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Accurate numerical bounds for the spectral points of singular Sturm–Liouville problems over $0 < x < \infty$

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Abstract

The eigenvalues of singular Sturm–Liouville problems defined over the semi-infinite positive real axis are examined on a truncated interval $0 < x < \ell$ as functions of the boundary point ℓ. As a basic theoretical result, it is shown that the eigenvalues of the truncated interval problems satisfying Dirichlet and Neumann boundary conditions provide, respectively, upper and lower bounds to the eigenvalues of the original problem. Moreover, the unperturbed system in a perturbation problem, where ℓ remains sufficiently small, admits analytical solutions in terms of the Bessel functions of the first kind. Applications to the Schrödinger equations of diatomic molecules and a harmonic oscillator confirm the practical implementation of this approach in calculating highly accurate numerical eigenvalue enclosures. It is worth mentioning that this study is, therefore, a completion of the paper (J. Comput. Appl. Math. 115 (2000) 535) where similar problems on the whole real axis $-\infty < x < \infty$ were treated along the same lines.

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1. Introduction

Linear differential equations of the second order are of crucial importance in the study of differential equations not only for theoretical reasons but also their appearences in any serious investigation of the classical areas of mathematical physics and applied sciences. It is a well-known fact that any second order linear equation can always be transformed to Sturm–Liouville form having nice

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mathematical properties. Let us consider such an equation in Sturm–Liouville form

$$\hat{\mathscr{L}}y = 0, \quad \hat{\mathscr{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[(x-x_0)^2 p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right] + q(x) - \lambda(x-x_0)^2 r(x) \tag{1.1}$$

defined on the interval $x \in (x_0, \infty)$, say I_∞, where x_0 and λ are real parameters. We suppose that the functions p, p', q and r are real analytic at the point x_0 and continuous on any subinterval of I_∞. Besides p and r are assumed to be positive throughout I_∞.

We are interested in the eigenvalue problems associated with the differential operator $\hat{\mathscr{L}}$ subject to suitable boundary conditions. More precisely, we are looking for solutions of class $L^2(x_0, \infty)$, where

$$\int_{x_0}^{\infty} (x-x_0)^2 r(x)[y(x)]^2 \,\mathrm{d}x < \infty \tag{1.2}$$

and take into account operators $\hat{\mathscr{L}}$ of the limit-point type [1]. That is, if the equation $\hat{\mathscr{L}}y = 0$ admits a non-trivial solution $g(x)$ of class $L^2(x_0, \infty)$ the parameter λ must then be necessarily an eigenvalue and $g(x)$ the corresponding eigenfunction. In such a limit-point case, no boundary conditions are needed at infinity.

It is obvious that we have a singular system because of the infinite interval I_∞ under consideration. Furthermore, the differential equation has an additional singularity, namely, a regular singular point located at $x = x_0$ so that the required solution should behave correctly there as well. From this argument it follows that the eigenfunctions possess the asymptotic form

$$y(x) \sim (x-x_0)^{\alpha-1/2}, \quad \alpha > 0 \tag{1.3}$$

as $x \to x_0$. Here, the parameter α in the exponent of the singularity at x_0 can easily be determined by

$$\alpha = \tfrac{1}{2}\sqrt{1 + 4q_0/p_0}, \tag{1.4}$$

where $q_0 = q(x_0)$ and $p_0 = p(x_0)$. Note that α should be positive for the square integrability of solutions. In fact, we may equate p_0 to unity and, without loss of generality, set $x_0 = 0$ since a linear transformation always takes x_0 into the origin of a rescaled coordinate system.

In a recent article [10], we treated singular eigenvalue problems over $-\infty < x < \infty$ with no further singularity at a finite point of the whole real axis by means of the purely regular problem defined on the finite interval $(-\ell, \ell)$ of length 2ℓ. Similarly, instead of (1.1) on the unbounded interval I_∞, we consider here the same differential equation over a finite interval I_ℓ, where $x \in (0, \ell)$ with $x_0 = 0$, which has a singularity only at the origin. The present work can, therefore, be viewed as an extension of the method and techniques in [10] along the same lines to systems having a sufficiently singular behaviour at a point x_0, say $x_0 = 0$. Hence the mathematical problem in question consists of the differential equation in (1.1) on I_ℓ as well as a regularity condition of type (1.3) as $x \to 0$ and a common condition

$$y(x)\cos\theta + x^2 p(x) y'(x)\sin\theta = 0, \quad \theta \in \mathbb{R} \tag{1.5}$$

at $x = \ell$. Clearly, the particular values of $\theta = 0$ and $\pi/2$ correspond to Dirichlet and Neumann type boundary conditions, respectively.

In Section 2 we show how to examine the variation of an eigenvalue as a function of the boundary parameter ℓ in the cases of both Dirichlet and Neumann problems. Section 3 finds out the behaviours

of eigenvalues while ℓ remains small in a regular perturbation problem. The application of the suggested method to the radial Schrödinger equation is included in Section 4. Accurate computations of eigenvalue enclosures, using Rayleigh–Ritz and Lehmann methods, are presented in the last section together with concluding remarks.

2. Dependence of eigenvalues on the boundary point ℓ

The Sturm–Liouville equation on I_ℓ can be thought for a moment as a partial differential equation

$$\mathscr{L} f(x,\ell) = 0, \quad \mathscr{L} = -\frac{\partial}{\partial x}\left[x\,p(x)\,\frac{\partial}{\partial x}\right] + s(x) - \lambda(\ell)xr(x) \tag{2.1}$$

in independent variables x and ℓ and the transformed dependent variable

$$f(x,\ell) = \sqrt{x}\,y(x,\ell), \tag{2.2}$$

where

$$s(x) = \frac{1}{x}\left[q(x) + \tfrac{1}{4}\,p(x)\right] + \tfrac{1}{2}\,p'(x). \tag{2.3}$$

The required solution $f(x,\ell)$ of the transformed equation (2.1) obeys the regularity condition

$$f(x,\ell) \sim x^{\alpha}, \quad \alpha = \tfrac{1}{2}\sqrt{1+4q_0}, \quad p_0 = 1, \tag{2.4}$$

for all ℓ as $x \to 0$, and the boundary condition

$$f(x,\ell)\cos\theta + x\,p(x) f_x(x,\ell)\sin\theta = 0 \tag{2.5}$$

at $x = \ell$ where, as usual, the subscript x denotes the partial derivative with respect to x. Such a solution is obviously square integrable over I_ℓ which can be normalized to obtain

$$\int_0^\ell xr(x)[f(x,\ell)]^2\,\mathrm{d}x = 1 \tag{2.6}$$

for all $\ell > 0$. On the other hand, the differentiation of $\mathscr{L} f = 0$ with respect to ℓ gives

$$\mathscr{L} f_\ell(x,\ell) = xr(x) f(x,\ell)\,\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} \tag{2.7}$$

from which we arrive at the relation

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = \int_0^\ell [\mathscr{L} f_\ell(x,\ell)] f(x,\ell)\,\mathrm{d}x. \tag{2.8}$$

Equation (2.8) can be put into a form

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = \text{Boundary Terms} + \int_0^\ell f_\ell(x,\ell)[\mathscr{L}^\star f(x,\ell)]\,\mathrm{d}x \tag{2.9}$$

upon introducing the adjoint differential operator $\mathscr{L}^\star$. However, the integral term in (2.9) vanishes since $\mathscr{L}$ is formally self-adjoint and, hence, $\mathscr{L}^\star y = \mathscr{L} y = 0$. Thus the eigenvalues of the finite

interval problem satisfy the relation

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ell} = x\,p(x)[f_x(x,\ell)f_\ell(x,\ell) - f(x,\ell)f_{x\ell}(x,\ell)]|_{x=0}^{\ell} \tag{2.10}$$

which may be simplified on using (2.5). Actually, the total differential of the function $f(x,\ell)$ implies the operational equivalence

$$\frac{\mathrm{d}}{\mathrm{d}\ell} = \frac{\partial}{\partial x} + \frac{\partial}{\partial \ell} \tag{2.11}$$

if $x = \ell$ with $\mathrm{d}x = \mathrm{d}\ell$. Then the implicit derivative of the boundary condition in (2.5) with respect to ℓ leads to the identities

$$f_\ell(\ell,\ell) = -f_x(\ell,\ell) \tag{2.12}$$

and

$$f_{x\ell}(\ell,\ell) = -f_{xx}(\ell,\ell), \tag{2.13}$$

whenever $\theta = 0$ and $\pi/2$, respectively. Now if we use the formulation above, we obtain the following propositions.

Proposition 1. *Let $\lambda^+(\ell)$ and $f^+(x,\ell)$ denote an eigensolution of the Dirichlet problem. Then it follows from* (2.10), *in conjunction with* (2.12), (2.4) *and* (2.5), *that*

$$\frac{\mathrm{d}\lambda^+}{\mathrm{d}\ell} = -\ell\,p(\ell)[f_x^+(\ell,\ell)]^2 < 0 \tag{2.14}$$

for all ℓ. Therefore, as ℓ increases the eigenvalues of the Dirichlet problem decreases monotonically to the eigenvalues, denoted by λ^∞, of the original problem over I_∞.

Proposition 2. *Let $\lambda^-(\ell)$ and $f^-(x,\ell)$ denote an eigensolution of the Neumann problem. Then we see, after some algebra, that the relation in* (2.10) *reads as*

$$\frac{\mathrm{d}\lambda^-}{\mathrm{d}\ell} = [s(\ell) - \lambda^-(\ell)\ell r(\ell)][f^-(\ell,\ell)]^2. \tag{2.15}$$

In many cases in which the mathematical problem describes a physical phenomena such as the Schrödinger form of the operator $\mathscr{L}$ with $p(x) = r(x)$, it is reasonable to define a turning point $\ell = \ell_0$ for which

$$\lambda^-(\ell_0) = \hat{v}(\ell_0) \tag{2.16}$$

where $\hat{v}(x)$,

$$\hat{v}(x) = \frac{s(x)}{xr(x)}, \tag{2.17}$$

is an effective potential function. Furthermore, $\hat{v}(\ell) < \lambda^-(\ell)$ for $\ell < \ell_0$ and $\hat{v}(\ell) > \lambda^-(\ell)$ for $\ell > \ell_0$. Hence, Proposition 2 implies that the eigenvalues $\lambda^-(\ell)$ of the Neumann problem decrease when $\ell < \ell_0$, take on minimum values at $\ell = \ell_0$ and increase when $\ell > \ell_0$.

As a significant result, providing ℓ is large enough we deduce that $\lambda^+(\ell)$ and $\lambda^-(\ell)$ converge to λ^∞ from above and from below as ℓ increases, respectively. In other words, the difference $\lambda^+(\ell)-\lambda^-(\ell)$ can be regarded as an error bound in the computation of eigenvalues λ^∞ of the singular problem on I_∞. Note that this conclusion on the behaviours of Dirichlet and Neumann eigenvalues as ℓ varies, is a word for word repeat of the corollary given in [10] for the purely regular system over $(-\ell,\ell)$.

3. Small values of ℓ as a perturbation parameter

By making use of the scaling transformation

$$x=\ell\xi \tag{3.1}$$

Eq. (2.1) is written as

$$\left\{-\frac{\partial}{\partial\xi}\left[\xi\,p(\ell\xi)\,\frac{\partial}{\partial\xi}\right]+\ell s(\ell\xi)-\ell^2\lambda(\ell)\xi r(\ell\xi)\right\}f(\xi,\ell)=0,\quad \xi\in I_1 \tag{3.2}$$

on the unit interval I_1, where $\xi\in(0,1]$. Note that p, p' and q contained in the function s in (2.3), and r are all analytic at $x=0$ and so at $\ell=0$ as well. In what follows, for sufficiently small values of ℓ, we try an eigensolution of the type

$$f(\xi,\ell)=F_0(\xi)+F_1(\xi)\ell+\cdots \tag{3.3}$$

and

$$\ell^2\lambda(\ell)=v_0+v_1\ell+\cdots \tag{3.4}$$

and deduce that the leading order term $F_0(\xi)$ satisfies the Bessel differential equation

$$\mathscr{L}_0F_0(\xi)=\mu^2F_0(\xi),\qquad \mathscr{L}_0=-\frac{1}{\xi}\,\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\xi\,\frac{\mathrm{d}}{\mathrm{d}\xi}\right)+\frac{\alpha^2}{\xi^2} \tag{3.5}$$

where

$$\mu^2=r_0v_0=r_0\lim_{\ell\to0^+}\ell^2\lambda(\ell),\quad r_0=r(0). \tag{3.6}$$

To derive boundary conditions for the functions $F_k(\xi)$ at $\xi=1$, we write down the left hand side of (2.5) as a power series in ℓ and set each coefficient of ℓ to zero. Thus the conditions imposed on $F_0(\xi)$ are the boundary condition

$$F_0(1)\cos\theta+F_0'(1)\sin\theta=0 \tag{3.7}$$

and, from (2.4), the regularity condition $F_0(\xi)\sim\xi^\alpha$ as $\xi\to0$.

Obviously, the solution of (3.5), which behaves correctly at the origin, is the Bessel function of the first kind of order α denoted conventionally by $J_\alpha(\mu\xi)$. So the dominant solution of the asymptotic problem satisfying the boundary condition as well is given, for small values of ℓ, by

$$f(\xi,\ell)\sim AJ_\alpha(\mu\xi),\quad A\in\mathbb{R} \tag{3.8}$$

provided that μ is a positive zero of the equation $J_\alpha(\mu)\cos\theta+\mu J_\alpha'(\mu)\sin\theta=0$. As is well known this transcendental equation has an infinite number of real positive roots, all of which are simple

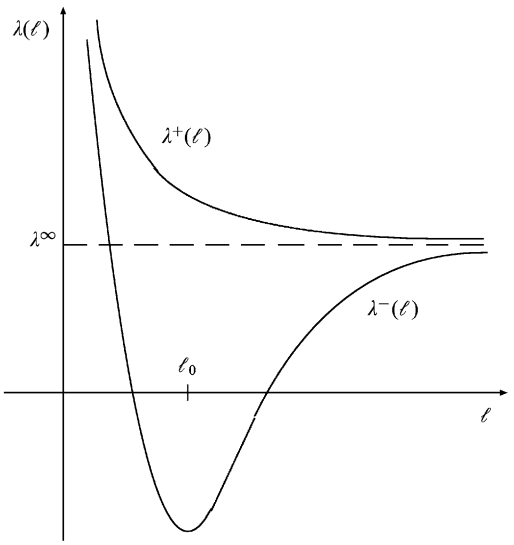

Fig. 1. Typical variations of the Dirichlet and Neumann eigenvalues.

[6]. Notice also that the existence of such μ values justifies at the same time the existence of the limit in (3.6).

Therefore, the eigenvalues $\lambda(\ell)$ of the problem on the finite interval in Section 2 grows like $1/\ell^2$ as $(0,\ell)$ becomes finer and finer, that is,

$$\lambda(\ell) \sim \frac{\mu^2}{r_0 \ell^2} \tag{3.9}$$

as $\ell \to 0$. Recalling the two propositions of Section 2, we now estimate the behaviour of a typical eigenvalue of each problem of the Dirichlet and Neumann type, as a function of ℓ as shown in Fig. 1.

4. Applications to the Schrödinger equation

Let us consider the radial Schrödinger equation of the form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{2}{x}\frac{\mathrm{d}}{\mathrm{d}x} + \frac{l(l-1)}{x^2} + v(x)\right] \Psi(x) = E\Psi(x), \quad x \in I_\infty, \tag{4.1}$$

where $\Psi(x)$, $v(x)$ and E denote the wavefunction, potential function and the energy eigenvalues, respectively, and the integral values $l=1,2,\ldots$, are the eigenvalues of the angular momentum operator originating from the separation of a three-dimensional quantum system. Eq. (4.1) is a particular form of our differential equation, which can be recovered from (1.1) by setting

$$x_0 = 0, \quad p(x) = r(x) = 1, \quad q(x) = l(l-1) + x^2 v(x), \quad \lambda = E. \tag{4.2}$$

Two very famous analytically solvable cases corresponding to the wave mechanical treatment of the harmonic oscillator, where

$$v(x) = x^2, \tag{4.3}$$

and diatomic molecules via the Morse potential

$$v(x) = Z^2[\mathrm{e}^{-(x-c)} - 1]^2 = 2Z^2\mathrm{e}^{-(x-c)}[\cosh(x-c) - 1], \quad Z, c > 0 \tag{4.4}$$

provide a convenient testing ground for the present approach. For all quantum numbers $n, l = 1, 2, \ldots$, the analytical solutions derived on I_∞ for the harmonic oscillator are given by

$$\Psi_{n,l}(x) = A_{n,l}x^{l-1}\mathrm{e}^{-\frac{1}{2}x^2}L_{n-1}^{l-1/2}(x^2), \quad E_{n,l} = 4n + 2l - 3, \tag{4.5}$$

where the $A_{n,l}$ are some normalization constants, and the L_m^n stand for the associated Laguerre polynomials. However, only the eigen-pair of the Schrödinger equation with $l = 1$, corresponding to the purely vibrational energy levels of diatomic molecules modeled by the Morse potential, is expressible in closed form

$$\Psi_n(x) = B_n x[u(x)]^{d_n}\mathrm{e}^{-Zu(x)}L_{n-1}^{2d_n}[2Zu(x)], \quad E_{n,1} = (2n-1)\left[Z - \tfrac{1}{4}(2n-1)\right] \tag{4.6}$$

for $n = 1, \ldots, K$, where K is the integer part of the parameter $Z + \frac{1}{2}$, the B_n are some constants, and

$$u(x) = \mathrm{e}^{-(x-c)}, \quad d_n = Z - \tfrac{1}{2}(2n-1) > 0. \tag{4.7}$$

Despite the similarity in form of the two eigensolutions, they in fact possess different spectral structures. The harmonic oscillator has purely a discrete spectrum whereas the Morse problem has both a discrete and a continuous spectra. More precisely, the Morse potential has a finite number K of real spectral points lying between $0 < E < Z^2$ and a continuous spectrum for all $E \geqslant Z^2$ in the E-complex plane. Note that the number K of the spectral points depends completely on Z, a kind of atomic charge parameter, and the system has no bound states if $Z < \frac{1}{2}$.

Another important remark is that the analytical solution in (4.6) is obtainable over the interval $(-\infty, \infty)$, which contains the unphysical region $-\infty < x < 0$ [4]. Since, here, x denotes the internuclear distance it should be non-negative. Nevertheless we proved numerically in [9] that Morse's original assumption of the inclusion of the unphysical portion $(-\infty, 0)$ does not cause any deviation from the correct eigenvalues representing the physical domain.

Under the assumption that $v(x)$ does not grow faster than $1/x^2$ at the origin, as is the case for the potentials in (4.3) and (4.4), we see from (4.2) that the parameter α in (2.4) is written as

$$\alpha = l - \tfrac{1}{2}, \quad l = 1, 2, \ldots \tag{4.8}$$

and the Schrödinger equation (4.1) on the unit truncated interval I_1 takes the form

$$T\Phi(\xi) = E(\ell)\Phi(\xi), \quad T = \frac{1}{\ell^2}\mathscr{L}_0 + v(\ell\xi), \quad \xi \in I_1 \tag{4.9}$$

for a given $\ell > 0$, where ξ is again the scaled variable in (3.1) and $\Phi(\xi) = \sqrt{\xi}\Psi(\xi)$. In this setting the transformed dependent variable Φ obeys the conditions of the same forms as that of $F_0(\xi)$ in Section 3.

From a computational viewpoint, we have to introduce a numerical algorithm to cope with the eigenvalue problem for a prescribed ℓ at which the differences between the Dirichlet and Neumann

eigenvalues are reasonably small. The analytical solutions in closed form of the asymptotic problem in Section 3 suggest evidently two approximation methods to use. Firstly, the series in (3.3) and (3.4) have nonzero radii of convergence in the ℓ-complex plane because they are regular perturbation expansions of an eigensolution. So the higher-order corrections can be evaluated by a Rayleigh–Schrödinger perturbative scheme, which results in a formula to approximate eigenvalues $E(\ell)$ for every ℓ sufficiently close to $\ell = 0$.

Alternatively, since the eigenfunctions of the operator $\mathscr{L}_0$ in (3.5) constitute a set of orthogonal functions on I_1, they can be used as an expansion basis in a Rayleigh–Ritz variational method to approximate the eigenfunctions of the operator T in (4.9). As a matter of fact, we get a sequence of normalized functions $\{\phi_n(\xi)\}$ in the sense that

$$\int_0^1 \xi \phi_m(\xi)\phi_n(\xi)\,\mathrm{d}\xi = \delta_{mn}, \tag{4.10}$$

where δ_{mn} is the Kronecker's delta. Explicitly speaking, the basis functions $\phi_n(\xi)$ satisfying the equation $\mathscr{L}_0\phi_n = \mu_n^2\phi_n$ and appropriate conditions are of the form

$$\phi_n(\xi) = \mathscr{N}_n J_\alpha(\mu_n\xi), \quad n = 1, 2, \ldots, \tag{4.11}$$

where the μ_n stand for the positive roots of the equation

$$J_\alpha(\mu)\cos\theta + \mu J'_\alpha(\mu)\sin\theta = 0, \tag{4.12}$$

and the normalization constants $\mathscr{N}_n$ are defined by the relation

$$\mathscr{N}_n^2\{[J_\alpha(\mu_n)]^2 - J_{\alpha-1}(\mu_n)J_{\alpha+1}(\mu_n)\} = 2. \tag{4.13}$$

These relations can be simplified in the Dirichlet and Neumann problems. Indeed, for the Dirichlet type boundary conditions the μ_n are the roots of the simpler equation $J_\alpha(\mu) = 0$, and hence

$$\mathscr{N}_n = \frac{\sqrt{2}}{J_{\alpha-1}(\mu_n)}. \tag{4.14}$$

For the Neumann problem, on the other hand, $J'_\alpha(\mu) = 0$, and the normalization constants become

$$\mathscr{N}_n = \frac{\sqrt{2}\mu_n}{\sqrt{\mu_n^2 - \alpha^2}J_\alpha(\mu_n)} \tag{4.15}$$

where, in (4.13)–(4.15), we have used the functional relationships known for the Bessel functions.

Finally, we see from (4.8) that the exponent α is always half an odd integer, and, therefore, the basis elements ϕ_n contain Bessel functions of fractional orders, which are closely related to the spherical Bessel functions. These functions can simply be written in terms of the circular functions, the first two of which are

$$J_{1/2}(z) = \sqrt{\frac{2}{\pi z}}\sin z, \quad J_{-1/2}(z) = \sqrt{\frac{2}{\pi z}}\cos z. \tag{4.16}$$

The others may be evaluated by means of the recurrence relation

$$zJ_{k+3/2}(z) = (2k+1)J_{k+1/2}(z) - zJ_{k-1/2}(z) \tag{4.17}$$

for $k = 0, 1, \ldots$ [2].

5. Specimen numerical computations and discussion

The "state of art" about the numerical evaluation of the bound states of the differential eigenvalue problems is well discussed in [5]. There are indeed many existing software packages that can estimate to user requested precision eigenvalues of very general Sturm–Liouville problems. However, these do not provide two-sided bounds explaining why the present study may be interesting. More explicitly, the reliability and consistency of the eigenvalues can be rechecked by means of the lower and upper bounds. Of course, this is achieved at the cost of solving two boundary value problems of the Dirichlet and Neumann types instead of a single one.

Depending on the quality of the basis functions under consideration, we can find very accurate numerical results for the ground and the low-lying states eigenvalues by means of the Rayleigh–Ritz variational method. So proposing a trial solution for (4.9) of the form

$$\Phi_M(\xi) = \sum_{n=1}^{M} a_n \phi_n(\xi), \quad a_n \in \mathbb{R} \tag{5.1}$$

and making use of standard techniques, we convert the differential eigenvalue problem to a symmetric matrix eigenvalue problem

$$\sum_{n=1}^{M} [H_{mn}(\ell) - \mathscr{E}(M,\ell)\delta_{mn}]a_n = 0, \quad m = 1, 2, \ldots, M \tag{5.2}$$

with the matrix elements defined by

$$H_{mn}(\ell) = V_{mn}(\ell) + \frac{\mu_n^2}{\ell^2}\,\delta_{mn}, \tag{5.3}$$

where

$$V_{mn}(\ell) = \int_0^1 \xi \phi_m(\xi)\phi_n(\xi) v(\ell\xi)\,\mathrm{d}\xi, \tag{5.4}$$

and $\mathscr{E}(M,\ell)$ denotes the approximate matrix eigenvalues for $E(\ell)$. In general, the first N eigenvalues of (5.2) ordered by magnitude $\mathscr{E}_1 \leqslant \mathscr{E}_2 \leqslant \cdots \leqslant \mathscr{E}_N$ approximate $E_1 \leqslant E_2 \leqslant \cdots \leqslant E_N$ very well, if the approximation order M is about $2N$ [5].

Furthermore, it is known from the variational principle that the Rayleigh–Ritz matrix eigenvalues $\mathscr{E}(M,\ell)$ provide upper bounds to the exact eigenvalues $E(\ell)$. In the case of the Dirichlet problem this approach is, therefore, quite appropriate and natural due to the fact that the true Dirichlet eigenvalues $E^+(\ell)$ are already upper bounds, for all ℓ, to the target eigenvalues $E = E^\infty$ of the original problem (4.1) over I_∞. That is to say, concerning the kth representative eigenvalue E_k^∞ we have the inequalities

$$E_k^\infty < E_k^+(\ell) < \mathscr{E}_k^+(M,\ell) \tag{5.5}$$

valid for all $k \leqslant M$, M and ℓ, where the $\mathscr{E}_k^+$ denote the Rayleigh–Ritz eigenvalues corresponding to the Dirichlet boundary conditions.

Unfortunately, the situation seems to be complicated in the Neumann problem, where the correct eigenvalues $E^-(\ell)$ are lower bounds to E^∞, $E^-(\ell) < E^\infty$, if $\ell > \ell_0$. More specifically, the Rayleigh–Ritz method finds matrix eigenvalues $\mathscr{E}^-(M,\ell)$ which are upper bounds to the lower bound eigenvalues; that is, $\mathscr{E}^-(M,\ell) > E^-(\ell)$ for finite values of M. As a result it may be the case that $\mathscr{E}^-(M,\ell) > E^\infty$ due to the truncation errors, or otherwise. In order to overcome this trouble and introduce reliable eigenvalue enclosures for E^∞, we employ the so-called Lehmann method [3,5] for the calculation of the spectrum of the Neumann problem.

The Lehmann method uses again a trial solution of form (5.1) and determines lower bounds to the first N spectral points $E_1^-(\ell),\ldots,E_N^-(\ell)$. However, it requires an a priori lower bound $\eta(N,\ell)$ for $E_{N+1}^-(\ell)$ such that

$$E_N^-(\ell) < \mathscr{E}_N^-(N,\ell) < \eta(N,\ell) \leqslant E_{N+1}^-(\ell). \tag{5.6}$$

To apply the Lehmann method we define a new square matrix $\boldsymbol{W}$ of size N, whose common entry is defined by the integral

$$W_{mn}(\ell) = \int_0^1 \xi[T\phi_m(\xi)][T\phi_n(\xi)]\,\mathrm{d}\xi, \tag{5.7}$$

and can be written explicitly as

$$W_{mn}(\ell) = \frac{1}{\ell^4}[\mu_m^4\delta_{mn} + \ell^2(\mu_m^2+\mu_n^2)V_{mn}(\ell) + \ell^4 U_{mn}(\ell)], \tag{5.8}$$

where

$$U_{mn}(\ell) = \int_0^1 \xi\phi_m(\xi)\phi_n(\xi)[v(\ell\xi)]^2\,\mathrm{d}\xi, \tag{5.9}$$

for $m,n = 1,2,\ldots,N$. Then we consider the symmetric generalized matrix eigenvalue problem

$$\sum_{n=1}^{N}[\mathscr{A}_{mn}(\ell) - \beta(N,\ell)\mathscr{B}_{mn}(\ell)]a_n = 0, \quad m = 1,2,\ldots,N \tag{5.10}$$

containing the symmetric matrices $\mathscr{A}$ and $\mathscr{B}$ with general elements

$$\mathscr{A}_{mn}(\ell) = H_{mn}(\ell) - \eta(N,\ell)\delta_{mn} \tag{5.11}$$

and

$$\mathscr{B}_{mn}(\ell) = [\eta(N,\ell)]^2\delta_{mn} - 2\eta(N,\ell)H_{mn}(\ell) + W_{mn}(\ell), \tag{5.12}$$

respectively. Now if we introduce the ordered sequence

$$\mathscr{D}_k^-(N,\ell) = \eta(N,\ell) + \frac{1}{\beta_{N+1-k}(N,\ell)} \tag{5.13}$$

then Lehmann's theorem [5] states that the $\mathscr{D}_k^-(N,\ell)$ are lower bounds to the Neumann eigenvalues,

$$\mathscr{D}_k^-(N,\ell) < E_k^-(\ell) \tag{5.14}$$

for $k = 1, 2, \ldots, N$. Consequently, (5.5) and (5.14) generalize the two-sided inequality

$$\mathscr{D}_k^-(N,\ell) < E_k^-(\ell) < E_k^\infty < E_k^+(\ell) < \mathscr{E}_k^+(M,\ell), \quad M \geqslant N \tag{5.15}$$

for the first N spectral points $E_1^\infty, \ldots, E_N^\infty$ of the singular system.

Because of the left-hand side inequality in (5.6) the matrix $\mathscr{A}$ is negative definite whereas, it can be shown that $\mathscr{B}$ is positive definite. Hence the eigenvalues $\beta_i(N,\ell)$ of (5.10) are all negative for $i = 1, \ldots, N$. As another computationally important remark, if

$$\mathscr{B} = \boldsymbol{L}\boldsymbol{L}^{\mathrm{T}} \tag{5.16}$$

is the Cholesky decomposition of the positive definite matrix $\mathscr{B}$, then (5.10) can be replaced by the standard problem

$$\sum_{n=1}^{N} [\mathscr{C}_{mn}(\ell) - \beta(N,\ell)\delta_{mn}(\ell)]a_n = 0, \quad m = 1, 2, \ldots, N \tag{5.17}$$

implying that the eigenvalues $\beta(N,\ell)$ in (5.10) are precisely the eigenvalues of the symmetric matrix $\mathscr{C}$,

$$\mathscr{C} = \boldsymbol{L}^{-1}\mathscr{A}(\boldsymbol{L}^{-1})^{\mathrm{T}} \tag{5.18}$$

as it is similar to the matrix $\mathscr{B}^{-1}\mathscr{A}$ [7].

It should be noted that the application of the Lehmann method is not an easy task, even it may not always be possible because of the existence and computation of a lower bound $\eta(N,\ell)$ for $E_{N+1}^-(\ell)$ satisfying the conditions in (5.6) (see [5] for details). Fortunately, in this work we estimate such $\eta(N,\ell)$ values in many cases by means of the Nth Rayleigh–Ritz eigenvalues $\mathscr{E}_N^+(M,\ell)$ of the Dirichlet problem. Actually, for a second-order differential operator in Sturm–Liouville form, it is known from the Sturm oscillation and comparison theorems that the Dirichlet eigenvalues are always greater than the corresponding Neumann eigenvalues and that

$$E_N^-(\ell) < E_N^+(\ell) < E_{N+1}^-(\ell) \tag{5.19}$$

for all N [1]. Therefore, if M is large enough then $E_N^+(\ell) \cong \mathscr{E}_N^+(M,\ell)$, and choosing $\eta(N,\ell)$ as $\mathscr{E}_N^+(M,\ell)$ we have

$$\eta(N,\ell) \leqslant E_{N+1}^-(\ell) \tag{5.20}$$

as required. If we are lucky this estimation satisfies the left-hand side inequality in (5.6) as well, which is generally the case since the eigenvalues are well separated in our specific examples. Otherwise, the numerical implementation of the Neumann boundary value problem by using the Lehmann method fails.

In our tables, n is the state number of the eigenvalues, and the N stand for the sizes of matrices used in our numerical algorithm. Illustrative examples are performed for the Schrödinger equation with the angular quantum number $l = 1$, for which the exponent of the singularity at the origin is $\alpha = 1/2$. The Lehmann lower and the Rayleigh–Ritz upper eigenvalue bounds are presented as a function of the boundary point ℓ in Tables 1 and 2 for the harmonic oscillator and the Morse potential, with $Z = 50$ and $c = 0$, respectively. It is clearly shown that more accurate eigenvalue enclosures are determined as ℓ increases confirming the conclusions of the two propositions in

Table 1
Convergence rates of two-sided Rayleigh–Ritz and Lehmann bounds for the first three eigenvalues of the harmonic oscillator as a function of N and ℓ

n	ℓ	N	$\mathscr{D}_n^-(N,\ell)$	$\mathscr{E}_n^+(N,\ell)$	$E_{n,1}^{\infty}$
1	4.5	5	—	3.000 014	
		10	2.999 998 316	3.000 000 608	
		15	2.999 998 316	3.000 000 608	3
	6.0	10	—	3.000 000 000 006 370	
		15	2.999 999 999 999 770	3.000 000 000 000 216	
		20	2.999 999 999 999 770	3.000 000 000 000 216	3
	7.5	15	—	3.000 000 000 000 000 075	
		20	2.999 999 999 999 999 999 999 283	3.000 000 000 000 000 000 000 690	
		25	2.999 999 999 999 999 999 999 283	3.000 000 000 000 000 000 000 690	3
	10	30	3.000 000 000 000 000 000 000 000	3.000 000 000 000 000 000 000 000	3
2	4.5	5	—	7.002	
		10	6.999 854	7.000 125	
		15	6.999 854	7.000 125	7
	6.0	10	—	7.000 000 003 860	
		15	6.999 999 999 827	7.000 000 000 161	
		20	6.999 999 999 827	7.000 000 000 161	7
	7.5	15	—	7.000 000 000 000 088	
		20	6.999 999 999 999 999 998 619	7.000 000 000 000 000 001 326	
		25	6.999 999 999 999 999 998 619	7.000 000 000 000 000 001 325	7
	10	30	7.000 000 000 000 000 000 000 000	7.000 000 000 000 000 000 000 000	7
3	4.5	5	—	11.055	
		10	10.992	11.006	
		15	10.992	11.006	11
	6.0	10	—	11.000 000 598	
		15	10.999 999 965	11.000 000 031	
		20	10.999 999 965	11.000 000 031	11
	7.5	15	—	11.000 000 000 028	
		20	10.999 999 999 999 999 261	11.000 000 000 000 000 706	
		25	10.999 999 999 999 999 261	11.000 000 000 000 000 706	11
	10	30	11.000 000 000 000 000 000 000 000	11.000 000 000 000 000 000 000 000	11

The numerical bounds are compared with the exact analytical eigenvalues $E_{n,1}^{\infty} = 4n - 1$ of the singular problem on the unbounded domain I_{∞}.

Section 2. We see, from Table 1, that the upper and lower bounds of the harmonic oscillator eigenvalues coincide to the accuracy quoted at $\ell = 10$.

We prove that the basis set of Bessel functions is almost constantly efficient for both problems considered here numerically, whose spectral characteristics are quite different. A remarkable slowing down of convergence occurs only for the very weakly bound states of the Morse potential, where the state number n approaches the actual number of discrete spectral points K defined just after (4.6). In fact, most of the methods applied to a problem of this kind, wherein both discrete and continuous spectra appear, break down at the border of the continuum [8]. Furthermore, a random distribution of the matrix eigenvalues $\mathscr{E}_n$ (or $\mathscr{D}_n$), for which $n > K$, is encountered. In any case, however, the

Table 2
Convergence rates of two-sided Rayleigh–Ritz and Lehmann bounds for the first three eigenvalues of the Morse potential with $Z = 50$ as a function of N and ℓ

n	ℓ	N	$\mathscr{D}_n^-(N,\ell)$	$\mathscr{E}_n^+(N,\ell)$	$E_{n,1}^{\infty}$
1	0.8	15	—	49.750 005	
		20	49.749 999 992	49.750 000 007	
		25	49.749 999 993	49.750 000 007	49.75
	1.0	25	—	49.750 000 000 005	
		30	49.749 999 999 999 925	49.750 000 000 000 070	
		35	49.749 999 999 999 925	49.750 000 000 000 070	49.75
	1.2	30	—	49.750 000 000 062	
		35	—	49.750 000 000 000 005 848	
		40	49.749 999 999 999 999 999 584	49.750 000 000 000 000 000 282	
		45	49.749 999 999 999 999 999 715	49.750 000 000 000 000 000 153	49.75
2	0.8	15	—	147.750 097	
		20	147.749 999 215	147.750 000 871	
		25	147.749 999 215	147.750 000 871	147.75
	1.0	25	—	147.750 000 001	
		30	147.749 999 999 979	147.750 000 000 018	
		35	147.749 999 999 979	147.750 000 000 018	147.75
	1.2	30	—	147.750 000 001 689	
		35	—	147.750 000 000 000 139	
		40	147.749 999 999 999 999 922	147.750 000 000 000 000 074	
		45	147.749 999 999 999 999 925	147.750 000 000 000 000 072	147.75
3	0.8	15	—	243.750 283	
		20	243.749 950	243.750 046	
		25	243.749 950	243.750 046	243.75
	1.0	25	—	243.750 000 037	
		30	243.749 999 997	243.750 000 002	
		35	243.749 999 997	243.750 000 002	243.75
	1.2	30	—	243.750 000 007 960	
		35	—	243.750 000 000 000 811	
		40	243.749 999 999 999 981	243.750 000 000 000 015	
		45	243.749 999 999 999 982	243.750 000 000 000 015	243.75

The numerical bounds are compared with the exact analytical eigenvalues in (4.6) of the singular problem on the whole real line.

present algorithm, a sketch of which is outlined in the Appendix, is not restricted to the two specific potentials in (4.3)–(4.4) and is more generally applicable within the aforementioned limitations.

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Appendix. Sketch of the algorithm and the evaluation of matrix elements

For the numerical computation of the eigenvalues of the Dirichlet problem, it suffices to determine the matrix elements V_{mn} in (5.4). However, we have to calculate the V_{mn} as well as the matrix elements U_{mn} in (5.9) in the case of the Neumann boundary conditions. The other matrices are all constructed by means of either V_{mn} or U_{mn} or both. Thus, we evaluate the following integrals:

$$V_{mn}(\ell) = \mathcal{N}_m \mathcal{N}_n \int_0^1 \xi v(\ell\xi) J_\alpha(\mu_m \xi) J_\alpha(\mu_n \xi)\, \mathrm{d}\xi \tag{A.1}$$

and

$$U_{mn}(\ell) = \mathcal{N}_m \mathcal{N}_n \int_0^1 \xi [v(\ell\xi)]^2 J_\alpha(\mu_m \xi) J_\alpha(\mu_n \xi)\, \mathrm{d}\xi \tag{A.2}$$

for a given potential function, where $\alpha = 1/2$ in our illustrative examples. Notice that the μ_n should be taken as the positive roots of $J_{1/2}(\mu) = 0$ or, simply, $\sin\mu = 0$ in the Dirichlet problem whereas the Neumann problem requires the positive roots of the equation $J'_{1/2}(\mu) = 0$ or $2\mu - \tan\mu = 0$.

For the harmonic oscillator potential function $v(x) = x^2$ we find immediately that

$$V_{mn}(\ell) = 2\ell^2[(\mu_m - \mu_n)^{-2} - (\mu_m + \mu_n)^{-2}] \tag{A.3}$$

for $m \neq n$ and

$$V_{nn}(\ell) = \tfrac{1}{6}\ell^2(2 - 3\mu_n^{-2}) \tag{A.4}$$

for $m = n$ whenever the basis functions satisfy the Dirichlet boundary conditions. In fact, here the roots are nothing but $\mu_k = k\pi$ for $k = 1, 2, \ldots$.

Similarly, we obtain

$$V_{mn}(\ell) = \frac{2\ell^2}{\sqrt{(4\mu_m^2 - 1)(4\mu_n^2 - 1)}} \left[\frac{1 + 4\mu_m\mu_n}{(\mu_m + \mu_n)^2} - \frac{1 - 4\mu_m\mu_n}{(\mu_m - \mu_n)^2}\right] \tag{A.5}$$

for $m \neq n$ and

$$V_{nn}(\ell) = \tfrac{1}{6}\ell^2 \left[\frac{8\mu_n^4 + 2\mu_n^2 + 3}{\mu_n^2(4\mu_n^2 - 1)}\right] \tag{A.6}$$

for $m = n$, whenever the Neumann boundary value problem is under consideration. In this case, the elements of the matrix $\boldsymbol{U}$, which is encountered in the application of the Lehmann method, are of the form

$$U_{mn}(\ell) = \frac{4\ell^4}{\sqrt{(4\mu_m^2 - 1)(4\mu_n^2 - 1)}} \left\{\frac{(\mu_m + \mu_n)^2[(\mu_m - \mu_n)^2 - 6] + (\mu_m - \mu_n)^2 + 6}{(\mu_m - \mu_n)^4} - \frac{(\mu_m - \mu_n)^2[(\mu_m + \mu_n)^2 - 6] + (\mu_m + \mu_n)^2 + 6}{(\mu_m + \mu_n)^4}\right\} \tag{A.7}$$

for $m \neq n$ and

$$V_{nn}(\ell) = \tfrac{1}{10}\ell^4 \left[\frac{8\mu_n^6 + 22\mu_n^4 - 10\mu_n^2 - 15}{\mu_n^4(4\mu_n^2 - 1)}\right] \tag{A.8}$$

for $m = n$. It is noteworthy that the matrix elements involve elementary expressions in terms only of the zeros of (4.12), and no evaluation of any Bessel function is required.

On the other hand, the derivation of the matrix representation of the Morse potential results again in certain analytical formulas containing the elementary integrals $C(x,y)$ and $S(x,y)$ defined, respectively, by

$$C(x,y)=\int_0^1 \mathrm{e}^{-xt}\cos(yt)\,\mathrm{d}t$$

$$=\frac{x}{x^2+y^2}+\frac{\mathrm{e}^{-2x}}{x^2+y^2}(y\sin y-x\cos y),\quad C(0,0)=1 \tag{A.9}$$

and

$$S(x,y)=\int_0^1 \mathrm{e}^{-xt}\cosh(xt)\cos(yt)\,\mathrm{d}t$$

$$=\frac{x}{4x^2+y^2}+\frac{\sin y}{2y}+\frac{\mathrm{e}^{-2x}}{4x^2+y^2}\left(\tfrac{1}{2}\,y\sin y-x\cos y\right), \tag{A.10}$$

where

$$S(x,0)=\tfrac{1}{4}(1-\mathrm{e}^{-2x})/x+\tfrac{1}{2},\quad S(0,0)=1. \tag{A.11}$$

Now the required matrix elements can easily be calculated for two different sets of the roots μ_k corresponding to Dirichlet and Neumann end conditions.

To sum up and to allow a reader to implement the bounds for different examples than the two families given here, we may sketch step by step the numerical algorithm that solves the more general case, i.e., the Schrödinger equation in (4.1) to which the method is applied.

(a) Given the potential function $v(x)$ and the angular quantum number l. Find the parameter α in (4.8), and choose a boundary parameter ℓ which is large enough.

(b) Evaluate the matrix elements V_{mn} and U_{mn} in (A.1) and (A.2), respectively. Notice that the convergence of each integral is guaranteed because the Bessel and the potential functions behave correctly at the origin. The asymptotic form imposed on the potential function $v(x)$ as $x\to 0$ is directly a consequence of the regular singularity of the differential operator at $x_0=0$. When $\alpha\neq 1/2$, it is strongly recommended to use a multiprecision arithmetic on a symbolic software such as *Mathematica*, in order to get reliable enough roots of the corresponding Bessel functions or their derivatives. Furthermore, it is more appropriate to employ the functional equation in (4.17) for the reduction of the matrix elements to integrals containing the Bessel functions of order $\pm 1/2$, for simplicity.

(c) For the Dirichlet problem, identify the Rayleigh–Ritz eigenvalues as the eigenvalues of the real, symmetric matrix $\boldsymbol{H}$ whose general entry is defined by (5.3). In this work, we use EISPACK Fortran subroutines to diagonalize real, symmetric matrices. It should be noted that these routines use originally a double precision arithmetic, however, we modify them so as to use quadruple precision (32 digits) on an IBM-H70 (RISC) main frame.

(d) For the Neumann problem, we first use again an EISPACK subroutine called REDUC, which reduces the generalized eigenproblem in (5.10) to the standard one in (5.17). Then we find the eigenvalues of the resulting real, symmetric matrix $\mathscr{C}$ in (5.18) and determine the Lehmann bounds from (5.13). Recall that the constructions of the matrices in (5.10) fail unless an a priori lower bound satisfying (5.6) is estimated.

(e) Compare the Dirichlet and Neumann eigenvalues, i.e., Rayleigh–Ritz and Lehmann bounds, and increase the value of the boundary parameter ℓ systematically until the required precision within the machine limits is reached.

References

[1] E.A. Coddington, N. Levinson, Theory of Ordinary Differential Equations, TATA McGraw-Hill, New Delhi, 1990.
[2] I.S. Gradshteyn, I.M. Ryzhik, Table of Integrals, Series, and Products, Academic Press, London, 1980.
[3] N.J. Lehman, Optimale Eigenwerteinschließungen, Numer. Math. 5 (1963) 246–272.
[4] P.M. Morse, Diatomic molecules according to the wave mechanics. II. Vibrational levels, Phys. Rev. 34 (1929) 57–64.
[5] M. Plum, Eigenvalue problems for differential equations, in: M. Ainsworth, J. Levesley, W.A. Light, M. Marletta (Eds.), Wavelets, Multilevel Methods and Elliptic PDEs, Clarendon Press, Oxford, 1997.
[6] I.N. Sneddon, Special Functions of Mathematical Physics and Chemistry, Oliver and Boyd, Edinburgh, 1961.
[7] J. Stoer, R. Bulirsch, Introduction to Numerical Analysis, Springer, New York, 1980.
[8] H. Taşeli, Modified Laguerre basis for hydrogen-like systems, Int. J. Quantum Chem. 63 (1997) 949–959.
[9] H. Taşeli, Exact solutions for vibrational levels of the Morse potential, J. Phys. A 31 (1998) 779–788.
[10] H. Taşeli, Accurate numerical bounds for the spectral points of singular Sturm–Liouville problems over $-\infty < x < \infty$, J. Comput. Appl. Math. 115 (2000) 535–546.