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Accurate numerical bounds for the spectral points of singular Sturm–Liouville problems over $-\infty < x < \infty$

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Abstract

The eigenvalues of singular Sturm–Liouville problems are calculated very accurately by obtaining rigorous upper and lower bounds. The singular problem over the unbounded domain $(-\infty, \infty)$ is considered as the limiting case of an associated problem on the finite interval $[-\ell, \ell]$. It is then proved that the eigenvalues of the resulting regular systems satisfying Dirichlet and Neumann boundary conditions provide, respectively, upper and lower bounds converging monotonically to the required asymptotic eigenvalues. Numerical results for several quantum mechanical potentials illustrate that the eigenvalues can be calculated to an arbitrary accuracy, whenever the boundary parameter ℓ is in the neighborhood of some critical value, denoted by ℓ_{cr}. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Eigenvalue problems for differential equations are frequently encountered in practice in connection with physical and engineering problems (see [7] for a fairly detailed review). An important class of eigenvalue equations of this kind is described by the second-order self-adjoint differential operator in Sturm–Liouville form,

$$\mathscr{L}y = 0, \qquad \mathscr{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right] + q(x) - \lambda r(x). \tag{1.1}$$

The problem is regarded as singular when it is defined on an infinite interval of x, $x \in (-\infty, \infty)$. In this case, we assume that $p(x), p'(x), q(x)$ and $r(x)$ are real continuous, $p > 0$ and $r > 0$ on any real x interval under consideration. Furthermore, we do not suppose any integrability property of the functions $1/p, |q|$ and r over $(-\infty, \infty)$ so that the singular problem cannot be transformed to a regular problem on a finite interval [5].

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On the other hand, if the coefficients in $\mathscr{L}$ have a singular behavior at a specific point, $x = x_0$ say, then the problem may be treated on $[0, \infty)$ by means of a simple transformation, which is another singular case. In both cases, $q(x)$ is assumed to be a function which is bounded from below, and we are looking for solutions of class $L^2(-\infty, \infty)$ or $L^2(0, \infty)$. In this article, we deal with the former singular case in which

$$\int_{-\infty}^{\infty} r(x)|y(x)|^2 \, \mathrm{d}x < \infty \tag{1.2}$$

and are interested in problems of limit-point type. That is, if (1.1) has a nontrivial solution $u(x)$ of class $L^2(-\infty, \infty)$ then λ must be an eigenvalue and $u(x)$ the corresponding eigenfunction. Therefore, no boundary conditions are needed at infinity [1]. Note also that since $q(x)$ is bounded from below, such a boundary value problem (BVP) has a finite or enumerable infinite number of discrete eigenvalues λ.

The main objective of this study is to compute accurate eigenvalue enclosures, i.e., upper and lower bounds for the bound states of the singular problem over $-\infty < x < \infty$. In Section 2, we examine the behavior of the eigenvalues of the associated finite interval problems. The numerical applications are presented in Section 3, and the last section concludes the paper with a discussion of the results.

2. Associated regular boundary value problem

The main idea behind our method is to consider a regular BVP over a finite interval $x \in [\alpha, \beta]$ satisfying the condition

$$ay(x) + by'(x) = 0 \tag{2.1}$$

at $x = \alpha$ and β, where a and b are some constants. For simplicity, we may assume a fully symmetric problem about $x = 0$, and we take $x \in [-\ell, \ell]$ with $\ell > 0$. Now the eigensolutions of the BVP may be regarded as

$$y = y(x, \ell), \qquad \lambda = \lambda(\ell). \tag{2.2}$$

First of all, it is clear that the finite interval problem becomes singular as $\ell \to 0$. However, the differential operator $\mathscr{L}$ has no singularity at $x = 0$ which implies that the eigenvalue parameter λ is somehow singular at $\ell = 0$.

Proposition 1. *The eigenvalues of the finite interval problem grow like ℓ^{-2} for sufficiently small values of ℓ, i.e., $\lambda(\ell) = \mathcal{O}(\ell^{-2})$ as $\ell \to 0$.*

Proof. Making use of the linear transformation

$$x = \frac{\ell}{\pi}\xi, \quad \xi \in [-\pi, \pi] \tag{2.3}$$

we transform the equation $\mathscr{L}y = 0$ into the form

$$-\frac{\mathrm{d}}{\mathrm{d}\xi}\left[p(\ell\xi/\pi)\frac{\mathrm{d}y}{\mathrm{d}\xi}\right] + \frac{\ell^2}{\pi^2}[q(\ell\xi/\pi) - \lambda(\ell)r(\ell\xi/\pi)]y = 0. \tag{2.4}$$

Since

$$\lim_{\ell\to 0} p(\ell\xi/\pi) = p_0 > 0, \qquad \lim_{\ell\to 0} r(\ell\xi/\pi) = r_0 > 0 \tag{2.5}$$

and

$$\lim_{\ell\to 0} [\ell^2 q(\ell\xi/\pi)] = 0 \tag{2.6}$$

we obtain the simple BVP

$$\frac{d^2 y}{d\xi^2} + \mu y = 0, \qquad \bar{a}y(\mp\pi) + \bar{b}y'(\mp\pi) = 0, \tag{2.7}$$

where

$$\mu = \frac{1}{\pi^2}\frac{r_0}{p_0} \lim_{\ell\to 0} [\ell^2\lambda(\ell)]. \tag{2.8}$$

It is well known that the eigenvalues μ of the BVP in (2.7) exist so that

$$\lambda(\ell) = \mathcal{O}(\ell^{-2}), \quad \ell \to 0. \tag{2.9}$$

Notice that λ tends to $+\infty$ at $\ell = 0$, since μ should be nonnegative in order to satisfy the periodic boundary conditions. □

On the other hand, the conditions in (2.1) now read as

$$ay(\ell,\ell) + by_x(\ell,\ell) = 0 \tag{2.10}$$

and

$$ay(-\ell,\ell) + by_x(-\ell,\ell) = 0. \tag{2.11}$$

Note that the total differential of $y = y(x,\ell)$ is

$$dy = \frac{\partial y}{\partial x}dx + \frac{\partial y}{\partial \ell}d\ell \tag{2.12}$$

and if $x = \mp\ell$ with $dx = \mp d\ell$ then

$$dy = \left(\mp\frac{\partial y}{\partial x} + \frac{\partial y}{\partial \ell}\right)d\ell \tag{2.13}$$

implies that

$$\frac{dy}{d\ell} = \mp\frac{\partial y}{\partial x} + \frac{\partial y}{\partial \ell}. \tag{2.14}$$

Therefore, the implicit derivatives of (2.10) and (2.11) with respect to ℓ give the relations

$$a[y_x(\ell,\ell) + y_\ell(\ell,\ell)] + b[y_{xx}(\ell,\ell) + y_{x\ell}(\ell,\ell)] = 0 \tag{2.15}$$

and

$$a[-y_x(-\ell,\ell) + y_\ell(-\ell,\ell)] + b[-y_{xx}(-\ell,\ell) + y_{x\ell}(-\ell,\ell)] = 0, \tag{2.16}$$

respectively, which will be used in the later analysis.

Furthermore, differentiation of $\mathscr{L}y = 0$ with respect to ℓ leads to

$$\mathscr{L}y_\ell = r(x)\,y\,\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} \tag{2.17}$$

from which we write

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = \int_{-\ell}^{\ell} \mathscr{L}y_\ell \cdot y\,\mathrm{d}x, \tag{2.18}$$

where we have assumed a normalized solution in the finite interval $x \in [-\ell, \ell]$ such that

$$\int_{-\ell}^{\ell} r(x)|y(x)|^2\,\mathrm{d}x = 1. \tag{2.19}$$

It follows then that

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = \text{Boundary terms} + \int_{-\ell}^{\ell} y_\ell \cdot \mathscr{L}^\star y\,\mathrm{d}x \tag{2.20}$$

in which $\mathscr{L}^\star y = 0$ as $\mathscr{L}$ is formally self-adjoint, $\mathscr{L} = \mathscr{L}^\star$. Thus, we have the main relation

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = p(x)[y_x(x,\ell)\,y_\ell(x,\ell) - y(x,\ell)\,y_{x\ell}(x,\ell)]\big|_{x=-\ell}^{\ell} \tag{2.21}$$

which enables us to examine $\lambda(\ell)$ under various boundary conditions.

Proposition 2. *The eigenvalues, denoted by $\lambda^+(\ell)$, of the Dirichlet problem, where $(a,b) = (1,0)$, decrease monotonically as ℓ increases, providing upper bounds on the eigenvalues λ^∞ of the singular BVP.*

Proof. The boundary conditions in (2.10) and (2.11) reduce to

$$y(\ell,\ell) = y(-\ell,\ell) = 0 \tag{2.22}$$

for the Dirichlet problem. Furthermore, the relations in (2.15) and (2.16) imply that

$$y_x(\ell,\ell) = -y_\ell(\ell,\ell) \tag{2.23}$$

and

$$y_x(-\ell,\ell) = y_\ell(-\ell,\ell), \tag{2.24}$$

respectively. Now, substitution of (2.22)–(2.24) into (2.21) leads to

$$\frac{\mathrm{d}\lambda^+}{\mathrm{d}\ell} = -p(\ell)\,y_x^2(\ell,\ell) - p(-\ell)y_x^2(-\ell,\ell). \tag{2.25}$$

Exploiting the reflection symmetry of the problem we obtain

$$\frac{\mathrm{d}\lambda^+}{\mathrm{d}\ell} = -2p(\ell)y_x^2(\ell,\ell). \tag{2.26}$$

In any case, however, we see that

$$\frac{\mathrm{d}\lambda^+}{\mathrm{d}\ell} < 0 \tag{2.27}$$

for all $\ell > 0$, showing that $\lambda^+(\ell)$ decreases monotonically to its limit λ^∞ as $\ell \to \infty$, which completes the proof. □

Proposition 3. *The eigenvalues, denoted by* $\lambda^-(\ell)$, *of the Neumann problem, where* $(a,b)=(0,1)$, *increase monotonically for all* $\ell > \ell_0$ *such that*

$$\frac{q(\ell)}{r(\ell)} > \lambda^-(\ell) \tag{2.28}$$

and generate lower bounds on the eigenvalues λ^∞ *of the singular BVP. Here, we assume that there exists a value of* ℓ, *say* $\ell=\ell_0$, *for which*

$$\frac{q(\ell_0)}{r(\ell_0)} = \lambda^-(\ell_0) \tag{2.29}$$

and beyond which (2.28) *is satisfied.*

Proof. Using the Neumann boundary conditions

$$y_x(\ell,\ell) = y_x(-\ell,\ell) = 0 \tag{2.30}$$

and the relations

$$y_{xx}(\ell,\ell) = -y_{x\ell}(\ell,\ell) \tag{2.31}$$

and

$$y_{xx}(-\ell,\ell) = y_{x\ell}(-\ell,\ell) \tag{2.32}$$

obtained from (2.15) and (2.16), respectively, we deduce from (2.21) that

$$\frac{\mathrm{d}\lambda^-}{\mathrm{d}\ell} = p(\ell)y_{xx}(\ell,\ell)y(\ell,\ell) + p(-\ell)y_{xx}(-\ell,\ell)y(-\ell,\ell). \tag{2.33}$$

Now, solving the equation $\mathscr{L}y=0$ for $p(x)y_{xx}(x,\ell)$ we see that (2.33) takes the form

$$\frac{\mathrm{d}\lambda^-}{\mathrm{d}\ell} = \left[\frac{q(\ell)}{r(\ell)} - \lambda^-(\ell)\right] r(\ell)y^2(\ell,\ell) \tag{2.34}$$

which is positive valued for all ℓ provided that the condition in (2.28) holds.

The hypothesis about the existence of ℓ_0 is plausible since $q(x)$ is bounded from below. Physically, such a value of ℓ is called the *turning point*. Therefore, Neumann eigenvalues strictly increase as ℓ increases, for $\ell > \ell_0$. Moreover, it is known from Sturm–Liouville oscillation and comparison theorems [1] that the Dirichlet eigenvalues $\lambda_n^+(\ell)$ are always greater than the Neumann eigenvalues $\lambda_n^-(\ell)$ for any fixed state number n. As a result, the limiting value of $\lambda_n^-(\ell)$ as $\ell \to \infty$ is bounded from above by λ_n^∞, which completes the proof of Proposition 3. □

Corollary. *The eigenvalues of the Dirichlet and Neumann BVPs generate two-sided eigenvalue bounds for the eigenvalues of the singular BVP in the sense that*

$$\lambda^-(\ell) < \lambda^\infty < \lambda^+(\ell), \tag{2.35a}$$

where $\ell > \ell_0$ *to ensure the left-hand-side inequality. The difference* $\lambda^+(\ell) - \lambda^-(\ell)$ *is then a rigorous measure of the error in the computation of* λ^∞.

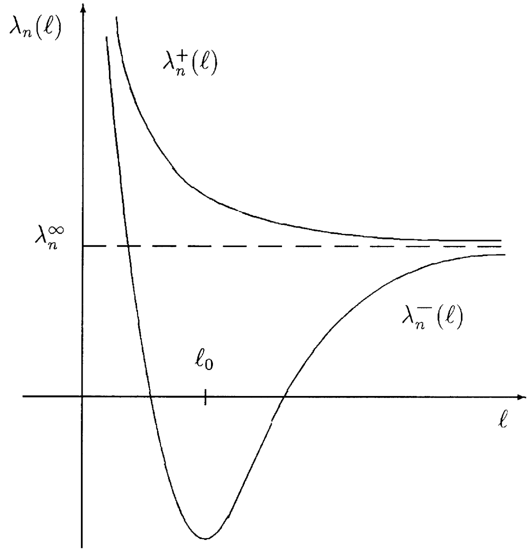

Fig. 1. Dirichlet and Neumann eigenvalues.

Moreover, since the differential operator is assumed to be of limit-point type at infinity, the required solution of the BVP tends to a unique limit as $\ell \to \infty$, independent of the choices of a and b in the boundary condition (2.1) [1]. Therefore, in the limiting case we have

$$\lim_{\ell\to\infty} [\lambda^+(\ell) - \lambda^-(\ell)] = 0. \tag{2.35b}$$

Now the qualitative behaviors of the eigenvalues of the Dirichlet and Neumann problems, whose graphs are illustrated in Fig. 1, as the boundary parameter ℓ varies from zero to infinity have been determined.

Remark. The sequences of eigenfunctions of the simple BVP in (2.7)

$$\phi_{2k}^+(x) = \frac{1}{\sqrt{\pi}} \cos(k+1/2)x, \quad k = 0,1,\ldots, \tag{2.36a}$$

$$\phi_{2k+1}^+(x) = \frac{1}{\sqrt{\pi}} \sin(k+1)x, \quad k = 0,1,\ldots \tag{2.36b}$$

and

$$\phi_0^-(x) = \frac{1}{\sqrt{2\pi}}, \qquad \phi_{2k}^-(x) = \frac{1}{\sqrt{\pi}} \cos kx, \quad k = 1,2,\ldots, \tag{2.37a}$$

$$\phi_{2k+1}^-(x) = \frac{1}{\sqrt{\pi}} \sin(k+1/2)x, \quad k = 0,1,\ldots \tag{2.37b}$$

satisfying Dirichlet and Neumann conditions, respectively, comprise complete orthonormal bases over $x \in [-\pi,\pi]$. As a result, any square integrable function $f(x)$ on $x \in [-\pi,\pi]$ has an expansion in terms of these eigenfunctions, which converges to $f(x)$ in the interval in the sense of least squares or in the mean [9].

It should be noted that the sets of eigenfunctions in (2.36a) and(2.37a) can only be used to expand an even function of x, while those in (2.36b) and (2.37b) are suitable for the representation of an odd function. However, even in the symmetric interval $-\ell < x < \ell$, if the differential operator $\mathscr{L}$ has no symmetry about $x = 0$, then the decomposition of even and odd parity eigensolutions is not possible. Therefore, in such a case it is more appropriate to modify (2.36) and (2.37) so as to reflect the asymmetric structure of the problem. Mapping of the domain from $x \in [-\ell, \ell]$ to $\xi \in [0, \pi]$, where

$$\xi = \frac{\pi}{2\ell}(x + \ell), \tag{2.38}$$

we handle the simple BVP in (2.7) over the asymmetric interval $\xi \in [0, \pi]$. Then the normalized eigenfunctions

$$\varphi_k^+(\xi) = \sqrt{\frac{2}{\pi}} \sin(k+1)\xi, \quad k = 0, 1, \ldots \tag{2.39}$$

and

$$\varphi_0^-(\xi) = \frac{1}{\sqrt{\pi}}, \qquad \varphi_k^-(\xi) = \sqrt{\frac{2}{\pi}} \cos k\xi, \quad k = 1, 2, \ldots \tag{2.40}$$

which obey Dirichlet and Neumann boundary conditions, respectively, may properly be used to expand an arbitrary square integrable function on $0 < \xi < \pi$.

3. Numerical applications

The well-known quantum mechanical harmonic oscillator problem for which

$$p(x) = r(x) = 1, \qquad q(x) = x^2 \tag{3.1}$$

provides a convenient testing ground for our method. In fact, Eq. (1.1) reduces to the Hermite–Weber equation

$$-\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (x^2 - \lambda)y = 0 \tag{3.2}$$

and the singular eigenvalue problem in $(-\infty, \infty)$ possesses exact analytical solutions of the form

$$y_n^\infty(x) = A_n \mathrm{e}^{-x^2/2} H_n(x), \qquad \lambda_n^\infty = 2n + 1, \quad n = 0, 1, \ldots, \tag{3.3}$$

where the $H_n(x)$ and A_n are the Hermite polynomials and some normalization constants, respectively. The scaled finite interval problem in $x \in [-\pi, \pi]$ gives rise to the orthonormal systems $\{\phi_k^+\}$ or $\{\phi_k^-\}$. Furthermore, the reflection symmetry of the problem yields the possibility of the treatment of even and odd eigensolutions separately. Thus, for the symmetric states of the harmonic oscillator, we propose expansions of the type

$$\Phi^{+}(x)=\sum_{k=0}^{\infty} h_k \phi_{2k}^{+}(x) \tag{3.4}$$

and

$$\Phi^{-}(x)=\sum_{k=0}^{\infty} f_k \phi_{2k}^{-}(x) \tag{3.5}$$

in order to handle Dirichlet and Neumann BVPs, respectively. The substitution of (3.4) into (3.2) results in the Galerkin equations

$$\sum_{j=0}^{\infty} [\mathscr{A}_{kj}-\lambda^{+}(\ell)\delta_{kj}]h_j=0, \quad k=0,1,\ldots, \tag{3.6}$$

where δ_{kj} is the Kronecker's delta, and $\mathscr{A}_{kj}$ stands for the matrix representation of the differential operator defined by

$$\mathscr{A}_{kj}=(k+1/2)^2(\pi/\ell)^2\delta_{kj}+(\ell/\pi)^2(R_{k-j}+R_{k+j+1}) \tag{3.7}$$

in which the R_m denote the simple integrals

$$R_m=\frac{1}{\pi}\int_0^{\pi} x^2\cos mx\,\mathrm{d}x. \tag{3.8}$$

Hence, truncating the solution in (3.4), we arrive at the standard matrix eigenvalue problem

$$\sum_{j=0}^{N-1} [\mathscr{A}_{kj}-\lambda^{+}(\ell)\delta_{kj}]h_j=0, \quad k=0,1,\ldots,N-1. \tag{3.9}$$

Similarly, the Neumann solution in (3.5) leads again to a matrix eigenvalue problem of form (3.9).

The numerical results for the first three symmetric state eigenvalues of the Hermite–Weber equation are presented in Table 1.

The method can also be applied to the problems where the differential operator $\mathscr{L}$ has no reflection symmetry. As such an example, we now consider again a problem in the Schrödinger form

$$-\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+(\mathrm{e}^{-\alpha x}-1)^2y=\lambda y, \quad \alpha>0 \tag{3.10}$$

which is known as the *Morse potential* problem to determine vibrational energy levels of diatomic molecules [4,8]. This singular eigenvalue problem over $-\infty<x<\infty$ has a finite number of eigenvalues lying between $0<\lambda<1$, and a continuous spectrum for all $\lambda\geqslant 1$. The solutions for the bound states are expressible as

$$y_n^{\infty}(x)=B_n(2/\alpha)^{v_n}\mathrm{e}^{-\alpha v_n x}L_n^{(2v_n)}(2\mathrm{e}^{-\alpha x}/\alpha), \quad \lambda_n^{\infty}=\beta_n(2-\beta_n) \tag{3.11}$$

for

$$n=0,1,\ldots,K \tag{3.12}$$

where

$$\beta_n=\tfrac{1}{2}\alpha(2n+1), \quad v_n=\frac{1}{\alpha}(1-\beta_n)>0 \tag{3.13}$$

Table 1
Convergence rates of the N-truncated bounds for the first three symmetric states eigenvalues of the harmonic oscillator as a function of ℓ. The numerical bounds are compared with the exact analytical eigenvalues $\lambda_n^\infty = 2n+1$ of the singular problem in the unbounded domain where $\ell \to \infty$

n	ℓ	N	$\lambda_n^-(\ell)$	$\lambda_n^+(\ell)$	λ_n^∞
0	4.5	5	1.000 065	1.000 006	
		8	0.999 999 983	1.000 000 015	
		10	0.999 999 983	1.000 000 015	1
	6.0	8	1.000 000 359	1.000 000 041	
		10	1.000 000 000 026	1.000 000 000 002	
		12	0.999 999 999 999 997	1.000 000 000 000 003	
		14	0.999 999 999 999 997	1.000 000 000 000 003	1
	7.5	14	1.000 000 000 000 026	1.000 000 000 000 002	
		16	1.000 000 000 000 000 000 872	1.000 000 000 000 000 000 052	
		18	1.000 000 000 000 000 000 000 010	1.000 000 000 000 000 000 000 007	
		20	0.999 999 999 999 999 999 999 994	1.000 000 000 000 000 000 000 006	1
2	4.5	5	5.012	5.002	
		8	4.999 998 118	5.000 011 010	
		10	4.999 998 115	5.000 011 008	5
	6.0	8	5.000 170	5.000 026	
		10	5.000 000 033	5.000 000 002 729	
		12	4.999 999 999 992 9	5.000 000 000 007 4	
		14	4.999 999 999 992 4	5.000 000 000 007 3	5
	7.5	14	5.000 000 000 055	5.000 000 000 006	
		16	5.000 000 000 000 003 195	5.000 000 000 000 000 221	
		18	5.000 000 000 000 000 000 003	5.000 000 000 000 000 000 039	
		20	4.999 999 999 999 999 999 962	5.000 000 000 000 000 000 037	5
4	4.5	5	9.255	9.064	
		8	9.998 884 7	9.000 985 6	
		10	8.998 884 5	9.000 985 4	9
	6.0	8	9.009 718	9.002 029	
		10	9.000 006 013	9.000 000 611	
		12	8.999 999 997 6	9.000 000 002 57	
		14	8.999 999 997 3	9.000 000 002 56	9
	7.5	14	9.000 000 017	9.000 000 002	
		16	9.000 000 000 001 765	9.000 000 000 000 139	
		18	9.000 000 000 000 000 003	9.000 000 000 000 000 036	
		20	8.999 999 999 999 999 964	9.000 000 000 000 000 035	9

and K, B_n and $L_n^{(m)}(x)$ are, respectively, the integer part of the parameter $1/\alpha - \frac{1}{2}$, a normalization constant and the generalized Laguerre polynomials. It is easy to show that the problem has no bound states if $\alpha > 2$.

We first consider Morse problem (3.10) over $-\ell \leqslant x \leqslant \ell$ and then transform it into the asymmetric interval $[0, \pi]$ by the substitution in (2.38). Therefore, expanding the solutions of the resulting equation into series of the φ_k^+ and φ_k^- in (2.39) and (2.40), we convert the BVP to matrix eigenvalue problems of the form (3.9) in order to determine numerical eigenvalue enclosures. Note that the

Table 2
Convergence rates of the N-truncated bounds for the first three eigenvalues of the asymmetrical problem in (3.10) with $\alpha=0.02$, as a function of ℓ. The numerical bounds are compared with the exact analytical eigenvalues λ_n^{∞}, expressed in (3.11), of the singular problem in the unbounded domain where $\ell \to \infty$

n	$\alpha\ell$	N	$\lambda_n^-(\ell)$	$\lambda_n^+(\ell)$	λ_n^{∞}
0	0.8	15	0.019 900 011	0.019 900 001 903	
		20	0.019 899 999 997 277	0.019 900 000 002 788	
		25	0.019 899 999 997 132	0.019 900 000 002 776	0.0199
	1.0	20	0.019 900 000 607	0.019 900 000 060	
		25	0.019 900 000 000 046	0.019 900 000 000 002 164	
		30	0.019 899 999 999 999 971	0.019 900 000 000 000 027 965	
		35	0.019 899 999 999 999 971	0.019 900 000 000 000 027 881	0.0199
	1.2	30	0.019 900 000 000 115	0.019 900 000 000 024 858	
		35	0.019 900 000 000 000 014	0.019 900 000 000 000 002 339	
		40	0.019 900 000 000 000 000 000 597	0.019 900 000 000 000 000 000 113	
		45	0.019 899 999 999 999 999 999 937	0.019 900 000 000 000 000 000 061	0.0199
1	0.8	15	0.059 100 356	0.059 100 039	
		20	0.059 099 999 641	0.059 100 000 348	
		25	0.059 099 999 636	0.059 100 000 348	0.0591
	1.0	20	0.059 100 022	0.059 100 005 973	
		25	0.059 100 000 001	0.059 100 000 000 413	
		30	0.059 099 999 999 992	0.059 100 000 000 007 099	
		35	0.059 099 999 999 992	0.059 100 000 000 007 090	0.0591
	1.2	30	0.059 100 000 005	0.059 100 000 000 675	
		35	0.059 100 000 000 000 601	0.059 100 000 000 000 055	
		40	0.059 099 999 999 999 999 984	0.059 100 000 000 000 000 029	
		45	0.059 099 999 999 999 999 970	0.059 100 000 000 000 000 028	0.0591
2	0.8	15	0.097 500 769	0.097 500 113	
		20	0.097 499 980	0.097 500 018	
		25	0.097 499 980	0.097 500 018	0.0975
	1.0	20	0.097 500 665	0.097 500 129	
		25	0.097 500 000 094	0.097 500 000 014	
		30	0.097 499 999 999 193	0.097 500 000 000 787	
		35	0.097 499 999 999 191	0.097 500 000 000 787	0.0975
	1.2	30	0.097 500 000 025	0.097 500 000 003 184	
		35	0.097 500 000 000 003	0.097 500 000 000 000 324	
		40	0.097 499 999 999 999 993	0.097 500 000 000 000 006 117	
		45	0.097 499 999 999 999 993	0.097 500 000 000 000 006 072	0.0975

matrix elements can be evaluated analytically in both cases. For instance, in the Dirichlet problem

$$\mathscr{A}_{kj} = \left[(k+1)^2\frac{\pi^2}{4\ell^2}+1\right]\delta_{kj} + \mathrm{e}^{2\alpha\ell}[I_{k-j}(4\alpha\ell/\pi) - I_{k+j+2}(4\alpha\ell/\pi)]$$
$$- 2\mathrm{e}^{\alpha\ell}[I_{k-j}(2\alpha\ell/\pi) - I_{k+j+2}(2\alpha\ell/\pi)], \tag{3.14}$$

where the $I_m(s)$ stand for the integrals

$$I_m(s) = \frac{1}{\pi}\int_0^{\pi} e^{-s\xi}\cos m\xi \, d\xi = \frac{s}{\pi}\left[\frac{1-(-1)^m e^{-s\pi}}{s^2+m^2}\right]. \tag{3.15}$$

Two-sided bounds on the low-lying state eigenvalues of (3.10) are shown in Table 2, for a specific value of α, $\alpha = 0.02$.

4. Concluding remarks

We solve two auxiliary regular BVPs subject to Dirichlet and Neumann boundary conditions, which provide us with a practical method of determining upper and lower bounds for the eigenvalues of the singular BVP. Furthermore, more accurate bounds are obtainable by way of increasing the boundary parameter ℓ, confirming the theoretical analysis. Therefore, there exists a critical value of ℓ, ℓ_{cr} say, at which

$$\lambda^+(\ell_{cr}) - \lambda^-(\ell_{cr}) < \varepsilon, \tag{4.1}$$

where $\varepsilon > 0$ stands for a prescribed accuracy, which can be made as small as we please. Another remark is that the present method is constantly efficient for both symmetrical and asymmetrical problems.

On the other hand, it is shown from the numerical tables that both lower and upper bounds converge from above as N increases, and their significant digits so determined yield indeed two-sided bounds on the asymptotic eigenvalues. This is due to the fact that we employ Rayleigh–Ritz-type trial solutions for the numerical implementation of the associated regular BVPs. It is well known that Rayleigh–Ritz method is based on the variational principle, so that it provides not only good approximations but also upper bounds to the eigenvalues. In the case of the Neumann problem, we, therefore, generate upper bounds for the lower bound eigenvalues. As a result, it is crucial to determine actually the correct digits of N-truncated matrix eigenvalues, or Galerkin approximations, as N increases. To overcome this difficulty, we should note that we do not calculate directly the target eigenvalue, namely λ^∞, but $\lambda^-(\ell)$ instead. Although N-truncated matrix eigenvalues give upper bounds on $\lambda^-(\ell)$, their last few digits with a possible uncertainty can be truncated since the exact value of $\lambda^-(\ell)$ is always less than λ^∞ for all $\ell < \infty$. Obviously, by the term 'significant digits' we mean both stable digits of successive Galerkin approximations and the digits confirming between different values of ℓ.

This strategy may be regarded as too experimental, nevertheless, it practically gives highly accurate results for λ^∞ provided that various values of ℓ are considered systematically to compute $\lambda^-(\ell)$ and $\lambda^+(\ell)$. This is why we include results corresponding to certain values of ℓ in our numerical tables. In fact, to be more accurate one may use, for instance, the interval arithmetic which controls all rounding errors made in the calculations. In general, the computation of lower bounds is a much more difficult task, and the established methods require an a priori lower bound for the Nth eigenvalue of the problem [2,3,6]

Finally, it is worth mentioning that singular problems in $x \in [0, \infty)$ may be treated by this method as well. In this case, the analysis has to be modified appropriately, which is presently an ongoing study.

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