 4, 8, 16, and 24. The computed error certainly falls in the bound guaranteed. Now consider the last column of Table 2 where $\alpha = \frac{1}{2}$ and N = 2M. The difference here is that the truncation error piece from N + 1 to ∞ is not balanced with the error integral and the lower truncation piece. The former truncation error can be seen by a short computation to be much smaller than the other two balanced pieces. What this situation seems to suggest is that even if the parameters α and β are not found exactly, the method still can work and the errors incurred are not necessarily larger than if the parameters were found exactly.

Table 2. Wood-Saxon Errors for $N = \frac{1}{2}M$ and N = 2M

AER	$\lvert\mu_1 - \lambda_1\rvert$ (N = ½M)	M	$\lvert\mu_1 - \lambda_1\rvert$ (N = 2M)
.0432	.069	4	.0027
.01176	.0181	8	.00015
.001867	.00117	16	.00021
.000454	.000097	24	0

In the comparison section $\alpha = \frac{1}{2}$, $\beta = 1$, and $N = 2M$ is used. Table 3 gives the computed data for this case.

In Table 4, the Wood-Saxon eigenvalues are calculated for $\alpha = \frac{1}{2}$, $\beta = 1$, and $N = \frac{1}{2}M$, the choices from the theory of the sinc-collocation method. Notice that the calculations of the first eigenvalue always fall within the guaranteed bounds. However, convergence of the eigenvalues is not seen as quickly as in the case of $N = 2M$ shown in Table 3.

Table 3. Wood-Saxon ($N = 2M$).

True Eigenvalues	4	8	16	24 = M
λ_p				
1.424333	1.427127	1.424484	1.424335	1.424333
λ_2	-----	2.447301	2.444763	2.444707
λ_3	-----	-----	3.972775	3.972332
λ_4	-----	-----	-----	5.993260

Table 4. Wood-Saxon (N = ½M).

True Eigenvalues	4	8	16	24 = M
	.432-1	.118-1	.187-2	.455-3 = AER
1.424333	1.494131	1.442476	1.425513	1.424430
λ_2	-----	2.562343	2.453885	2.445506
λ_3	-----	-----	4.007281	3.9756102
λ_4	-----	-----	-----	6.002765

Example 5.3: Mathieu's Equation

$$-u''(x) + (2\theta\cos 2x)u(x) = \lambda u(x)$$

$$u(0) = u(\pi) = 0$$

(the solutions u(x) and eigenvalues λ depend on θ)

For any θ, $g_0 = g_\pi = 0$ where $g(x) = 2\theta\cos 2x$ and $\rho_0 = \rho_\pi = 0$ where $\rho(x) = 1$. Hence, $\alpha = \beta = ½$ by (2.8), (2.9), and (5.7). Then $h = \pi/\sqrt{M}$ and M = N by (5.1) and (5.2). The map used is

$$\phi(x) = An\left(\frac{x}{\pi - x}\right) \quad ;$$

the matrix system is

$$\left\{ -\frac{1}{h^2} I^{(2)} + D\left(\frac{1}{4} + 2\theta\cos 2x_k\left(\frac{x_k^2(\pi - x_k)^2}{\pi^2}\right)\right)\right\} \vec{z}$$

$$= \lambda D\left(\frac{x_k^2(\pi - x_k)^2}{\pi^2}\right)\vec{z} \quad ;$$

and $$x_k = \frac{\pi e^{kh}}{e^{kh} + 1} \quad .$$

Note that for each choice of θ, all that is changed in the matrix system are the elements of a diagonal matrix. The elements come from the point evaluation of a known function. Note also that when $\theta = 0$, Mathieu's equation reduces to the Fourier equation, and the matrix system becomes

$$\left\{ -\frac{1}{h^2} I^{(2)} + D(1/4) \right\} \vec{z} = \lambda D\left(\frac{x_k^2 (\pi - x_k)^2}{\pi^2} \right) \vec{z} \quad .$$

Tables 5 and 6 display eigenvalues and errors for both $\theta = 0$ and $\theta = 1$. The true eigenvalues for Table 6 are found in Birkoff et. al. [8].

Table 5. Mathieu's Equation with $\theta = 0$ (Fourier).

True Eigenvalues	4	8	16	24 = M
λ_p	.432-1	.118-1	.187-2	.455-3 = AER
	$\lvert \mu_p - \lambda_p \rvert$			
1	.182-1	.659-3	.109-5	.370-6
4	----	.797-1	.173-2	.623-4
9	----	----	.716-1	.469-2
16	----	----	----	.940-1

Table 6. Mathieu's Equation with $\theta = 1$.

True Eigenvalues	4	8	16	24 = M
λ_p	.432-1	.118-1	.187-2	.455-3 = AER
		$\lvert u_p - \lambda_p \rvert$		
-.1102488	.4202	.8918-1	.5258-2	.4722-3
3.9170248	----	.4177	.3524-1	.3828-2
9.0477393	----	----	.2537	.3429-1
16.0329701	----	----	----	.2287

Example 5.4: Bessel's Equation

$$(5.16) \qquad \begin{cases} -u''(x) + \left(\dfrac{4n^2 - 1}{4x^2}\right)u(x) = \lambda u(x) \\ u(0) = u(1) = 0 \ , \ n \geq 1 \end{cases}$$

The exact eigenvalues, λ_p, of (5.16) are related to the zeros, j_{np}, of the Bessel function J_n, i.e. $\lambda_p = j_{np}^2$ where j_{np} is the pth positive zero of J_n.

For n a nonnegative integer, α and β are found by (2.8), (2.9), and (5.7) with $g(x) = \left(\dfrac{4n^2 - 1}{4x^2}\right)$ and $\rho(x) = 1$. Those equations yield $g_0 = \left(\dfrac{4n^2 - 1}{4}\right)$, $\rho_0 = 0$, $g_1 = 0$, and $\rho_1 = 0$; so $\alpha = n$ and $\beta = \frac{1}{2}$. From (5.4), it is obvious that $u \to 0$ much more rapidly as $x \to 0$ (as n gets large) than as $x \to 1$. The parameter selection will be based on how the

solution behaves as $x \to 1$. This selection seems somewhat more uniform with respect to parameter selection (for the calculation of the eigenvalues of (5.16) with differing values of n). Notice, however, that due to the balancing of the error terms in (4.29), the accuracy is unaffected by α coming first or β. So balancing the error terms $e^{-\beta Nh} = e^{-\pi d/h} = e^{-\alpha Mh}$ yields $h = \pi/\sqrt{N}$ and $N = 2nM$. The map for the interval (0,1) is

$$\phi(x) = \ln\left(\frac{x}{1 - x}\right) ,$$

and the matrix system is

$$\left\{ - \frac{1}{h^2} I^{(2)} + D\left(\frac{1}{4} + \frac{1}{4}(4n^2 - 1)(1 - x_k)^2\right) \right\} \vec{z}$$

$$= \lambda D(x_k^2(1 - x_k)^2)\vec{z}$$

with $$x_k = \frac{e^{kh}}{1 + e^{kh}} .$$

Table 7 gives the calculated error and asymptotic error rate for the eigenvalues of (5.14) with n = 1. The eigenvalues that will be used for comparison purposes are given in Watson [22].

Table 7. Bessel's Equation with n = 1.

True Eigenvalue	4	8	16	24 = M
λ_p	.1176-1	.1867-2	.1383-3	.187-4 = AER
		$\lvert\mu_p - \lambda_p\rvert$		
14.68197087	.15928-1	.353-4	.66-6	.21-6
49.21845675	-----	.03-1	.7198-4	.7-7
103.4994532	-----	-----	.633-2	.695-4

Example 5.5: Chebyshev

$$-u''(x) + (-3/4)(1 - x^2)^{-2}u(x) = \lambda(1 - x^2)^{-1}u(x)$$

$$u(-1) = u(1) = 0$$

In this example, $g(x) = (-3/4)(1 - x^2)^{-2} < 0$ on $(-1,1)$; hence, the development prior to Theorem 4.24 is not applicable. The nonnegativity assumption $g(x) \geq 0$, however, was needed only for the inequality (4.11), i.e. to bound $\gamma_g(t)$ away from zero. Given the map

$$\phi(x) = \ln\left(\frac{x + 1}{1 - x}\right)$$

and noting that $\phi'(x) = 1 / \psi'(t)$, $\gamma_g(x)$ from (4.8) can be rewritten as

$$\gamma_g(x) = \frac{-1}{(\phi'(x))^{3/2}}\left(\frac{1}{\phi'(x)}\right)'' + \frac{g(x)}{(\phi'(x))^2}$$

$$= 1/4 + 1/4(1 - x^2)(-3/4)(1 - x^2)^{-2}$$

$$\geq 1/4 - 3/16 = 1/16 .$$

So if δ in (4.11) is replaced by 16, the rest of the theorem development is applicable and Theorem 4.24 can be applied to this problem.

It turns out that for any example on a finite interval, if

$$\liminf_{x\in(a,b)}\left\{\frac{g(x)}{(\phi'(x))^2}\right\} > -1/4 , \tag{5.17}$$

Theorem 4.24 can be applied; that is, γ_g can be bounded below by a positive number and the assumption $g(x) \geq 0$ is not necessary.

To see this recall that from (4.12)

$$a_m \equiv \min_{a_j\in\sigma(A)} \{a_j\}$$

$$\geq \min_{d_j\in\sigma(D(\gamma_g))} \{d_j\}$$

by the spectral properties of $-I^{(2)}$. For any $g(x)$ and for

$$\phi(x) = \ln\left(\frac{x - a}{b - x}\right)$$

$$\gamma_g(x) = 1/4 + \frac{g(x)}{(\phi'(x))^2} .$$

Therefore, as long as (5.17) is satisfied, γ_g is bounded below by a positive number and a_m is also bounded below by a positive number. Hence, Theorem 4.24 is applicable.

The equations (2.8), (2.9), and (5.7) for $g(x) = (-3/4)(1 - x^2)^{-2}$ and $\rho(x) = (1 - x^2)^{-1}$ yield $g_{-1} = -3/16$, $g_1 = -3/16$, and $\rho_{-1} = \rho_1 = 0$. Therefore, $\alpha = 1/4$ and $\beta = 1/4$. This leads to $h = \sqrt{2}\pi/\sqrt{M}$ and $N = M$ from (5.1) and (5.2).

The true eigensolutions to the Chebyshev equation are

$$u_{\lambda_n}(x) = (1 - x^2)U_n(x)$$

and $\lambda_n = n^2 + 3/4$, $n = 0, 1, 2, \ldots$

where U_n is the nth Chebyshev polynomial of the second kind.

The matrix system for this example is given by

$$\left\{ - \frac{1}{h^2} I^{(2)} + D(1/16) \right\} \vec{z} = \lambda D \left(\frac{1 - x_k^2}{4} \right) \vec{z}$$

with $x_k = \dfrac{e^{kh} - 1}{e^{kh} + 1}$. The calculations done with this system are exhibited in Table 8.

Table 8. Chebyshev Equation.

True Eigenvalues	4	8	16	24 = M
λ_p	.108-0	.432-1	.118-1	.433-2 = AER
	$\lvert \mu_p - \lambda_p \rvert$			
3/4	.521-0	.181-1	.210-3	.319-4
15/4	-----	.536-1	.187-2	.170-3
35/4	-----	-----	.321-1	.183-2
63/4	-----	-----	-----	.381-1

Example 5.6: Laguerre

$$(5.18) \qquad -u''(x) + \left(\frac{x^2 + 3}{4x^2}\right) u(x) = \lambda\left(\frac{1}{2x}\right)u(x)$$

$$u(0) = u(\infty) = 0$$

The standard form of Laguerre's differential equation with parameter γ is given by

$$(5.19) \qquad y''(x) + \left(\frac{\gamma + 1 - x}{x}\right) y'(x) + \frac{n}{x}\, y(x) = 0 \ .$$

Letting $y(x) = u(x)(x^{-3/2}e^{x/2})$ and $\gamma = 2$ and substituting into (5.19) yields the normal form of Laguerre's equation, that is

$$(5.20) \qquad -u''(x) + \left(\frac{x^2 - 6x + 3}{4x^2}\right) u(x) = \frac{n}{x}\, u(x) \ .$$

To maintain the positivity of $g(x)$ and $\rho(x)$, let

$$\frac{x^2 - 6x + 3}{4x^2} = \frac{x^2 + 3}{4x^2} - \frac{6x}{4x^2} \ .$$

Rewriting (5.20) yields

$$-u''(x) + \left(\frac{x^2 + 3}{4x^2}\right) u(x) = \left(\lambda/2x\right)u(x)$$

where $\lambda = 3 + 2n$ for $n = 0, 1, 2, \ldots$, $g(x) = \dfrac{x^2 + 3}{4x^2}$,

and $\rho(x) = 1/2x$. Then $g_0 = 3/4$ and $\rho_0 = 0$ giving $\alpha = 1$.

As $x \to \infty$, $g(x) \to 1/4$ and $\rho(x) \to 0$; thus by the WKB approximation (2.4) and zero boundary conditions on (5.18)

$$u(x) \sim e^{-x/2} \quad \text{as} \quad x \to \infty \ ;$$

so $\beta = \frac{1}{2}$ by (5.6). By the discussion following (5.6), the

asymptotic behavior of u determines that the map to be used is

$$\phi(x) = \text{Ln}(x) \ .$$

This choice allows

$$N = \left[\left[(1/h)\text{Ln}(2Mh) + 1 \right]\right]$$

so the dimensions of the matrix system, given by

$$\left\{ -\frac{1}{h^2} I^{(2)} + D\left(\frac{1}{4} + \left(\frac{x_k(x_k^2 + 3)}{4} \right) \right) \right\} \vec{z} = \lambda D\left(\frac{x_k}{2} \right) \vec{z}$$

for $x_k = e^{kh}$ and $\lambda = 2n + 3$, $n = 0, 1, 2, \ldots,$ will be smaller than if the map $\phi(x) = \text{Ln}(\sinh(x))$ is chosen.

The true eigenfunctions for this differential equation are well-known and are

$$u_{\lambda_n}(x) = x^{3/2} e^{-x/2} \left\{ \frac{e^x}{n! x^2} \frac{d^n}{dx^n} \left(x^{n+2} e^{-x} \right) \right\}$$

where $\lambda_n = 2n + 3$, $n = 0, 1, 2, \ldots$.

Table 9. Laguerre's Equation.

True Eigenvalues	4	8	16	24 = M
λ_p	.118-1	.187-2	.138-3	.188-4 = AER
	.244-1	.197-2	.879-4	.376-5 = Q
		$\lvert\mu_p - \lambda_p\rvert$		
3	.242-1	.111-2	.283-4	.868-6
5	-----	.123-1	.101-2	.485-4
7	-----	-----	.172-1	.124-2
9	-----	-----	-----	.108-1

Notice in Table 9 that the calculated error was much better than the error rate predicted. Thus, included in the table is the value $Q = M^{3/2}|\cos\theta_p|\exp(-(\pi d\alpha M)^{1/2})$ which comes from the conclusion of Theorem 4.24 without bounding $|\cos\theta_p|$ by 1. Recall θ_p is the angle between $\vec{z}_p$ and $\Delta\vec{\omega}_0$. It seems from this example that bounding $|\cos\theta_p|$ by 1 is a very crude bound. No exact statement can be made at this time, but if a more precise bound could be placed on $|\cos\theta_p|$, then it appears that the conclusion of Theorem 4.24 could also be made more precise.

Comparison of Sinc-Collocation Method to Other Numerical Methods

Galerkin and collocation schemes, finite differences, finite elements, and spectral methods are well-known and often-used methods to calculate the eigenvalues of Sturm-Liouville problems. The purpose of this section is to compare the implementation, accuracy, and overall performance of the sinc-collocation method to several of these alternative methods.

Four of the examples in the previous section were chosen to do these comparisons. The harmonic oscillator, Wood-Saxon, and Mathieu's equations will be compared to the Rayleigh-Ritz method described in Chapter 2 using finite element basis function. The tau method using Chebyshev basis functions is a spectral method that is applied to

Bessel's equation. The tau method is described in detail in Comparison 3.

With each comparison a table is given which includes the absolute error in the true and computed eigenvalues. The error is listed for the compared method and the sinc-collocation method. The basis for the comparison is that in each method the same number of basis elements (roughly) are used; that is, comparable matrix sizes are used.

Comparison 1: Harmonic Oscillator

$$-u''(x) + (x^2 + 2/x^2)u(x) = \lambda u(x)$$

$$u(0) = u(\infty) = 0$$

Botha and Schoombie [10] use the Rayleigh-Ritz method with cubic splines and cubic hermite splines as the finite element basis functions. With these choices of bases the matrices A and B in the matrix system $A\vec{x} = \lambda B\vec{x}$ are symmetric and banded matrices with band width 7. Recall from Chapter 2 that to fill the nonzero elements of these matrices a numerical integration and a truncation of the infinite interval were necessary for each element. To maintain the order of error of the method, the numerical integration method used must be of comparable order.

Tables 10 and 11 display the compared results for $\lambda_2 = 9$. The only results given by Botha and Schoombie are for $\lambda_2 = 9$. In terms of the error in the computed and true

eigenvalues, the Rayleigh-Ritz method and the sinc-collocation method gave similar results. The sinc method yielded one more decimal place of accuracy than did the Rayleigh-Ritz with cubic hermite splines. The Rayleigh-Ritz method with cubic splines produced results of the same accuracy as the sinc method.

Table 10. Harmonic Oscillator: Absolute Error Between the True and Computed Second Eigenvalues for Rayleigh-Ritz Method with Cubic Hermite Splines and Sinc-Collocation Method.

Matrix Size	Error in Cubic Hermite	Error in Sinc-Collocation	Matrix Size
18 x 18	.39-3	.117378-2	18 x 18
38 x 38	.31-4	.211841-5	39 x 39
46 x 46	.91-5	.392814-6	47 x 47
58 x 58	.20-5	.189826-6	57 x 57

Table 11. Harmonic Oscillator: Absolute Error Between the True and Computed Second Eigenvalues for Rayleigh-Ritz Method with Cubic Splines and Sinc-Collocation Method.

Matrix Size	Error in Cubic	Error in Sinc-Collocation	Matrix Size
11 x 11	.19-2	.4497-1	10 x 10
25 x 25	.15-4	.662387-4	25 x 25
36 x 36	.30-5	.99758-5	36 x 36

Comparison 2: Wood-Saxon

$$-u''(x) + u(x) = \lambda(1 + e^{(x-r)/\mathfrak{a}})^{-1}u(x)$$

$$u(0) = u(\infty) = 0$$

$$r = 5.086855 \ , \ \mathfrak{a} = .929853$$

This example will also be compared to the work by Botha and Schoombie [10]. Again the method is Rayleigh-Ritz with cubic and cubic hermite splines.

Notice that to change from the harmonic oscillator problem to the Wood-Saxon problem, the numerical integrations and truncation of the infinite interval need to be completely redone to fill the matrices A and B of the Rayleigh-Ritz method. Changing the matrix system of the sinc-collocation method required only that two diagonal matrices be changed with those changes being point evaluations of known functions. Because of the ease in going from problem to problem, the sinc-collocation method has the obvious advantage of simplicity.

The eigenvalue comparison is done on the first eigenvalue $\lambda = 1.424333$. Tables 12 and 13 show that for both sets of basis functions the Rayleigh-Ritz method was more accurate in terms of the computation of the eigenvalue.

Table 12. Wood-Saxon: Absolute Error Between the True and Computed First Eigenvalues for Rayleigh-Ritz Method with Cubic Hermite Splines and Sinc-Collocation Method.

Matrix Size	Error in Cubic Hermite	Error in Sinc-Collocation	Matrix Size
18 x 18	.34-5	.59-3	19 x 19
24 x 24	.14-5	.15-3	25 x 25
28 x 28	.34-5	.818-4	28 x 28
30 x 30	.10-7	.453-4	31 x 31

Table 13. Wood-Saxon: Absolute Error Between the True and Computed First Eigenvalues for Rayleigh-Ritz Method with Cubic Splines and Sinc-Collocation Method.

Matrix Size	Error in Cubic	Error in Sinc-Collocation	Matrix Size
11 x 11	.10-4	.76-2	10 x 10
16 x 16	.92-5	.12-2	16 x 16
22 x 22	.10-5	.29-3	22 x 22

Comparison 3: Mathieu's Equation

$$-u''(x) + (2\theta\cos 2x)u(x) = \lambda u(x)$$

$$u(0) = u(\pi) = 0$$

Birkoff, DeBoor, Swartz, and Wendroff [8] use the Rayleigh-Ritz method with cubic and cubic hermite splines to calculate the eigenvalues of Mathieu's equation for

several values of θ. Compared here will be the eigenvalue computations for $\theta = 0$ (Fourier's equation) and $\theta = 1$. As θ changes the Rayleigh-Ritz method requires that the elements of the matrices of the method be recalculated with numerical integrations. The sinc-collocation method changes only by point evaluations of known functions in two diagonal matrices.

The following Tables 14-17 show that when comparing the two methods in the calculation of the eigenvalues, the Rayleigh-Ritz method gave significantly better results.

Table 14. Fourier Equation: Absolute Error Between the True and Computed Eigenvalues for Rayleigh-Ritz Method with Cubic Hermite Splines and Sinc-Collocation Method.

True Eigenvalue	Matrix Size	Error in Cubic Hermite	Error in Sinc-Collocation	Matrix Size
1	10 x 10	.640-6	.18216-1	9 x 9
	14 x 14	.12-6	.3273-2	13 x 13
	16 x 16	.68-8	.65678-3	17 x 17
4	10 x 10	.125-3	.822061	9 x 9
	14 x 14	.254-4	.237378	13 x 13
	16 x 16	.131-4	.794968-1	17 x 17

Table 15. Fourier Equation: Absolute Error Between the True and Computed Eigenvalues for Rayleigh-Ritz Method with Cubic Splines and Sinc-Collocation Method.

True Eigenvalue	Matrix Size	Error in Cubic	Error in Sinc-Collocation	Matrix Size
1	9 x 9	.0-5	.18216-1	9 x 9
	10 x 10	.0-5	.76545-2	11 x 11
4	9 x 9	.4-4	.82206	9 x 9
	10 x 10	.2-4	.42999	11 x 11

Table 16. Mathieu's Equation with $\theta = 1$: Absolute Error Between the True and Computed Eigenvalues for Rayleigh-Ritz Method with Cubic Hermite Splines and Sinc-Collocation Method.

True Eigenvalue	Matrix Size	Error in Hermite	Error in Sinc-Collocation	Matrix Size
-.1102488	10 x 10	.313-4	.4202	9 x 9
	14 x 14	.701-5	.19388	13 x 13
	16 x 16	.373-5	.89-1	17 x 17

Table 17. Mathieu's Equation with $\theta = 1$: Absolute Error Between the True and Computed Eigenvalues for Rayleigh-Ritz Method with Cubic Splines and Sinc-Collocation Method.

True Eigenvalue	Matrix Size	Error in Hermite	Error in Sinc-Collocation	Matrix Size
-.1102488	9 x 9	.23-4	.4202	9 x 9
	10 x 10	.10-4	.28658	11 x 11

Comparison 4: Bessel's Equation

$$-u''(x) + \left(\frac{4n^2 - 1}{4x^2}\right)u(x) = \lambda u(x)$$

$$u(0) = u(1) = 0 \ , \ n \geq 1$$

In the calculation of the eigenvalues of Bessel's equation, Gottlieb and Orszag [4] consider

$$y'' + \frac{1}{x}\, y' - \frac{n^2}{x^2}\, y = -\lambda y$$

with n = 7. This form of Bessel's equations comes from letting $u(x) = \sqrt{x}\, y(x)$ in (5.16). The method of Gottlieb and Orszag is the tau-method with Chebyshev basis functions. Let

$$\tilde{y}(x) = \sum_{m=1}^{M} y_m T_{2m-1}(x)$$

where the y_m are constants to be found and T_{2m-1} is the Chebyshev polynomial of the first kind of degree 2m - 1. The differential equation to be solved is

$$y'' + \frac{1}{x} y' - \frac{n^2}{x^2} y = -\lambda y + \tau T_{2M-1} .$$

Substituting $\tilde{y}$ into the differential equation and taking an inner product with T_{2j-1} $(1 \le j \le M)$ yields the system

$$\sum_{m=1}^{M} y_m (T''_{2m-1}, T_{2j-1}) + \frac{1}{x} \sum_{m=1}^{M} y_m (T'_{2m-1}, T_{2j-1})$$

(5.21)

$$- \frac{n^2}{x^2} y_j c_j = -\lambda y_j c_j + \tau c_j , \quad 1 \le j \le M ,$$

where

$$c_j = \begin{cases} \pi & j = 1 \\ \pi/2 & j \ge 2 \end{cases}$$

and

$$\tau = -(T_{2M-1}, L\tilde{y} + \lambda\tilde{y}) .$$

The boundary condition implies

$$\sum_{m=1}^{M} y_m = 0 \quad . \tag{5.22}$$

The inner product used is

$$(f,g) = \int_0^1 f(x)g(x) \frac{1}{\sqrt{1 - x^2}} \, dx .$$

As can be seen from (5.21), every element of the matrix system using the tau-method necessitates doing two numerical integrations. To maintain the accuracy of the method, these integrations need to be calculated to at least this same accuracy.

Gottlieb and Orszag also introduce a "pole condition" to improve convergence of their method. This condition, $y'(0) = 0$, gives

$$\sum_{m=1}^{M} y_m T'_{2m-1}(0) = 0$$

as another equation of their system, along with (5.21) and (5.22). Gottlieb and Orszag themselves point out that the pole condition must be applied properly so as not "to degrade significantly the accuracy of the spectral computations." Also note that, for n = 1, for example, the pole condition does not apply (the solution of (5.20) for n = 1 is $J_1(x)$ with $J_1'(0) = \frac{1}{2}$) and cannot be used to speed up convergence of their method.

The matrix system just prior to Table 7 can be used to approximate the eigenvalues of (5.20) with the parameters $h = \pi/\sqrt{N}$ and $N = 2nM$ with effectively no change, that is, change the parameter N and change a constant in a diagonal matrix as n changes.

The final Table 18 gives a comparison of the results of Gottlieb and Orszag for the first eigenvalue for n = 7 in (5.20), with and without the pole condition, to the results of this thesis. The exact eigenvalue used is given in Gottlieb and Orszag as $\lambda_1 = 122.907600204$. Notice that the sinc-collocation did as well as the tau method without the pole condition. The tau method with the pole condition

did speed the convergence of the calculation for the problem.

Table 18. Bessel's Equation with n = 7: Absolute Error Between the True and Computed First Eigenvalue for Chebyshev-Tau Method With and Without Pole Condition and Sinc-Collocation Method.

Matrix Size	Tau Without Pole	Tau With Pole	Sinc-Collocation	Matrix Size
18 x 18	3.36023	.2-4	.152017	15 x 15
26 x 26	.6506-3	.0-9	.5365-3	30 x 30

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