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Correction of Numerov's Eigenvalue Estimates

Alan L. Andrew[1] and John W. Paine[2]*

[1] Mathematics Department, La Trobe University, Bundoora, Victoria, 3083, Australia
[2] Mathematics Department, Simon Fraser University, Burnaby, BC V5A 1S6, Canada

Summary. The error in the estimate of the kth eigenvalue of a regular Sturm-Liouville problem obtained by Numerov's method with mesh length h is $O(k^6 h^4)$. We show that a simple correction technique of Paine, de Hoog and Anderssen reduces the error to one of $O(k^3 h^4)$. Numerical examples demonstrate the usefulness of this correction even for low values of k.

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I. Introduction

There has been much recent interest in problems requiring efficient and accurate computation of a long sequence of eigenvalues of regular Sturm-Liouville problems. (See [2] for References.) It is usually advantageous [2] first to transform the problem to the Liouville normal form

$$-y'' + qy = \lambda y. \tag{1a}$$

We consider the case of essential boundary conditions which may, without loss of generality, be written as

$$y(0) = y(\pi) = 0. \tag{1b}$$

When finite difference methods are used to approximate the eigenvalues, $\lambda_1 < \lambda_2 < \lambda_3 < \dots$, of (1), the error in the approximation to λ_k is known to increase rapidly with k. For example the usual centred difference approximation to (1a) with uniform mesh length $h := \pi/(n+1)$ approximates $\lambda_1, \dots, \lambda_n$ by the eigenvalues $\lambda_1^{(n)} < \dots < \lambda_n^{(n)}$ of the $n \times n$ matrix $-A+Q$ where $A := (a_{ij})$ is symmetric tridiagonal with

$$a_{ii} := -2/h^2, \quad i = 1, \dots, n, \quad a_{i,i+1} := 1/h^2, \quad i = 1, \dots, n-1 \tag{2}$$

and $Q := \operatorname{diag}[q(x_1), \dots, q(x_n)]$ where $x_j := jh$. In this case the errors satisfy $|\lambda_k - \lambda_k^{(n)}| = O(k^4 h^2)$. For example when $q = 0$, $\lambda_k = k^2$ and $\lambda_k^{(n)} = 4\sin^2(kh/2)/h^2$.

* *Present address:* Dept. of Geology and Geophysics, University of Adelaide, South Australia, 5001

Recently Paine, de Hoog and Anderssen [8] observed that this known closed form solution when $q=0$ could be used to improve dramatically the accuracy of the computed higher eigenvalues with negligible extra effort. They showed that, for all $q \in C^2\,[0,\pi]$ and all $\alpha<1$, there exists a constant $c(\alpha)$ such that, for all n and all $k<\alpha\pi/h$, the approximations

$$\tilde{\lambda}_k^{(n)} := \lambda_k^{(n)} + k^2 - 4\sin^2(kh/2)/h^2$$

satisfy

$$|\tilde{\lambda}_k^{(n)} - \lambda_k| \leqq c(\alpha)\,k h^2. \tag{3}$$

Although the improvement is obviously greatest for large k, their numerical results indicate that $|\tilde{\lambda}_k^{(n)} - \lambda_k| < |\lambda_k^{(n)} - \lambda_k|$ even for small k. This analysis has subsequently been extended [1] to the problem with (1b) replaced by the more general boundary conditions

$$\sigma_1\,y(0) + \sigma_2\,y'(0) = \sigma_3\,y(\pi) + \sigma_4\,y'(\pi) = 0.$$

Also Paine [7] has shown that the correction technique of [8] can greatly increase the efficiency of a certain method for the numerical solution of the inverse eigenvalue problem.

A deservedly popular technique for computation of the lowest eigenvalues of (1) is Numerov's method, which approximates $\lambda_1, \ldots, \lambda_n$ by the eigenvalues $\Lambda_1^{(n)} < \ldots < \Lambda_n^{(n)}$ of

$$-A\,\mathbf{u} + BQ\,\mathbf{u} = \Lambda B\,\mathbf{u} \tag{4}$$

where

$$B := I + h^2 A/12 \tag{5}$$

and I is the identity. Since $\|y_k^{(j)}\| = O(k^j \|y_k\|)$, $j=1,2,\ldots$, where y_k is the eigenfunction of (1) corresponding to λ_k, it follows from Taylor's theorem that

$$(-A + BQ - \lambda_k B)\,\mathbf{y}_k = O(k^6 h^4\,\|\mathbf{y}_k\|_\infty)$$

and hence since, as shown in [3],

$$\|B^{-1}\|_\infty = O(1), \tag{6}$$

an analysis similar to that in [5], pp. 133–134, shows that

$$|\Lambda_k^{(n)} - \lambda_k| = O(k^6 h^4). \tag{7}$$

When $q=0$ (and hence $Q=0$), it is readily verified that

$$-A\,\mathbf{s}_k^{(n)} = \mu_k^{(n)}\,B\,\mathbf{s}_k^{(n)} \tag{8}$$

where $\mathbf{s}_k^{(n)} := (\sin(k x_1), \ldots, \sin(k x_n))^T$ and

$$\mu_k^{(n)} := \frac{12\,[1-\cos(kh)]}{h^2\,[5+\cos(kh)]} = k^2 + O(k^6 h^4). \tag{9}$$

We show here that the error in the estimates

$$\tilde{\Lambda}_k^{(n)} := \Lambda_k^{(n)} + k^2 - \mu_k^{(n)} \tag{10}$$

given by the correction technique of [8] grows more slowly with k than the error in the original estimates $\Lambda_k^{(n)}$. Specifically we show that, for all functions $q \in C^4[0,\pi]$ and all $\alpha<1$, there exists a constant $c^*(\alpha)$ such that, for all n and all $k<\alpha\pi/h$,

$$|\tilde{\Lambda}_k^{(n)}-\lambda_k|<c^*(\alpha)k^3h^4. \tag{11}$$

This can be deduced by a modification of the proof used in [8]. We use instead a slightly different approach which establishes the following stronger result.

Theorem 1. *If $q \in C^4[0,\pi]$ then there exists a constant c_0 depending only on q such that for all $n \in \mathbb{N}$ and $k=1,\dots,n$,*

$$|\tilde{\Lambda}_k^{(n)}-\lambda_k| \leqq c_0 k^4 h^5/\sin(kh).$$

Since $\alpha/\sin(\alpha\pi)$ increases monotonically with α for $0<\alpha<1$, (11) follows immediately from Theorem 1 and we have as a bonus the formula

$$c^*(\alpha)=c_0\,\alpha\pi/\sin(\alpha\pi).$$

The method of proof used here can also be used to show that $c(\alpha)$ in (3) has a similar form.

Although $c^*(\alpha)\to\infty$ as $\alpha\to 1$, $c^*(\alpha)$ increases slowly at first and $c^*(\frac{1}{2})/c^*(0+)$ is only $\pi/2$. This suggests that, if the first k eigenvalues are required, the choice $n=2k$ (suggested in [8] for the second order method) will be suitable and numerical results confirm this.

Comparison of (3), (7) and (11) makes it clear that, as an approximation to λ_k, $\tilde{\Lambda}_k^{(n)}$ will be better than $\Lambda_k^{(n)}$ for sufficiently large k and better than $\tilde{\lambda}_k^{(n)}$ for sufficiently small h. Our numerical results, which are summarized in Sect. 3, indicate that the restriction to "sufficiently large k" and "sufficiently small h" is not serious in practice, at least for reasonably smooth q. In all cases we found $\tilde{\Lambda}_k^{(n)}$ to be a better approximation than $\Lambda_k^{(n)}$, even for $k=1$. In all cases with $k \leqq n/2$ (as recommended), and most cases with $k>n/2$, we also found $\tilde{\Lambda}_k^{(n)}$ to be a better approximation than $\tilde{\lambda}_k^{(n)}$.

2. Proof of Theorem 1

Since increasing q by a constant increases λ_k and $\Lambda_k^{(n)}$ by the same constant, we can assume without loss of generality (as in [8]) that

$$\int_0^\pi q(x)\,dx=0.$$

This implies [8] that

$$\lambda_k=k^2+O(k^{-2}). \tag{12}$$

For notational convenience, the subscript k and the superscript (n) are supressed throughout this proof. Thus y denotes the eigenfunction of (1) corresponding to the kth eigenvalue and $\mathbf{u}:=(u_1,\dots,u_n)^T$ the eigenvector corresponding to the kth eigenvalue of (4). For any function p: $[0,\pi]\to\mathbb{R}$ we use the notation $p_i:=p(x_i)$, $p_i':=p'(x_i)$ etc, $i=1,\dots,n$ and $\mathbf{p}:=(p_1,\dots,p_n)^T$, $\mathbf{p}':=(p_1',\dots,p_n')^T$.

Since A and B are symmetric commuting invertible matrices

$$AB^{-1}=B^{-1}A=(B^{-1}A)^T. \tag{13}$$

Hence by (4)

$$-\mathbf{u}^T B^{-1}A+\mathbf{u}^T Q=\Lambda \mathbf{u}^T. \tag{14}$$

Hence $\Lambda \mathbf{u}^T \mathbf{y}+\mathbf{u}^T B^{-1} A\mathbf{y}=\mathbf{u}^T Q\mathbf{y}=\lambda \mathbf{u}^T \mathbf{y}+\mathbf{u}^T \mathbf{y}''$ by (1), that is

$$(\Lambda-\lambda)\mathbf{u}^T\mathbf{y}=\mathbf{u}^T(\mathbf{y}''-B^{-1}A\mathbf{y}). \tag{15}$$

Since

$$\mathbf{s}''=-k^2\mathbf{s} \tag{16}$$

it follows from (15) and (8) that

$$(\Lambda-\lambda)\mathbf{u}^T\mathbf{y}=(\mu-k^2)\mathbf{u}^T\mathbf{s}+\mathbf{s}^T(\mathbf{e}''-B^{-1}A\mathbf{e})+\boldsymbol{\varepsilon}^T(\mathbf{e}''-B^{-1}A\mathbf{e}), \tag{17}$$

where

$$\boldsymbol{\varepsilon}:=\mathbf{u}-\mathbf{s}, \tag{18}$$

$$e(x):=y(x)-\sin(kx) \tag{19}$$

and hence $\mathbf{e}=\mathbf{y}-\mathbf{s}$. The following lemmas enable us to estimate the various terms arising in (17). We assume y normalized as in [8], with analogous normalization for $\mathbf{u}$, and show that $\boldsymbol{\varepsilon}$ and $\mathbf{e}$ are then $O(k^{-1})$.

Lemma 1. $\|\boldsymbol{\varepsilon}\|_\infty \leqq 2h\pi\,\|q\|_\infty\,\|\mathbf{u}\|_\infty/\sin(kh)$.

Proof. Subtracting $\mu B\mathbf{u}+BQ\mathbf{u}$ from both sides of (4) and multiplying by $-[5+\cos(kh)]h^2/6$ yields

$$u_{j-1}-2\cos(kh)u_j+u_{j+1}=[5+\cos(kh)]h^2[(\mu-\Lambda)B\mathbf{u}+BQ\mathbf{u}]_j/6,\ j=1,\dots,n. \tag{20}$$

Hence, using an argument analogous to that in the proof of Theorem 2.1 of [8], it follows from Lemma 2.3 of [8] that

$$\varepsilon_j=\frac{[5+\cos(kh)]h^2}{72\sin(kh)}\sum_{i=1}^{j-1}\sin(k(x_j-x_i))[(\mu-\Lambda+q_{i-1})u_{i-1} +10(\mu-\Lambda+q_i)u_i+(\mu-\Lambda+q_{i+1})u_{i+1}],\quad j=1,\dots,n. \tag{21}$$

Since $B^{-1}A$ and Q are real symmetric it follows from (4), (8) and standard perturbation theory [9, p. 102] that

$$|\mu-\Lambda|\leqq\|Q\|_\infty=\|\mathbf{q}\|_\infty\leqq\|q\|_\infty. \tag{22}$$

Hence by (21) and the triangle inequality

$$\begin{aligned}|\varepsilon_j|&\leqq|h^2(j-1)/\sin(kh)|\max_i(|\mu-\Lambda+q_i|\,|u_i|)\\&\leqq[2(j-1)h^2/\sin(kh)]\,\|q\|_\infty\,\|\mathbf{u}\|_\infty\\&\leqq[2\pi h/\sin(kh)]\,\|q\|_\infty\,\|\mathbf{u}\|_\infty,\quad\text{since } h(j-1)\leqq\pi.\ \square\end{aligned}$$

Lemma 2. *For y normalised as in* [8],

$$e(x)=k^{-1}\int_0^x (k^2-\lambda+q(t))\sin[k(x-t)]\,y(t)\,dt, \tag{23}$$

$$e^{(j)}(x)=O(k^{j-1}), \qquad j=0,1,2,\ldots \tag{24}$$

and

$$e(0)=e(\pi)=e''(0)=e''(\pi)=0. \tag{25}$$

Proof. Equations (23) and (25) are proved in [8] and (24) follows from (23) and (12) since $y^{(j)}=O(k^j)$. □

Lemma 3. *Let*

$$f:=(k^2-\lambda+q)\,y, \tag{26}$$

$$\alpha(x,h):=\int_x^{x+h} f(t)\sin[k(x+h-t)]\,dt \tag{27}$$

and

$$E_j:=\alpha(x_j,h)+\alpha(x_j,-h). \tag{28}$$

Then

$$A\,\mathbf{e}-B\,\mathbf{e}''-(k^2-\mu)\,B\,\mathbf{e}=(1+h^2\mu/12)\,\mathbf{E}/kh^2-B\,\mathbf{f}. \tag{29}$$

Proof. By (23), $\mathbf{e}''=\mathbf{f}-k^2\,\mathbf{e}$ and hence

$$B\,\mathbf{e}''=B\,\mathbf{f}-k^2 B\,\mathbf{e}. \tag{30}$$

Also by (2), (23), (28) and (9),

$$\begin{aligned} kh^2(A\,\mathbf{e})_j &= k(e_{j+1}-2e_j+e_{j-1})\\ &=\int_0^{x_j} f(t)\{\sin[k(x_{j+1}-t)]-2\sin[k(x_j-t)]+\sin[k(x_{j-1}-t)]\}\,dt+E_j\\ &=-\frac{h^2\mu}{12}\int_0^{x_j} f(t)\{\sin[k(x_{j+1}-t)]+10\sin[k(x_j-t)]+\sin[k(x_{j-1}-t)]\}\,dt+E_j\\ &=-h^2\mu k[e(x_{j+1})+10e(x_j)+e(x_{j-1})]/12+(1+h^2\mu/12)\,E_j. \end{aligned}$$

Hence

$$A\,\mathbf{e}=-\mu B\,\mathbf{e}+(1+h^2\mu/12)\,\mathbf{E}/kh^2. \tag{31}$$

Subtracting (30) from (31) and rearranging gives (29). □

Lemma 4. *For all $q\in C^4[0,\pi]$ there exists a constant c_1 such that*

$$|\boldsymbol{\varepsilon}^T[B^{-1}A\,\mathbf{e}-\mathbf{e}''+(\mu-k^2)\,\mathbf{e}]|\le c_1\,k^4h^4/\sin(kh), \qquad k=1,\ldots,n.$$

Proof. By (28) and (27),

$$E_j=\int_{x_j}^{x_{j+1}} f(t)\sin[k(x_{j+1}-t)]\,dt+\int_{x_j}^{x_{j-1}} f(t)\sin[k(x_{j-1}-t)]\,dt.$$

Expanding f about x_j by Taylor's theorem in both integrals and integrating by parts shows that

$$E_j=(2/k)[1-\cos(kh)]f_j+\{(h^2/k)-(2/k^3)[1-\cos(kh)]\}f_j''+O(kh^6\,\|f^{(4)}\|_\infty). \tag{32}$$

Also $B\mathbf{f}=\mathbf{f}+h^2A\mathbf{f}/12=f+h^2\mathbf{f}''/12+O(h^4\,\|f^{(4)}\|_\infty)$.

Combining this result with (32) and then using the easily verified equation

$$2[1-\cos(kh)](1+h^2\mu/12)=h^2\mu$$

shows that

$$\begin{aligned}(1/k)(1+h^2\mu/12)E_j-h^2(B\mathbf{f})_j&=\{(2/k^2)[1-\cos(kh)](1+h^2\mu/12)-h^2\}f_j\\&+h^2\{k^{-2}[1-(2/h^2k^2)(1-\cos(kh))](1+h^2\mu/12)-h^2/12\}f_j''\\&+O(h^6\,\|f^{(4)}\|_\infty)=(h^2/k^2)(\mu-k^2)f_j+(h^2/k^4)(k^2-\mu)(1-h^2k^2/12)f_j''\\&+O(h^6\,\|f^{(4)}\|_\infty)=O(k^4h^6),\end{aligned} \tag{33}$$

since $\mu-k^2=O(k^6h^4)$, $1-h^2k^2/12=O(1)$ and

$$f_j(p):=f^{(p)}(x_j)=O(\|f^{(p)}\|_\infty)=O(k^p).$$

Since also

$$|\boldsymbol{\varepsilon}^T(B^{-1}A\mathbf{e}-\mathbf{e}''+(\mu-k^2)\mathbf{e})|\leqq n\,\|\boldsymbol{\varepsilon}\|_\infty\,\|B^{-1}\|_\infty\,\|A\mathbf{e}-B\mathbf{e}''+(\mu-k^2)B\mathbf{e}\|_\infty$$

and $n=O(1/h)$, the result follows from (6), (33) and Lemmas 1 and 3. □

Lemma 5. *For all* $\theta\in C^1[0,\pi]$,

$$\left|\sum_{i=0}^{n}\theta_{i+\frac12}\cos(2kx_{i+\frac12})\right|\leqq\pi\,\|\theta'\|_\infty/2\sin(kh),\qquad k=1,\dots,n,$$

where $x_{i\pm\frac12}:=(x_i+x_{i\pm1})/2$ *and* $\theta_{i\pm\frac12}:=\theta(x_{i\pm\frac12})$.

Proof. Since

$$\begin{aligned}&\sum_{i=0}^{m-1}2\sin(kh)\cos(2kx_{i+\frac12})\\&\quad=\sum_{i=0}^{m-1}[\sin(2kx_{i+1})-\sin(2kx_i)]=\sin(2kx_m)\quad\text{and}\quad\sin(kh)>0\end{aligned}$$

for $1\leqq k\leqq n$, summation by parts gives

$$\begin{aligned}\sum_{i=0}^{n}\theta_{i+\frac12}\cos(2kx_{i+\frac12})&=\theta_{n+\frac12}\sum_{i=0}^{n}\cos(2kx_{i+\frac12})\\&-\sum_{i=1}^{n}(\theta_{i+\frac12}-\theta_{i-\frac12})\sum_{j=0}^{i-1}\cos(2kx_{j+\frac12})\\&=-\sum_{i=1}^{n}(\theta_{i+\frac12}-\theta_{i-\frac12})\sin(2kx_i)/2\sin(kh).\end{aligned}$$

Since $|(\theta_{i+\frac12}-\theta_{i-\frac12})\sin(2kx_i)|\leqq h\,\|\theta'\|_\infty=\pi\,\|\theta'\|_\infty/(n+1)$, the result follows. □

Lemma 6. *For all $q \in C^4[0,\pi]$ there exists a constant c_2 such that*

$$|\mathbf{s}^T \mathbf{f}| \leqq c_2 k^4 h^4/\sin(kh), \qquad k=1,\dots,n.$$

Proof. Let $F(x) := f(x)\sin(kx)$ and let $T_h F$ be the approximation to $\int_0^\pi F(x)\,dx$ obtained by the trapezoidal rule with subintervals of uniform length h. Then by (26) $F \in C^4[0,\pi]$ and since $F(0)=F(\pi)=0$, it follows from the Euler-Maclaurin summation formula [4] that

$$\mathbf{s}^T \mathbf{f} = h^{-1} T_h F = h^{-1}\left\{\int_0^\pi F(x)\,dx + \frac{B_2}{2!} h^2 [F'(\pi) - F'(0)] + \frac{B_4}{4!} h^4 [F'''(\pi) - F'''(0)] - h^4 \int_0^\pi P_4(x/h) F^{(4)}(x)\,dx\right\} \tag{34}$$

where, as in [4], the B_j are the Bernouilli numbers and $P_1, \dots, P_4$ are piecewise polynomials of period one satisfying

$$P'_{j+1} = P_j \quad \text{on } (0,1), \qquad P_{2j+1}(0) = P_{2j+1}(1) = 0, \quad j=1,2,\dots \tag{35}$$

and $P_1(x) = x - \frac{1}{2}$, $0<x<1$.

It follows from Lemma 2 that $\int_0^\pi F(x)\,dx = 0$ and from (1) and (26) that $F'(\pi) = F'(0) = 0$ and $F'''(\pi) - F'''(0) = O(k^2)$. Hence by (34),

$$|\mathbf{s}^T \mathbf{f}| = \left| h^3 \int_0^\pi P_4(x/h) F^{(4)}(x)\,dx \right| + O(k^2 h^3). \tag{36}$$

Since, by Lemma 2, $y(x) = \sin(kx) + O(1/k)$ it follows from (26) and (12) that

$$F^{(4)}(x) = -8k^4 g(x) \cos(2kx) + O(k^3) \tag{37}$$

where $g := k^2 - \lambda + q$. Now define

$$g^*(x) := g(x_{i+\frac{1}{2}}) \qquad \text{for } x_i \leqq x < x_{i+1}, \quad i=0,\dots,n.$$

By Eq. (2.9.7) of [4],

$$|P_4(x)| \leqq \zeta(4)/8\pi^4 = O(1) \tag{38}$$

where ζ is the Riemann zeta function. Hence by (37),

$$\int_0^\pi P_4(x/h) F^{(4)}(x)\,dx = 8k^4 \int_0^\pi P_4(x/h)(g^* - g)(x)\cos(2kx)\,dx - 8k^4 \int_0^\pi P_4(x/h) g^*(x) \cos(2kx)\,dx + O(k^3). \tag{39}$$

By (38),

$$\left| \int_0^\pi P_4(x/h)(g^* - g)(x)\cos(2kx)\,dx \right| \leqq \|g^* - g\|_\infty \zeta(4)/8\pi^3 \leqq h\, \|g'\|_\infty \zeta(4)/16\pi^3 = O(h) = O(1/k)$$

since $kh<\pi$. Hence by (39),

$$\int_0^\pi P_4(x/h)F^{(4)}(x)\,dx=-8k^4\int_0^\pi P_4(x/h)\,g^*(x)\cos(2kx)\,dx+O(k^3). \tag{40}$$

Integration by parts using (35) shows that

$$\begin{aligned}\int_{x_i}^{x_{i+1}} P_4(x/h)\cos(2kx)\,dx&=h\int_0^1 P_4(t)\cos[2k(x_i+th)]\,dt\\
&=h\left\{\frac{B_4}{4!\,2kh}[\sin(2kx_{i+1})-\sin(2kx_i)]-\frac{B_2}{2!(2kh)^3}[\sin(2kx_{i+1})\right.\\
&\quad-\sin(2kx_i)]-\frac{1}{2(2kh)^4}[\cos(2kx_{i+1})+\cos(2kx_i)]\\
&\quad\left.+(2kh)^{-5}[\sin(2kx_{i+1})-\sin(2kx_i)]\right\}\\
&=2h\left\{\frac{-\sin(kh)}{4!(2kh)30}-\frac{\sin(kh)}{2!(2kh)^3 6}-\frac{\cos(kh)}{2(2kh)^4}\right.\\
&\quad\left.+\frac{\sin(kh)}{(2kh)^5}\right\}\cos(2kx_{i+\frac{1}{2}})\\
&=\frac{h\sin(kh)}{16(kh)^4}\left\{-\frac{(kh)^3}{45}-\frac{kh}{3}-\cot(kh)+\frac{1}{kh}\right\}\cos(2kx_{i+\frac{1}{2}}).\end{aligned}$$

Hence

$$\begin{aligned}&\left|\int_0^\pi P_4(x/h)\,g^*(x)\cos(2kx)\,dx\right|\\
&=\left|\sum_{i=0}^n g_{i+\frac{1}{2}}\int_{x_i}^{x_{i+1}} P_4(x/h)\cos(2kx)\,dx\right|\\
&=\left|\frac{h\sin(kh)}{16(kh)^4}\left[\cot(kh)-\frac{1}{kh}+\frac{kh}{3}+\frac{(kh)^3}{45}\right]\sum_{i=0}^n g_{i+\frac{1}{2}}\cos(2kx_{i+\frac{1}{2}})\right|\\
&\leqq\left|\frac{h\sin(kh)}{16(kh)^4}\left[\cot(kh)-\frac{1}{kh}+\frac{kh}{3}+\frac{(kh)^3}{45}\right]\frac{\pi\,\|g'\|_\infty}{2\sin(kh)}\right|\end{aligned}$$

by Lemma 5

$$\leqq\left|\frac{h\pi\,\|g'\|_\infty M(kh)^6}{32(kh)^4\sin(kh)}\right| \qquad \text{where } M:=\sup_{[0,\pi]}|G^{(7)}|/7!$$

and $G(x):=x\cos(x)+(-1+x^2/3+x^4/45)\sin(x)=x\sin(x)[\cot(x)-1/x+x/3+x^3/45]$, since it is readily verified by Taylor's theorem that $|G(x)|\leqq Mx^7$ when $0<x<\pi$.

Hence

$$\begin{aligned}\left|\int_0^\pi P_4(x/h)\,g^*(x)\cos(2kx)\,dx\right|&\leqq|\pi\,\|g'\|_\infty Mk^2h^3/32\sin(kh)|\\
&<\pi^3\,\|g'\|_\infty Mh/32\sin(kh) \qquad \text{since } 0<kh<\pi.\end{aligned}$$

The result now follows from (36) and (40) since $0<\sin(kh)<kh$. □

The proof of Theorem 1 is now easily completed. By (8), (13), (16) and (30), $\mathbf{s}^T(\mathbf{e}''-B^{-1}A\mathbf{e})=\mathbf{s}^T(\mathbf{e}''+k^2\mathbf{e})+(\mu-k^2)\mathbf{s}^T\mathbf{e}=\mathbf{s}^T\mathbf{f}+(\mu-k^2)\mathbf{s}^T\mathbf{e}$. Hence, since $\mathbf{u}^T\mathbf{s}+\mathbf{s}^T\mathbf{e}+\varepsilon^T\mathbf{e}=\mathbf{u}^T\mathbf{y}$, it follows from (17) and Lemmas 4 and 6 that

$$|\tilde{A}-\lambda|\,|\mathbf{u}^T\mathbf{y}|=|(A-\lambda)-(\mu-k^2)|\,|\mathbf{u}^T\mathbf{y}|\leqq c_3 k^4 h^4/\sin(kh) \tag{41}$$

where c_3 is the sum of the constants c_1 and c_2 in Lemmas 4 and 6. By Lemmas 1 and 2, $\|\mathbf{u}-\mathbf{s}\|_\infty$ and $\|\mathbf{y}-\mathbf{s}\|_\infty$ are both $O(k^{-1})$ for large k. Hence, since $(\mathbf{s}^T\mathbf{s})^{-1}=O(h)$, there exist positive constants k_0 and c_4 such that

$$\mathbf{u}^T\mathbf{y}\geqq c_4/h, \qquad \forall k\geqq k_0. \tag{42}$$

Combining (41) and (42) proves the theorem for $k\geqq k_0$. For $k<k_0$ the result follows from the fact that (7), (9) and (10) imply that there exists a constant c_5 such that

$$|\tilde{A}-\lambda|\leqq c_5 k^6 h^4\leqq c_5 k_0^3 k^4 h^5/\sin(kh). \quad □ \tag{43}$$

3. Numerical Results

The form of $\mu_k^{(n)}$ given by (9), though it simplifies some calculations in the proof, should not be used in numerical work as it is too sensitive to roundoff. In the practical evaluation of $\tilde{A}_k^{(n)}$ by (10) it is better to use the theoretically equivalent form

$$\mu_k^{(n)}=\frac{12\sin^2(kh/2)}{h^2[3-\sin^2(kh/2)]} \tag{44}$$

which was used in all calculations reported here.

In order to facilitate comparison with the results of [8], we chose the same functions q in (1) for our numerical examples, namely $q(x)=e^x$ and $q(x)=(x+0.1)^{-2}$. We calculated $A_k^{(n)}$ and $\tilde{A}_k^{(n)}$ for $k=1,\dots,n$ with $n=9$ and 19 and for $k=1,\dots,25$ with $n=39$, 79, 159 for each q and also for $k=1,\dots,4$ with $n=4$ for $q(x)=e^x$. All results shown were computed in double precision so that the structure of the error (which is very small for small kh) can be seen clearly.

For $q(x)=e^x$ and $n=39$, Table 1 shows, in order, for $k=1,\dots,20$: (i) the exact eigenvalue λ_k, (ii) the error $\lambda_k-A_k^{(n)}$in the uncorrected Numerov estimates, (iii) the error $\lambda_k-\tilde{A}_k^{(n)}$ in the corrected Numerov estimates, (iv) the error $\lambda_k-\tilde{\lambda}_k^{(n)}$ in the corrected second order estimates of [8] and finally (v) the ratio $(k^2-\mu_k^{(n)})/(\lambda_k-A_k^{(n)})$. For each q and all n, this ratio increased monotonically with k and was always positive (so that the correction, $k^2-\mu_k^{(n)}$, was always of the appropriate sign), and, for all $k<n$, was less than one (so that the correction was too small). Even for $k=n$, the ratio was less than one for $q(x)=(x+0.1)^{-2}$ and so close to one for $q(x)=e^x$ that $|\lambda_n-\tilde{A}_n^{(n)}|<|\lambda_{n-1}-\tilde{A}_{n-1}^{(n)}|$.

To confirm the prediction of Theorem 1, Table 2 gives the value of $(\lambda_k-\tilde{A}_k^{(n)})\sin(kh)/k^4h^5$ with $q(x)=e^x$ for $n=9$, 19, 39, 79 and 159. Table 3 compares the error, $\lambda_k-\tilde{A}_k^{(n)}$, in the corrected Numerov estimates obtained with $n=19$, 39 and 79 for $q(x)=(x+0.1)^{-2}$ with the exact eigenvalues in that case. For ease of tabulation, the errors in Table 3 and the three sets of errors in Table 1 are multiplied by 10^3.

Table 1. Errors ($\times 10^3$) in various estimates with $n=39$ and $q(x)=e^x$

k	λ_k	$(\lambda_k - \Lambda_k^{(n)}) \times 10^3$	$(\lambda_k - \tilde{\Lambda}_k^{(n)}) \times 10^3$	$(\lambda_k - \tilde{\lambda}_k^{(n)}) \times 10^3$	$\frac{(k^2 - \mu_k^{(n)})}{(\lambda_k - \Lambda_k^{(n)})}$
1	4.8966694	0.00282	0.0027	2.4	0.0563
2	10.045190	0.04268	0.0325	9.1	0.2380
3	16.019267	0.22720	0.1137	13.1	0.5098
4	23.266271	0.88366	0.2317	12.4	0.7377
5	32.263707	2.88017	0.3879	11.3	0.8653
6	43.220020	8.04318	0.5820	10.7	0.9276
7	56.181594	19.6872	0.8158	10.7	0.9586
8	71.152998	43.2849	1.0913	11.0	0.9748
9	88.132119	87.2765	1.4108	11.3	0.9838
10	107.11668	164.024	1.7778	11.8	0.9892
11	128.10502	290.917	2.1962	12.4	0.9925
12	151.09604	491.634	2.6709	13.2	0.9946
13	176.08900	797.568	3.2082	14.0	0.9960
14	203.08337	1249.40	3.8153	15.0	0.9969
15	232.07881	1898.85	4.5015	16.0	0.9976
16	263.07507	2810.51	5.2781	17.3	0.9981
17	296.07196	4063.87	6.1589	19.0	0.9985
18	331.06934	5755.41	7.1615	20.4	0.9988
19	368.06713	8000.64	8.3076	22.4	0.9990
20	407.06524	10936.3	9.6248	24.5	0.9991

Table 2. Scaled errors, $(\lambda_k - \tilde{\Lambda}_k^{(n)}) \sin(kh)/k^4 h^5$, with $q(x)=e^x$

	n				
k	9	19	39	79	159
1	0.069	0.070	0.070	0.070	0.070
2	0.103	0.106	0.106	0.107	0.107
3	0.099	0.106	0.107	0.108	0.108
4	0.081	0.091	0.093	0.094	0.094
9	−0.007	0.043	0.047	0.048	0.048
14		0.028	0.030	0.031	0.032
19		−0.004	0.021	0.023	0.023
25			0.016	0.017	0.018

The last two sentences of the proof of Theorem 1 suggest that, for $k<k_0$ in (42), $(\lambda_k - \tilde{\Lambda}_k^{(n)})$ could initially grow as fast as $O(k^6)$ but our examples did not exhibit this rapid initial growth of error. The maximum of $(\lambda_k - \tilde{\Lambda}_k^{(n)}) \sin(kh)/k^4 h^5$ occurred at $k=1$ for $q(x)=(x+0.1)^{-2}$ and at $k=2$ or 3 for $q(x)=e^x$ (after which it decreased monotonically in all cases) and the increase in $(\lambda_k - \tilde{\Lambda}_k^{(n)})$ for $k \leqq 3$ with $q(x)=e^x$ was less than $O(k^4)$. Indeed our results indicate that the relative error $(\lambda_k - \tilde{\Lambda}_k^{(n)})/\lambda_k$ increases only slightly with k until $(kh)/\sin(kh)$ begins to increase significantly. We conjecture that for a wide class of problems the error in $\tilde{\Lambda}_k^{(n)}$ is in fact $O(k^3 h^5/\sin(kh))$ and have made some progress towards proving this. We hope to return to this in a later paper.

Table 3. Errors ($\times 10^3$) in corrected Numerov estimates with $q(x)=(x+0.1)^{-2}$

k	λ_k	$(\lambda_k-\tilde{\Lambda}_k^{(n)})\times 10^3$		
		$n=19$	$n=39$	$n=79$
1	1.5198658	0.4325	0.046	0.004
2	4.9433098	2.7664	0.293	0.024
3	10.284663	8.6229	0.903	0.073
4	17.559958	19.436	2.011	0.162
5	26.782863	36.391	3.717	0.299
6	37.964426	60.481	6.095	0.486
7	51.113358	92.608	9.198	0.729
8	66.236448	133.70	13.07	1.029
9	83.338962	184.81	17.75	1.386
10	102.42499	247.30	23.29	1.802
11	123.49771	322.89	29.72	2.278
12	146.55961	413.94	37.10	2.814
13	171.61264	523.64	45.49	3.412
14	198.65837	656.47	54.97	4.072
15	227.69803	818.84	65.63	4.795
16	258.73262	1020.4	77.57	5.584
17	291.76293	1276.4	90.92	6.440
18	326.78963	1614.4	105.8	7.365
19	363.81325	2096.3	122.5	8.361
20	402.83424		141.0	9.432

Comparison of $|\lambda_k-\tilde{\Lambda}_k^{(n)}|$ with the values of $|\lambda_k-\tilde{\lambda}_k^{(n)}|$ given in [8] and [6] for $n=19$, 39 and 79 and $k\leqq 20$ shows that $\tilde{\Lambda}_k^{(n)}$ is more accurate (much more accurate for small kh) than $\tilde{\lambda}_k^{(n)}$ in *all* cases when $q(x)=e^x$ and all cases with $k<3n/4$ when $q(x)=(x+0.1)^{-2}$. This is not surprising since the relative advantage of Numerov's method is greatest when kh is small and $\|q^{(4)}\|_\infty/\|q''\|_\infty$ is not too large. Since computation of the eigenvalues of (4) requires only slightly more effort than calculating the eigenvalues of $(-A+Q)$, we recommend that the corrected Numerov estimates $\tilde{\Lambda}_k^{(n)}$ studied here be used in preference to the corrected second order estimates $\tilde{\lambda}_k^{(n)}$ of [8], at least for reasonably smooth q, provided $k<n/2$.

The "improvement factor" $|\lambda_k-\Lambda_k^{(n)}|/|\lambda_k-\tilde{\Lambda}_k^{(n)}|$ was always greater for $q(x)=e^x$ than for the nearly singular $q(x)=(x+0.1)^{-2}$. With $k=25$ and $n=79$ for example it was over 3,000 for $q(x)=e^x$ but only just over 150 for $q(x)=(x+0.1)^{-2}$. However perhaps of greatest interest is the fact that for *both* q and *all* k and n we found $|\lambda_k-\tilde{\Lambda}_k^{(n)}|<|\lambda_k-\Lambda_k^{(n)}|$. Since the extra work involved in computing the correction (10) is negligible, we believe the correction is potentially useful even for the lowest eigenvalues.

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