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Galerkin Schemes and the Sinc-Galerkin Method for Singular Sturm–Liouville Problems

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Galerkin schemes for the computation of the eigenvalues of both regular and singular Sturm–Liouville problems are compared to the sinc–Galerkin method. Contrasted are numerical results as well as qualitative features. The schemes discussed include finite element, spectral, and collocation. The equivalence of the spectral method with sinc basis functions to the sinc–collocation scheme provides this technique with many distinctive features. Highlighted among these features through the course of the computational comparisons is its ease of implementation, its exponential accuracy in the presence of singularities and its all-around versatility. © 1990 Academic Press, Inc.

I. INTRODUCTION

The computation of the eigenvalues of the Sturm–Liouville problem

$$\begin{gathered} Lu(x) \equiv -u''(x) + q(x)\,u(x) = \lambda \rho(x)\,u(x), \qquad a < x < b \\ u(a) = u(b) = 0 \end{gathered} \tag{1.1}$$

can be accomplished in many ways. One of the most commonly used techniques is a Galerkin method. This broad category of methods is generally considered to include spectral, finite element, and collocation schemes, the type being determined by the basis functions chosen. In a terse review, a Galerkin scheme may be summarized as follows. On the interval (c, d) let $\{f_i\}$ denote a complete orthonormal set in the Hilbert space $H(c, d)$. Denote by u_λ the solution of (1.1). Let χ be a "nice"

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map of (a, b) onto (c, d) and put $\tilde{f}_i = f_i \circ \chi$. Denote an approximate eigensolution of (1.1) by

$$U_M(x) = \sum_{i=0}^{M} c_i \tilde{f}_i(x), \tag{1.2}$$

where the c_i are found by solving

$$\langle LU_M - \lambda \rho U_M, \tilde{f}_j \rangle = 0, \qquad j = 0, 1, 2, ..., M, \tag{1.3}$$

and $\langle *, * \rangle$ is the inner product in $H(a, b)$.

A simple point of view is to refer to (1.3) as a spectral method if the basis functions $\{\tilde{f}_i\}$ are defined globally on the interval (a, b) and as a finite element method if they are compactly supported. If point evaluation is used in (1.3) the method is referred to as collocation. Standard basis functions used in finite element methods as well as a description of the collocation method are found in [2, 8]. An excellent survey of the role of the classical sets of orthogonal functions used in spectral methods is found in [9].

The qualities of the Galerkin scheme depend on the set $\{f_i\}$ as well as the map χ. Once a set $\{f_i\}$ has been selected, the choice of a map χ can be based on a wide range of considerations. Near the top of the hierarchy of these considerations is the fact that the mapped basis functions should preserve (and if possible, enhance) the approximating properties of the set $\{f_i\}$.

Depending on the nature of the coefficient functions q and ρ, each of the aforementioned schemes has its own particular advantages when applied to (1.1). Specific advantages sought include having high accuracy, having a rapid convergence rate, being easy to implement, and requiring a small amount of modification when q and ρ are changed. For example, an appropriately chosen spectral or finite element scheme typically is a more accurate method than is a collocation scheme whereas the latter is usually simpler to implement than are the former. For any one specific problem(1.1), there are equations where the previous sentence can be computationally misrepresentative (see Comparison 3.1 in Section III). On the other hand, one is often forced to sacrifice simplicity due to the inherent difficulties of a problem. This is frequently associated with problems that have singular coefficients and/or problems on infinite domains. These are called singular Sturm–Liouville problems (otherwise they are called regular). What is often desired in practice is a method that has (i) a known error estimate on a wide class of problems, (ii) a user-friendly mode of implementation relative to varying (1.1) (either changing q and ρ and/or the domain (a, b)), and (iii) a rate of convergence, sufficiently rapid, so that the desired accuracy is obtained within a reasonable (computationally measured) amount of time.

In [12] a collocation scheme was developed to approximate the eigenvalues of the Sturm–Liouville problem (1.1). Therein it was shown that the convergence rate of this sinc-collocation method is $\exp(-\kappa\sqrt{M})$ $(\kappa > 0)$, where $2M + 1$ sinc basis

elements are employed in the collocation scheme. This convergence rate was established for both the finite interval and the semi-infinite interval, and for non-negative coefficient functions q and ρ. The convergence rate is maintained for problems having regular singular points at a and/or b. In the case that the latter situation gives rise to eigenfunctions with algebraic or logarithmic singularities (at a and/or b), the previously cited convergence rate persists. Comparison 3.4 exhibits a case where a small change in the coefficient function q in (1.1) perturbs the eigenfunctions in such a fashion that these eigenfunctions change from entire to singular functions. It is perhaps in the case of singular problems where one of the strongest features of this sinc-collocation scheme is exhibited.

Another feature of the sinc-collocation method is that the discrete system which arises is the same as that for a spectral method using sinc basis functions. Thus the sinc-collocation method and the sinc-Galerkin method are equivalent in this setting. As such, this method exhibits collectively many of the advantages that are typically associated with either a spectral or collocation method. This non-classical set of orthogonal basis functions has many desirable properties [20].

The sinc-collocation scheme has the earlier mentioned properties ((i)–(iii) above) that a prospective user seeks. The purpose of the present paper is to explore these properties of the sinc function method in a comparative fashion. In an attempt not to prejudicially represent the sinc method, problems from the literature have been selected that have been discussed by other authors. Other problems have been chosen wherein the eigenvalues of (1.1) have been computed by different methods and fully reported. When the sinc method is implemented on (1.1) it is implemented on this specific (Liouville normal) form of the Sturm–Liouville problem (as opposed to its various equivalent forms: standard or self-adjoint). This choice was originally motivated by implementing the method on the radial Schrödinger equation and it appears in this case that (1.1) is the form of the equation most frequently cited. These various forms are all easily obtained from one another by a change of variables. The Liouville normal form produces a symmetric discrete approximating system whereas the standard fom of (1.1) typically does not. In the case that a competing numerical method is better suited to be applied to the Sturm–Liouville problem in its standard form, that will be done (see Comparison 3.2 in Section III).

In all cases the numerical method applied to any of the forms of (1.1) gives rise to an algebraic eigenvalue problem

$$A\mathbf{c} = \mu B\mathbf{c}, \tag{1.4}$$

where the matrices A and B are defined by the particular methodology. Within each comparison the distinguishing properties of these matrices (symmetry, positive definiteness, bandedness, conditioning, ease of assembly, etc.) are identified. As a case in point here, it is often easy to argue that a banded matrix is to be more highly regarded than is a full matrix (given that assembly is roughly the same amount of work). However, if the QR algorithm is applied to the problem (1.4)

then the sparse structure is quickly lost. Comparisons 3.3 and 3.4 point to a situation where a banded matrix is not necessarily more desirable than a full matrix. Comparisons 3.4 and 3.5 further illustrate some of the considerations that should go into the choice of a map. Comparison 3.5 also includes a discussion of the special features associated with the discrete sinc-collocation system. In particular this comparison takes advantage of problem symmetry in a manner that differs from the point of view in [10]. The matrix splitting herein described could also prove useful in other approximating schemes whose discrete system (1.4) has Toeplitz structure.

Section II briefly reviews the sinc-collocation method and the associated error estimates. The commonly used maps for sinc methods are described and illustrated. Section III includes the comparisons previously discussed. The essential features of each method are included in the comparisons.

The sinc-collocation method illustrates a great versatility on all of the examples in Section III. While for a given problem a better method can often be found, as an all purpose eigenvalue routine it performs reliably and predictably on a wide class of problems. This robustness, coupled with ease of implementation, exponential convergence rate, and a matrix splitting (described in Comparison 3.5) make this method a serious competitor with other discretization techniques for the computation of the eigenvalues for Sturm–Liouville problems.

II. Sinc Function Approximation

The sinc function is defined by

$$\operatorname{sinc}(t) = \frac{\sin(\pi t)}{\pi t}, \qquad t \in (-\infty, \infty). \tag{2.1}$$

If the function w is defined on the whole real line, then for $h > 0$ the series

$$C(w, h)(t) = \sum_{k=-\infty}^{\infty} w(kh)\, S(k, h)(t), \tag{2.2}$$

where

$$S(k, h)(t) = \operatorname{sinc}\left(\frac{t - kh}{h}\right) \tag{2.3}$$

is called the Whittaker cardinal expansion of w whenever the series converges. An extensive survey of the properties of (2.2) is contained in [20]. The properties necessary for the development of the sinc-collocation method will be summarized here.

The approximation of a function w by its Whittaker cardinal expansion is

described for the class of functions in $B(S_d)$. This family is defined as follows. The function w is in $B(S_d)$ if w is analytic in the infinite strip

$$S_d \equiv \{t+is: |s| < d \leqslant \pi/2\} \tag{2.4}$$

and satisfies both of

$$\int_{-d}^{d} |w(t+is)|\, ds \to 0, \qquad t \to \pm\infty \tag{2.5}$$

and

$$N_2(w) \equiv \lim_{s \to d^-} \int_{-\infty}^{\infty} (|w(t+is)|^2 + |w(t-is)|^2)\, dt < \infty. \tag{2.6}$$

An analysis of the error incurred in approximating a function $w \in B(S_d)$ by its cardinal expansion is found in [19]. When $w \in B(S_d)$ and w and d^2w/dt^2 are approximated by

$$C_{M,N}(w, h)(t) \equiv \sum_{k=-M}^{N} w(kh)\, S(k, h)(t) \tag{2.7}$$

and

$$\frac{d^2}{dt^2} C_{M,N}(w, h)(t) \equiv \sum_{k=-M}^{N} w(kh) \frac{d^2}{dt^2} S(k, h)(t), \tag{2.8}$$

respectively, then (2.7) converges to w and (2.8) converges to d^2w/dt^2. For practical computation assume there are positive constants α, β, and C so that

$$|w(t)| \leqslant C \begin{cases} \exp(\alpha t), & t \in (-\infty, 0] \\ \exp(-\beta t), & t \in (0, \infty). \end{cases} \tag{2.9}$$

If $w \in B(S_d)$, (2.9) is satisfied, and the selections

$$h = (\pi d/(\alpha M))^{1/2} \tag{2.10}$$

and

$$N = [\![(\alpha/\beta)\, M]\!] \tag{2.11}$$

are made, then, as shown in [15] the L^2-error of the second derivative satisfies

$$\| d^2w/dt^2 - (d^2/dt^2)(C_{M,N}(w, h))\|_2 \leqslant KM^{5/4} \exp(-(\pi d \alpha M)^{1/2}), \tag{2.12}$$

where K is a positive constant depending on w and d.

The Sturm–Liouville problem (1.1) was posed on the arbitrary interval (a, b). Because the error estimate for the eigenvalues is given on the whole real line, when (a, b) is not the real line the problem must be formulated for this different interval. The following definition is needed in mapping the problem (1.1) to the real line.

DEFINITION 2.1. Let D_d be a simply connected domain in the complex $z = x + iy$ plane with boundary ponts $a \neq b$ (Fig. 1). Let ϕ be a conformal map of D_d onto the infinite strip S_d (2.4) with $\phi(a) = -\infty$ and $\phi(b) = \infty$. Let the inverse map of ϕ be ψ and define

$$\Gamma = \{\psi(t) : -\infty < t < \infty\} \tag{2.13}$$

and

$$z_k = \psi(kh), \qquad k = 0, \pm 1, \ldots . \tag{2.14}$$

If the change of variable

$$w(t) = (\sqrt{\phi'}\, u) \circ \psi(t) \tag{2.15}$$

is made in (1.1), the transformed problem, as shown in [7], takes the form

$$\begin{gathered} -w''(t) + \gamma_q(t)\, w(t) = \lambda \rho(\psi(t))(\psi'(t))^2\, w(t), \qquad -\infty < t < \infty, \\ \lim_{t \to \pm\infty} w(t) = 0, \end{gathered} \tag{2.16}$$

where

$$\gamma_q(t) = -(\psi'(t))^{1/2} \frac{d}{dt}\left\{(1/\psi'(t)) \frac{d}{dt}((\psi'(t))^{1/2})\right\} + [\psi'(t)]^2\, q(\psi(t)). \tag{2.17}$$

If the transformed problem is approximated by collocating the sinc expansion (2.7) at the nodes $t_i = ih$, $-M \leqslant i \leqslant N$, the generalized eigenvalue problem (of the form (1.4)) results

$$\{-(1/h^2)\, I^{(2)} + D(\gamma_q)\}\, \mathbf{w} = \mu D(\rho(\psi')^2)\mathbf{w} \tag{2.18}$$

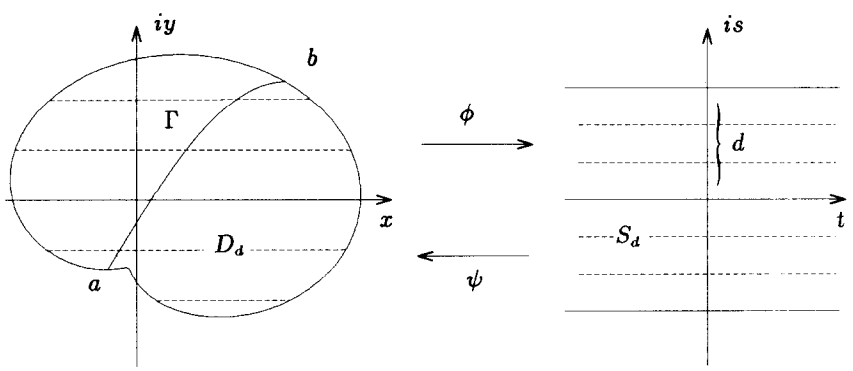

FIG. 1. The map ϕ and its inverse ψ.

with

$$I^{(2)} = \begin{bmatrix} \frac{\pi^2}{3} & \frac{-2}{1^2} & \frac{2}{2^2} & \cdots & & \frac{(-1)^{m-1}2}{(m-1)^2} \\ \frac{-2}{1^2} & \frac{\pi^2}{3} & & & & \\ \frac{2}{2^2} & & \ddots & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & \ddots & \ddots & \frac{2}{2^2} \\ & & & & \frac{\pi^2}{3} & \frac{-2}{1^2} \\ \frac{(-1)^{m-1}2}{(m-1)^2} & & \cdots & \frac{2}{2^2} & \frac{-2}{1^2} & \frac{\pi^2}{3} \end{bmatrix}. \tag{2.19}$$

Here $m = M + N + 1$, $D(r)$ is a diagonal matrix of dimension $m \times m$ with the (i, i)th element given by $r(t_i)$, $\mathbf{w}$ is an $m \times 1$ vector with ith element $w(t_i)$, and μ is the approximation of the eigenvalues λ of the continuous Sturm–Liouville problem.

The importance of known error bounds in the usefulness of a method has already been stated. The following Theorem 2.1 gives this error in the eigenvalue approximation. This theorem was stated and proven in [7] for the differential equation (1.1) transformed to the whole real line. The eigenvalues, however, of the transformed problem (2.16) and the Sturm-Liouville problem (1.1) are identical; hence the eigenvalue error bound given holds for the original differential equation without doing the transformation. Thus in practice the transformation need not be done. It merely facilitates the proof of the eigenvalue error bound. The generalized eigenvalue problem for the original Sturm–Liouville problem (1.1) is given by

$$\{-(1/h^2)\, I^{(2)} + D(-(\phi')^{-3/2}((\phi')^{-1/2})'' + q/(\phi')^2)\}\, \mathbf{z} = \mu D(\rho/(\phi')^2)\, \mathbf{z} \tag{2.20}$$

or

$$A\mathbf{z} = \mu \mathscr{D}^2 \mathbf{z} \tag{2.21}$$

where

$$\mathscr{D} = D(\sqrt{\rho}/(\phi')). \tag{2.22}$$

The following theorem then holds.

THEOREM 2.1. *Let λ_0, u_0 be an eigenpair of the Sturm–Liouville problem* (1.1). *Assume that $\sqrt{\phi'}\, u_0 \circ \psi \in B(S_d)$ and there are positive constants α, β, and C so that*

$$|\sqrt{\phi'(x)}\, u(x)| \leqslant C \begin{cases} \exp(-\alpha\,|\phi(x)|), & x \in \Gamma_a \\ \exp(-\beta\,|\phi(x)|), & x \in \Gamma_b \end{cases} \tag{2.23}$$

where

$$\Gamma_a = \{\psi(t): t \in (-\infty, 0]\}, \quad \Gamma_b = \{\psi(t): t \in (0, \infty)\}. \tag{2.24}$$

If there is a constant $\delta > 0$ so that $|\gamma_q(x)| \geqslant \delta^{-1}$, where

$$\gamma_q(x) = -(\phi'(x))^{-3/2}\,((\phi'(x))^{-1/2})'' + (\phi'(x))^{-2}\, q(x) \tag{2.25}$$

and the selections $h = (\pi d/(\alpha M))^{1/2}$ and $N = [\![(\alpha/\beta)\, M]\!]$ are made, then there is an eigenvalue μ_p of the generalized eigenvalue problem (2.20) *satisfying*

$$|\mu_p - \lambda_0| \leqslant K(\delta\lambda_0)^{1/2}\, M^{3/2} \exp(-(\pi d \alpha M)^{1/2}). \tag{2.26}$$

The inequality (2.26) holds for arbitrary eigenvalues λ_0. The factor $\sqrt{\lambda_0}$ indicates that the smaller spectral values are approximated more accurately than the larger spectral values.

The appropriate conformal map for (1.1) is determined by the interval (a, b) and the asymptotic behavior of the eigenfunctions. If the interval is finite the map used is

$$\phi_1(x) = \ln\left(\frac{x-a}{b-x}\right). \tag{2.27}$$

For the semi-infinite interval $(0, \infty)$, there are two available maps. For the user this causes little problem as both typically work quite well. Careful selection may produce even further improvement for a given problem. The choice is described in [7] and will be further discussed in the appropriate comparisons of Section III. One must choose between

$$\phi_2(x) = \ln(x) \tag{2.28}$$

and

$$\phi_3(x) = \ln(\sinh(x)). \tag{2.29}$$

These maps and the terms of the discrete system (2.20) are given in Fig. 2. While (2.20) appears complicated, note that the terms for these maps simplify dramatically so that the implementation is straightforward. The last line of Fig. 2 corresponds to either the identity map or no map (due to (2.12)) depending on one's point of view. It plays a role in problems on the entire real line whose solutions have the decay rates indicated in (2.9).

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

$$A\mathbf{z} = \mu \mathscr{D}^2 \mathbf{z}, \qquad \mathscr{D} = D(\sqrt{\rho}/\phi')$$

Interval	ϕ	$(\phi')^{-1}$	$-(\phi')^{-3/2}((\phi')^{-1/2})''$	x_k
(a, b)	$\phi_1(x) = \ln\left(\frac{x-a}{b-x}\right)$	$\frac{(x-a)(b-x)}{b-a}$	$\frac{1}{4}$	$\frac{be^{kh}+a}{e^{kh}+1}$
$(0, \infty)$	$\phi_2(x) = \ln(x)$	x	$\frac{1}{4}$	e^{kh}
$(0, \infty)$	$\phi_3(x) = \ln(\sinh(x))$	$\tanh(x)$	$\frac{4\cosh^2 x - 3}{4\cosh^4 x}$	$\ln[e^{kh} + \sqrt{e^{2kh}+1}]$
$(-\infty, \infty)$	$\phi_4(x) = x$	1	0	kh

FIG. 2. Terms for the discrete system (2.20).

The implementation of the method has been fully described in [7]. All parameter choices are made as in Theorem 2.1. The determination of the quantity α when the left endpoint is finite comes from the Frobenius technique. Thus for the comparisons in Section III choose

$$\alpha = s_+ - \tfrac{1}{2}, \tag{2.30}$$

where s_+ is the positive root of the indicial equation

$$s(s-1) - q_a = 0 \tag{2.31}$$

and

$$q_a = \lim_{x \to a^+} (x-a)^2 q(x). \tag{2.32}$$

If the interval (a, b) is finite, then β is determined similarly. In the case of the semi-infinite interval $(0, \infty)$ the WKB method determines β. Over the interval $(-\infty, \infty)$ the WKB method also determines α. In the case that the eigenfunctions are symmetric $\alpha = \beta$. In this latter case (symmetry of eigenfunctions) advantage may also be taken of the form of the discrete system (2.20). This is described in Comparison 3.5. The comparison of the performance of various Galerkin methods to this sinc-Galerkin method is reported in detail in the following section.

III. Comparisons

Galerkin schemes are well-known and often-used methods implemented for the numerical calculation of 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 (i.e., sinc-Galerkin) to several of these alternative schemes.

Because of the inherent differences in the methods (in some cases they are dramatically different), it is difficult to formulate in a precise manner a single criterion by which Method A may be declared "better" than Method B. If on one problem Method A performs better than Method B based on a single criterion, the roles of the methods may reverse on another problem. This role reversal can also occur in the assessment of the merits of the methods even on the same problem if one's criteria changes. Hence in an attempt to avoid prejudicial comparions this section will include both quantitative criteria (size of discrete system, work required to assemble the matrices and the accuracy attained) and qualitative criteria (factors such as symmetry and matrix structure, effort involved in changing q, ρ or the interval (a, b), ease of implementation and applicability to a broad class of singular as well as regular Sturm–Liouville problems).

Five examples are used in making the comparisons. The Fourier equation is used in Comparison 3.1 as representative of a regular Sturm–Liouville problem. Comparison 3.2 is a singular problem (Bessel's equation) on a finite interval ($q(x)$ has a singularity at $x=0$). The radial Schrödinger equation with the Woods–Saxon and harmonic oscillator type potentials is used in Comparison 3.3 and 3.4, respectively. These are representative of commonly occurring singular problems on the half-line $(0, \infty)$. The Hermite equation is an example on the whole real line $(-\infty, \infty)$ and is discussed in Comparison 3.5.

Several methods easily found in the literature are discussed in the comparisons. These include (i) the Rayleigh–Ritz (finite element) method with cubic spline and piecewise cubic Hermite basis functions, (ii) a spectral method with Chebyshev basis functions, (iii) a tau (spectral) method, and (iv) other mappings and/or domain truncation in combination with spectral or collocation methods.

Comparison 3.1 (Fourier).

$$\begin{aligned} -u''(x) &= \lambda u(x), \qquad 0 < x < 1 \\ u(0) &= u(1) = 0. \end{aligned} \tag{3.1}$$

This regular problem is useful in highlighting numerous aspects of eigenvalue approximation. Since the problem is so well behaved, the literature abounds with the application of many standard methods that work well. While many of these same schemes encounter difficulties on singular problems, this problem serves to emphasize the point that when results are acceptable, "the simpler the method is, the better."

The parameters necessary to implement the sinc method are $\alpha = \beta = \frac{1}{2}$ which yields $h = \pi/\sqrt{N}$. Since $\alpha = \beta$, the choice $M = N$ is also made. The map ϕ_1 in (2.27) is used and the discrete system (2.20) reduces to (by Fig. 2)

$$\left[-\frac{1}{h^2} I^{(2)} + D\left(\frac{1}{4}\right) \right] \mathbf{z} = \mu D((x(1-x))^2)\, \mathbf{z}. \tag{3.2}$$

The sinc method applied to this problem has the advertised exponential rate of convergence of Theorem 2.1. In general, spectral methods will have an exponential convergence rate of $O(\exp(-1/h^v))$, $v > 0$. Finite element methods have an algebraic convergence rate of $O(h^p)$, p a positive integer. Whereas the former is always more rapid than the latter ($\exp(-1/h^v)/h^p \to 0$ as $h \to 0$), computationally the method with algebraic convergence may be superior for modestly small h. In the case of the sinc method the convergence rate is

$$O(\exp(-(\pi d/h))) = O(\exp(-(\pi^2/(2h))))$$

for the Fourier equation since d may be chosen to be $\pi/2$. The convergence rate for the Rayleigh–Ritz (finite element) method with linear spline basis functions is $O(h^2)$. The results for the first eigenvalue (using the linear spline basis) are given in Table I along with those for the sinc method. The corresponding size of the matrices is included, where it must be remembered that the matrix A in (1.4) is full for the sinc method and tridiagonal for this particular Rayleigh–Ritz method.

The Rayleigh–Ritz method (even with algebraic convergence) is more accurate for small discrete systems. The sinc method uses $h = \pi/\sqrt{N} = \pi/\sqrt{(m-1)/2}$ ($m = 2N+1$ being the order of the coefficient matrix A in (1.4)) while the Rayleigh–Ritz method with linear spline basis uses $h = 1/m$. Thus the sinc method has exponential convergence rate $O(\exp(-\pi\sqrt{N}/2)) = O(\exp(-\pi\sqrt{(m-1)}/(2\sqrt{2})))$ while the Rayleigh–Ritz method with linear spline basis has algebraic convergence rate $O(1/m^2)$. The function

$$f(m) = m^2 e^{-\pi\sqrt{(m-1)}/(2\sqrt{2})}$$

TABLE I

Fourier Equation: Error in Computed Eigenvalues for the Rayleigh–Ritz Method with Linear Spline Basis and for the Sinc Method

	Rayleigh–Ritz method		Sinc method	
True eigenvalue	Matrix size	Error	Error	Matrix size
π^2	10×10	$0.669 - 1$	$0.179 - 1$	9×9
	20×20	$0.184 - 1$	$0.299 - 2$	19×19
	40×40	$0.483 - 2$	$0.119 - 4$	39×39

is bounded below by 1 for all $m \leqslant 50$. That is, the asymptotic exponential convergence rate of the sinc method is not dominant until $m \geqslant 51$. As can be seen in Table I the sinc method error decreases below that of the Rayleigh–Ritz method by the time the system is 20×20. There is a splitting (described in Comparison 3.5) of the discrete system that essentially reduces the system size reported in the last column of Table I for the sinc method to 5×5, 10×10, and 20×20.

However, if the Rayleigh–Ritz method is used with cubic splines or piecewise cubic Hermite basis functions (these are $O(h^6)$ methods) the exponential convergence rate of the sinc method lags behind until $m \geqslant 1194$. In these cases the discrete system has bandwidth seven and results far superior to those in Table I are obtained, [1].

As this indicates, for a Sturm–Liouville problem with eigenfunctions analytic in a domain in the complex plane containing the closed interval $[a, b]$, the algebraic rate of convergence of low order Rayleigh–Ritz methods is sufficiently accurate. If however q and/or ρ have singularities at a and/or b (as in Bessel's equation of Comparison 3.2) the algebraic convergence rate of the Rayleigh–Ritz method is no longer guaranteed. As will be seen (and justified by Theorem 2.1) the sinc method maintains its exponential convergence rate in these singular problems.

Comparison 3.2 (Bessel).

$$-u''(x) + \left(\frac{4n^2 - 1}{4x^2}\right) u(x) = \lambda u(x), \qquad 0 < x < 1, \, n \geqslant 1$$
$$u(0) = u(1) = 0. \tag{3.3}$$

This family (for varying parameter n) of singular Sturm–Liouville problems (due to the singularity in $q(x) = (4n^2 - 1)/(4x^2)$ at $x = 0$) illustrates the differences in the comparison of methods when the problem is not regular. Theorem 2.1 guarantees the same convergence rate for this problem as for the Fourier equation when the sinc method is applied. The parameters for the sinc method are $\alpha = n$ and $\beta = \frac{1}{2}$ which yield $h = \pi/\sqrt{N}$, where $N = 2nM$. The discrete system (2.20), with the map ϕ_1 in (2.27), takes the form

$$\left[-\frac{1}{h^2} I^{(2)} + D\left(\frac{1}{4} + \frac{1}{4}(4n^2 - 1)(1 - x)^2\right)\right] \mathbf{z} = \mu D((x(1-x))^2)\, \mathbf{z}. \tag{3.4}$$

Referring to (3.2), the only modification in the discrete system to arrive at (3.4) is a different diagonal matrix which is filled by point evaluations. The parameters α and β (governed by the possible high order root of the eigenfunctions near zero) dictate that fewer basis functions are required near zero and this difference is magnified as n increases ($N = 2nM$). Asymptotically the convergence rate is the same as in the regular Sturm–Liouville problem used in Comparison 3.1 ($O(\exp(-\pi\sqrt{N}/2))$), however M (and thus the number of basis functions m) is much smaller.

Another method that takes advantage of the high order zero of the eigenfunctions is the tau method [13]. In [9] the first eigenvalue of (3.3) for $n=7$ is computed using the tau method with Chebyshev basis functions. They use the standard form of (3.3) which can be obtained by letting

$$u(x)=\sqrt{x}\,y(x). \tag{3.5}$$

This yields

$$\begin{gathered}-y''(x)-\frac{1}{x}y'(x)+\frac{n^2}{x^2}y(x)=\lambda y(x), \qquad 0<x<1,\ n\geqslant 1 \\ y(0)=y(1)=0.\end{gathered} \tag{3.6}$$

This form does not produce a symmetric discrete system, however it can be argued that the exponential convergence rate of the tau method offsets this drawback.

When applying the tau method, two inner products defined by the integration of the Chebyshev basis functions against their first and second derivatives, respectively, are required. Therefore every element of this nonsymmetric discrete system requires two numerical quadratures, which must be calculated to at least the same accuracy as the method. This additional preliminary work detracts from this method. However the results in Table II are certainly satisfactory and are similar to those of the sinc method.

Here $J_n(x)$ denotes the Bessel function of order n. A "pole condition" is also described in [9] which improves the convergence of the tau method. This condition, $y'(0)=0$, adds an additional equation to the discrete system. Gottlieb and Orszag point out that the pole condition must be applied properly so as not "to degrade significantly the accuracy of spectral computations." In particular, for $n=1$ the pole condition must be modified as $J_1'(0)\neq 0$. Thus the pole condition does not have widespread applicability. However, for Bessel's equation with $n=7$ excellent results for the tau method with the pole condition are reported in [9].

Spectral methods using Chebyshev basis functions are used widely. When the problem is posed on an interval other than $(-1, 1)$, an intermediate mapping is commonly employed. Further discussion of this is included in Comparisons 3.4 and 3.5.

TABLE II

Bessel Equation for $n=7$: Error in Computed Eigenvalues for the Chebyshev Tau Method and for the Sinc Method

True eigenvalue $\lambda_1=j_{71}^2$, where $J_7(j_{71})=0$	Spectral method		Sinc method	
	Matrix size	Error	Error	Matrix size
122.907600204	18×18	$3.650-0$	$0.152-0$	15×15
	26×26	$0.651-3$	$0.537-3$	30×30

Comparison 3.3 (Woods–Saxon).

$$-u''(x)+u(x)=\lambda(1+e^{(x-r)/\varepsilon})^{-1}u(x), \qquad 0<x<\infty$$
$$u(0)=u(\infty)=0. \tag{3.7}$$

This is a singular Sturm–Liouville problem due to the semi-infinite domain, $(0, \infty)$. The coefficient function $\rho(x)=(1+e^{(x-r)/\varepsilon})^{-1}$ also has singularities in the complex plane at $z=r+\varepsilon(2n+1)\pi i$. The eigenfunctions satisfy

$$u_\lambda(x)\sim\exp(-(x-r)/\varepsilon), \qquad x\to\infty \tag{3.8}$$

and as the domain of (3.7) is $(0, \infty)$ either of the maps ϕ_2 in (2.28) or ϕ_3 in (2.29) are applicable (they both satisfy the bound in (2.23)). While the choice of map is not critical the reasoning which follows indicates a slightly more rapid convergence rate for ϕ_3 as opposed to ϕ_2 (note, however, that the discrete system for the choice ϕ_2 is simpler). The angle d for the sector denoted D_2 determined by ϕ_2 is limited by the coefficient singularity of $\rho(x)$. Using the values $r=5.086855$ and $\varepsilon=0.929853$ found in [17] the restriction on d for D_2 is $d=\mathrm{Tan}^{-1}(\varepsilon\pi/r)\sim\pi/6$. Since $\varepsilon\pi>\pi/2$ the domain denoted D_3 for the map ϕ_3 is not restricted and so here the choice $d=\pi/2$ is suitable. Thus the convergence rate for the sinc method with the map ϕ_2 is (from Theorem 2.1) $O(\exp(-\pi\sqrt{\alpha M/6}))$ while for the map ϕ_3 it is $O(\exp(-\pi\sqrt{\alpha M/2}))=O((\exp(-\pi\sqrt{\alpha M/6}))^{\sqrt{3}})$. The factor of $\sqrt{3}$ is not dramatic; however, it can easily be detected in the numerical results.

The parameters for the discrete system (2.20) with the map ϕ_3 are $\alpha=\frac{1}{2}$ and $\beta=1$ which yields (with $d=\pi/2$) $h=\pi/\sqrt{2N}$, where $M=2N$. The system becomes (see Fig. 2)

$$\left[-\frac{1}{h^2}I^{(2)}+D\left(\frac{4\cosh^3 x-3}{4\cosh^4 x}+\tanh^2 x\right)\right]\mathbf{z}=\mu D\left(\frac{\tanh^2 x}{1+e^{(x-r)/\varepsilon}}\right)\mathbf{z}. \tag{3.9}$$

Even here the differences in the discrete systems (3.2), (3.4), and (3.9) are merely different diagonal matrices filled by point evaluations.

A typical finite element treatment of (3.7) proceeds along the following lines. Select $T>0$ and solve (3.7) with $u(T)=0$ replacing $u(\infty)=0$. The error incurred in the Rayleigh–Ritz method (with either cubic spline or piecewise cubic Hermite bases) for the perturbed but now regular Sturm–Liouville problem is $O(h^6)$, where $h=T/n$, n being the number of basis functions. This procedure was implemented in [18]. The error due to the truncation of the domain to $(0, T)$ is in [17] for both of the above-mentioned bases. There the piecewise cubic Hermite basis yielded a slightly better approximation.

Once the truncation level T has been selected these methods reduce to a generalized matrix problem of the form (1.4) where A and B have bandwidth seven. The matrix A is extremely simple to fill since in (1.1) $q(x)\equiv 1$. To fill B, a quadrature of the same order as that of the method employed (here $O(h^6)$) is

required. Thus A and B each have $30+7(m-8)$ nonzero entries when they are $m \times m$. However, B involves considerable effort as each nonzero entry requires an integration of the form

$$\int_0^T (1+e^{(x-r)/\varepsilon})^{-1} H_i(x) H_j(x)\, dx, \tag{3.10}$$

where H_i is the ith basis function. The sinc method requires m point evaluations for each of A and B. Table III contains some of the results reported in [17].

The accuracy of the Rayleigh–Ritz method is certainly more favorable if the criterion is solely accuracy for a given matrix size. This example does not, however, convey the necessary interaction between the choices of T and h for the Rayleigh–Ritz method. It appears that only the choice of h affects the error in the eigenvalue approximation. However, simply increasing the number of basis functions does not necessarily decrease the error. As is pointed out in [17] the error is governed by both the number of basis elements and the truncation level T and they give bounds on each. However, the crucial concurrent choice of both of these parameters needs further study. The next Comparion 3.4 more accurately depicts the impact that these parameter choices may have on the eigenvalue approximation.

A convenience in the sinc method is that to obtain an error of $10^{-\delta}$ (remembering that these are asymptotic bounds), the right-hand side of (2.26) dictates equating $e^{-\pi\sqrt{2N}/2}$ to $10^{-\delta}$. Thus conservatively, the choice of N given by

$$N = \left[\!\!\left[\frac{2(\delta \ln 10)^2}{\pi^2} + 1 \right]\!\!\right] \tag{3.11}$$

is sufficient. Although N in (3.11) is typically an overestimate (from Table III four digits of accuracy is attained with $N=9$ whereas (3.11) with $\delta=4$ predicts $N=18$)

TABLE III

Radial Schrödinger Equation with Woods–Saxon Potential: Error in Computed Eigenvalues for the Rayleigh–Ritz Method with Piecewise Cubic Hermite Basis and for the Sinc Method

	Rayleigh–Ritz method			Sinc method	
True eigenvalue	Truncation level and step size	Matrix size	Error	Error	Matrix size
1.424333	$T=12$ $h=1.2$	18×18	$0.34-5$	$0.590-3$	19×19
	$T=13$ $h=1.0$	24×24	$0.14-5$	$0.15-3$	25×25
	$T=18$ $h=1.2$	28×28	$0.35-5$	$0.818-4$	28×28

the bound in (2.26) clearly indicates that increasing N (equivalently increasing $m = M + N + 1$, the number of basis functions) will decrease the error in the estimate.

The above mentioned points are not unique to the discussion of the Rayleigh–Ritz method with piecewise cubic Hermite basis versus the sinc method. They arise in the comparison of finite element and collocation methods in general when applied to problems on $(0, \infty)$. The latter is, in general, more easily implemented due to the point evaluation used in defining the matrices of the discrete system (which may be full) while the former has a banded structure that may create a bit more work to fill. The finite element method involves a domain truncation whereas collocation, with a globally defined basis deals with the "analogue" of this difficulty via coefficient damping or mapping. More discussion of these techniques is included in Comparison 3.4. The important point is that the Galerkin method with sinc basis functions has the exponential convergence typically associated with a spectral method as well as the ease of implementation in filling the discrete system via point evaluations typically associated with collocation.

Comparison 3.4 (Harmonic Oscillator Type).

$$\begin{gathered} -u''(x) + (x^2 + \gamma x^{-2})\, u(x) = \lambda u(x), \qquad 0 < x < \infty \\ u(0) = u(\infty) = 0 \end{gathered} \tag{3.12}$$

This is a singular Sturm–Liouville problem due to both the infinite interval $(0, \infty)$ and the singularity in the coefficient function $q(x) = x^2 + \gamma x^{-2}$ at $x = 0$ (for $\gamma \neq 0$). The eigenfunctions may have singularities depending on the value of γ. If $\gamma = 2$ (3.12) is the radial Schrödinger equation with harmonic oscillator potential which has been considered by numerous authors ([7, 17, 18] in particular). For arbitrary γ the eigenfunctions of (3.12) are given by

$$u_\lambda(x) = x^{r(\gamma)} y_\lambda(x)\, e^{-x^2/2}, \tag{3.13}$$

where

$$r(\gamma) = (1 + \sqrt{4\gamma + 1})/2 \tag{3.14}$$

and the $y_\lambda(x)$ satisfy

$$-xy''(x) + 2(x^2 - r(\gamma))\, y'(x) + (2r(\gamma) + 1)\, xy(x) = \lambda(\gamma)\, xy(x). \tag{3.15}$$

The associated eigenvalues $\lambda(\gamma)$ are given by

$$\lambda_j(\gamma) = 2r(\gamma) + 1 + 4(j - 1), \qquad j = 1, 2, 3, \ldots. \tag{3.16}$$

Hence in the case of the harmonic oscillator, $r(2) = 2$, and the eigenfunctions (3.13) are entire functions. If $\gamma = 0$, the eigenfunctions are a subset of the Hermite functions (Comparison 3.5); however, if $\gamma = \frac{3}{4}$, the eigenfunctions have a branch

singularity at $x=0$. Each of these distinctly different cases may require a different numerical treatment and will be discussed in what follows.

As in Comparison 3.3, since the domain of (3.12) is $(0, \infty)$ either ϕ_2 in (2.28) or ϕ_3 in (2.29) is appropriate (again both satisfy the bound (2.23)). When ϕ_3 is used as was done in Comparison 3.3, the discrete system (3.9) is obtained with $\tanh^2 x$ replaced by $(x^2+\gamma x^{-2})\tanh^2 x$ on the left-hand side and $\rho(x)=(1+e^{(x-r)/\varepsilon})^{-1}$ replaced by $\rho(x)\equiv 1$ on the right-hand side. With $\gamma=2$ in (3.12), the solutions were computed in [7] using ϕ_3 since for this map d may be taken to be $\pi/2$. As pointed out in [7], this is the preferred method corresponding to the two maps since d is bounded above by $\pi/4$ in the case of the map ϕ_2.

However, for the purpose of illustrating the map ϕ_2, the discrete system (2.20) with ϕ_2 was used to approximate the eigenvalues of (3.12). The system becomes (see Fig. 2)

$$\left[-\frac{1}{h^2}I^{(2)}+D\left(\frac{1}{4}+x^4+\gamma\right)\right]\mathbf{z}=\mu D(x^2)\,\mathbf{z}. \tag{3.17}$$

Again the modifications to arrive at this discrete system are simple point evaluations to fill the diagonal matrices. The parameters used are $\alpha(\gamma)=r(\gamma)-1/2$, $d=\pi/4$, and $h=\pi/(2\sqrt{\alpha(\gamma)M})$, where $N=[\![\ln(\alpha(\gamma)Mh)/h+1]\!]$.

The harmonic oscillator ($\gamma=2$) was reported in [17], where the Rayleigh–Ritz method was used with either piecewise cubic Hermite basis or cubic splines (similar to what was discussed in Comparison 3.3). Due to the much more rapid decrease of the eigenfunctions as compared to those of the Woods–Saxon potential, the truncation level T is considerably smaller for the harmonic oscillator. The matrices A and B in (1.4) again have bandwidth seven, however, with regard to filling these matrices, the roles of A and B have been reversed. The matrix A requires quadratures while B is simple to fill, since $\rho(x)\equiv 1$. Table IV contains some of the numerical results.

Here and in the further numerical results of [17], the interconnected choice of T and h for this Rayleigh–Ritz method on the truncated domain is more clearly seen. Results for $T=7$ are also given there and they are the same as for $T=6$ reported above. This indicates that the truncation level has increased to the point where the decaying solution is not significantly different (computationally) from zero at T. This choice of T (intimately related to the choice of h) requires careful estimations. The number N (the upper limit in the sum for the sinc method) gives a corresponding largest gridpoint for the sinc method of $t_N=e^{Nh}=7.71$. This in a vague way relates to the truncation level T used in the Rayleigh–Ritz method.

A procedure which has the interval truncation of this Rayleigh–Ritz method and the globally defined basis functions of a spectral method was implemented on a modified form of (3.12) (with $\gamma=0$) in [10]. The technique for (3.12) is to truncate the interval to $(0, T)$ and assume an approximate solution of the form

$$u_M(x)=\sum_{j=0}^{M} c_j T_j(\chi(x)), \tag{3.18}$$

TABLE IV

Radial Schrödinger Equation with Harmonic Oscillator Potential ($\gamma = 2$): Error in Computed Eigenvalue for the Rayleigh–Ritz Method with Piecewise Cubic Hermite Basis and for the Sinc Method

	Rayleigh–Ritz method			Sinc method	
True eigenvalue	Truncation level and step size	Matrix size	Error	Error	Matrix size
9	$T=5$ $h=0.5$	18×18	$0.39-3$	$0.974-2$	19×19
	$T=6$ $h=0.5$	22×22	$0.37-3$	$0.204-2$	24×24
	$T=5$ $h=0.25$	38×38	$0.31-4$	$0.105-3$	34×34
	$T=6$ $h=0.25$	46×46	$0.91-5$	$0.215-5$	47×47

where

$$\chi(x) = 2x/T - 1 \tag{3.19}$$

and

$$T_j(\xi) = \cos(j\cos^{-1}(\xi)). \tag{3.20}$$

T_j is the jth Chebyshev polynomial of the first kind. Note that (3.19) maps the domain $(0, T)$ to $(-1, 1)$ so that the Chebyshev basis may be used. This technique of domain truncation was satisfactory; however, [10] favored algebraically mapping the semi-infinite interval to $(-1, 1)$ directly. A mapping such as

$$\chi(x) = 2\left(\frac{x}{L+x}\right) - 1 \tag{3.21}$$

for a contant L accomplishes this and thus no truncation of the infinite interval is necessary. Both of these approaches have merit. A comparative study of domain truncation versus algebraic mapping for the expansion of certain model functions was reported in [3]. That study favored domain truncation in the case of entire functions (for example, when $\gamma = 0$ or 2 in (3.12)) and algebraic mapping in the case of singular functions (for example, when $\gamma = \frac{3}{4}$ in (3.12)). Each method works well as a spectral method and the choice is problem dependent. As is to be expected the sinc method works for the singular case, $\gamma = \frac{3}{4}$, and results are reported in [14].

Comparison 3.5 (Hermite).

$$\begin{aligned} -u''(x) + (x^2/4)\,u(x) &= \mu u(x), \qquad -\infty < x < \infty \\ u(-\infty) = u(\infty) &= 0. \end{aligned} \tag{3.22}$$

The computation of the eigenvalues of the Hermite equation was dealt with in [10] by considering the even and odd eigenfunctions separately. The eigenvalues are $\mu_n = n + \frac{1}{2}$ and the corresponding eigenfunctions are the Hermite functions. These are even or odd functions as n is even or odd. To calculate the odd eigenvalues it is only necessary to solve

$$\begin{aligned} -u''(t) + (t^2/4)\,u(t) &= \mu_{2n-1} u(t), \qquad 0 < t < \infty \\ u(0) = 0,\ u(\infty) &= 0. \end{aligned} \tag{3.23}$$

Setting $t = \sqrt{2}x$ reduces (3.23) to the form (3.12) where $\lambda_{2n-1} = 2\mu_{2n-1} = 4n - 1$ for $n = 1, 2, 3, \ldots$. Similarly the even eigenvalues may be calculated from

$$\begin{aligned} -u''(t) + (t^2/4)\,u(t) &= \mu_{2n} u(t), \qquad 0 < t < \infty \\ u(0) = c,\ u(\infty) &= 0, \end{aligned} \tag{3.24}$$

where the eigenfunctions are normalized by $u(0) = c$. As in Comparison 3.2 these special conditions (there the pole condition, here even and odd eigenfunctions) are problem dependent. This appears to be a considerable amount of work which could be avoided by merely dealing directly with the Hermite equation (3.22). This problem, as well as others that have symmetric potential and weight functions, may be treated as just described in order to reduce the computational work. Due to the Toeplitz structure of the system (2.20) the sinc-collocation method applied to (3.22) admits a splitting in the discrete system analogous to the even and odd eigenfunction splitting of (3.22) cited above. To see this, use centered sums ($M = N$), where $m = 2M + 1\,(M = N)$ and write (see Fig. 2) in the form

$$A = -\frac{1}{h^2} I^{(2)} + \kappa I + D(r), \tag{3.25}$$

where κ is a constant and $r(-x) = r(x)$ in the diagonal matrix $D(r)$. Here $r(x) = q(x)/(\phi'(x))^2$. The matrix in (3.25) admits the representation

$$A = \frac{-1}{h^2} \begin{pmatrix} I_M^{(2)} & \mathbf{c}_{M\times 1} & L_M' \\ (\mathbf{c}_{M\times 1})' & \pi^2/3 & (\mathbf{c}_{M\times 1})' J \\ L_M & J\mathbf{c}_{M\times 1} & I_M^{(2)} \end{pmatrix} + \kappa I_m + \begin{pmatrix} D_-(r) & & \bigcirc \\ & r(0) & \\ \bigcirc & & D_+(r) \end{pmatrix}, \tag{3.26}$$

where the subscripts denote the block sizes, $I_M^{(2)}$ is the $M \times M$ matrix $I^{(2)}$ as in (2.19), $\mathbf{c}_{M\times 1}$ consists of the first M elements of the $(M+1)$th column of $I_m^{(2)}$ and L_M is the $M \times M$ portion of $I_m^{(2)}$ in its lower left-hand corner. The $M \times M$ matrices

$$D_{\mp}(r) = \operatorname{diag}(r(x_{\mp k})) \tag{3.27}$$

are connected by the $M \times M$ matrix

$$J = \begin{pmatrix} & & & 1 \\ & \bigcirc & \iddots & \\ & 1 & \bigcirc & \\ 1 & & & \end{pmatrix} \tag{3.28}$$

via

$$D_-(r) = JD_+(r)\,J, \tag{3.29}$$

since r is an even function and $x_{-k} = -x_k$.

The $m \times m$ orthogonal matrix

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} I_M & \mathbf{O}_{M\times 1} & I_M \\ (\mathbf{O}_{M\times 1})^t & \sqrt{2} & (\mathbf{O}_{M\times 1})^t \\ -J_M & \mathbf{O}_{M\times 1} & J_M \end{pmatrix}$$

block diagonalizes A as follows:

$$\begin{aligned} Q^*AQ = \frac{-1}{h^2} &\begin{pmatrix} I_M^{(2)} - JL_M & \mathbf{O}_{M\times 1} & O_M \\ (\mathbf{O}_{M\times 1})^t & \pi^2/3 & \sqrt{2}(\mathbf{c}_{M\times 1})^t \\ O_M & \sqrt{2}\,\mathbf{c}_{M\times 1} & I_M^{(2)} + JL_M \end{pmatrix} \\ &+ \kappa I_m + \begin{pmatrix} D_-(r) & \mathbf{O}_{M\times 1} & O_M \\ (\mathbf{O}_{M\times 1})^t & r(0) & (\mathbf{O}_{M\times 1})^t \\ O_M & \mathbf{O}_{M\times 1} & D_+(r) \end{pmatrix}. \end{aligned} \tag{3.30}$$

Hence the spectrum of A is the same as the union of the spectrums of the two matrices

$$A^- = \frac{-1}{h^2}\,(I_M^{(2)} - JL_M) + \kappa I_M + D_-(r) \tag{3.31}$$

and

$$A^+ = \frac{-1}{h^2} \begin{pmatrix} \pi^2/3 & \sqrt{2}\,(\mathbf{c}_{M\times 1})^t \\ \sqrt{2}\,\mathbf{c}_{M\times 1} & I_M^{(2)} + JL_M \end{pmatrix} + \kappa I_{M+1} + \begin{pmatrix} r(0) & (\mathbf{O}_{M\times 1})^t \\ \mathbf{O}_{M\times 1} & D_+(r) \end{pmatrix}. \tag{3.32}$$

In the case that ρ in (1.1) is symmetric (it is identically one in (3.22)) the eigenvalues of $A_{\mp}$ are the approximate eigenvalues of the continuous problem. In the case that ρ is nonconstant but symmetric, this follows from (3.29) with r replaced by ρ.

This splitting would be aesthetically complete if one could assert that the spectrums of A^- and A^+ interlace one another. Such a result implies for example that the approximate smallest eigenvalue of the continuous problem is contained in the

spectrum of A^+. Whereas this is the authors' experience in numerical computation, an analytic statement along these lines does not appear to be an elementary argument. Such techniques as Weyl's separation theorem [21] give only crude estimates due to the large size of A^+ (or A^-) relative to the size of A.

Before turning to the computations for the Hermite example (3.22), note that the splitting that occurs in the first matrix on the right-hand side of (3.30) is independent of the problem. This statement remains true with the addition of κI in the case of problems on (a, b) and $(0, \infty)$ $(\phi(x) = \ln(x))$ since, from Fig. 2, κ may be taken to be $\frac{1}{4}$. The final matrix in (3.30) is obtained for the finite interval $(-a, a)$ for symmetric q and ρ, since (3.29) follows from $x_k = a(e^{kh} - 1)/(e^{kh} + 1) = -x_{-k}$. Hence the splitting in (3.30) trivially applies to the Fourier example in Comparison 3.1 and the matrix sizes reported in Table I can effectively be cut in half. A less trivial example is provided by the Chebyshev example in [7]. In the case of the half-line any such splitting would require very special properties of the functions q and ρ.

In Table V below the sinc method is used in conjunction with the splitting described above. The results listed under Chebyshev are taken from [10] where an n-term Chebyshev expansion was used for (3.22) in conjunction with the algebraic map

$$\chi(x) = \frac{2x^2}{x^2 + L^2} - 1, \tag{3.33}$$

where L is a scaling parameter. Here, similar to Comparison 3.4, the interconnected choice of L and n needs to be carefully addressed. Based upon accuracy for matrix size the sinc method does somewhat better, though both methods are clearly powerful techniques for this problem.

TABLE V

Hermite Equation: Error in Computed Eigenvalues for the Chebyshev Method and for the Sinc Method

	Chebyshev method			Sinc method (with splitting)	
True eigenvalue	L	Matrix size	Error	Error	Matrix size $(M+1)\times(M+1)$
$\lambda_5 = 9/2$	4	20×20	$0.29 - 3$		
	4	30×30	$0.36 - 7$	$0.10 - 1$	5×5
	8	10×10	$0.68 - 1$		
	8	20×20	$0.27 - 4$	$0.12 - 4$	9×9
	8	30×30	$0.15 - 8$		
	16	20×20	$0.29 - 6$	$0.30 - 9$	12×12
	16	30×30	†		

Note. The † indicates that the eigenvalue was accurate to all eleven digits reported in [10].

Another algebraic mapping for the problem (3.22) is

$$\chi(x) = \frac{x}{\sqrt{x^2 + L^2}}. \tag{3.34}$$

Both maps (3.33) and (3.34) directly map $(-\infty, \infty)$ to $(-1, 1)$, where the Chebyshev basis may be used. The map (3.34) is analyzed in [4] wherein a detailed study of the rational basis $\{T_j(x/(x^2+L^2)^{1/2})\}$ is undertaken. Similarly the rational basis $\{T_j((x-L)/(x+L))\}$ arising with the map (3.21) is studied in [5]. These rational functions have surfaced in many settings. They were used in connection with quadratures in [16]. Later [11] used them in rational function quadratures, while as distinguished elements of certain finite orthogonal sets they were studied in [6].

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