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Two-sided eigenvalue bounds for the spherically symmetric states of the Schrödinger equation

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Abstract

The eigenvalues of the radial Schrödinger equation are calculated very accurately by obtaining exact upper and lower bounds. By truncating the usual unbounded domain $[0,\infty)$ of the system to a finite interval of the form $[0,\ell]$, two auxiliary eigenvalue problems are defined. It is then proved that the eigenvalues of the resulting confined systems provide upper and lower bounds converging monotonically to the true eigenvalues required. Moreover, each auxiliary eigenvalue problem gives rise to an orthonormal set involving Bessel functions. The matrix representation of the Hamiltonian is, therefore, derived by expanding the wave function into a Fourier–Bessel series. Numerical results for single- and double-well polynomial oscillators as well as Gaussian type non-polynomial 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}.

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1. Introduction

In the last decade there has been a great deal of interest in studying the discrete spectrum of the radial Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{q-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l(l+q-2)}{r^2}+V(r)\right]\Psi=E\Psi,\quad r\in[0,\infty) \tag{1.1}$$

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in q space dimensions, where $q=2,3,\ldots$ and $l=0,1,\ldots$, subject to

$$\lim_{r\to\infty} \Psi(r)=0, \tag{1.2}$$

assuring the square integrability of the wave function Ψ. Furthermore, the solution should behave like

$$\Psi(r)=\mathcal{O}(r^l) \quad \text{as } r\to 0^+ \tag{1.3}$$

to compensate the regular singularity of the differential equation at the origin, provided that the potential function $V(r)$ does not grow faster than r^{-2} as $r\to 0^+$. Essentially, two main classes of simple quantum mechanical systems of this kind are described by the potentials

$$V(r)=\lim_{M\to\infty}\sum_{k=0}^{M} v_{2k}r^{2k} \tag{1.4}$$

and

$$V(r)=-\frac{\zeta}{r}+\lim_{M\to\infty}\sum_{k=0}^{M} c_k r^k, \tag{1.5}$$

where ζ, v_{2k} and c_k denote the coupling constants. Anharmonic oscillators and well potentials remain in the first class whenever the limit operation is removed and M is set to be a positive integer in (1.4), giving simply a polynomial of degree $2M$ with $v_{2M}>0$. In general, any potential, for instance, the Gaussian potential of the form $-A\,\mathrm{e}^{-\mu r^2}$, which possesses a convergent power series in r^2 about $r=0$ can be represented by (1.4). The second class includes the hydrogen-like systems such as the screened Coulomb potentials. In particular, a perturbed Coulomb problem is encountered when the series in (1.5) is truncated. Hence, the problem of solving a radial Schrödinger equation occurs frequently in quantum field theory and molecular physics and is of importance for both theory and applications [1, 12].

The mathematical problem in (1.1)–(1.3) is a singular Sturm–Liouville problem for which the closed form analytical eigensolutions are available only for a few classes of potentials [16, 26]. It is, therefore, necessary to solve the eigenvalue problem approximately. Several particular forms of potentials in (1.4) and (1.5) have been treated by direct numerical integration techniques [5–7, 15, 23, 27, 32] by Rayleigh–Ritz variational and Hill determinant approaches [4, 17, 18, 21, 22, 30, 31] by Rayleigh–Schrödinger and inner product perturbation series [1, 10, 24, 25, 29] and by moment [2, 8] and phase-integral methods [13]. We do not feel that it would be appropriate here to attempt comparing the relative efficiencies of established methods. Indeed, they could be regarded as useful and worthy depending on their special limitations. For more discussions on the methods in [1, 2, 4–8, 10, 13, 15–18, 21–27, 29–32] we refer the reader to the aforementioned papers and references cited therein.

Although many methods produce good numerical results, almost all of them are potential function dependent and, in fact, their applicability is usually not uniform with respect to the parameters of a chosen potential function. Furthermore, most of them provide only some approximations to the eigenvalues, giving no bounds at all. For some methods providing eigenvalue bounds, see [27, 30, 31]. In the preceding papers [21, 22] of the present authors, highly accurate results were achieved

by finding approximations which converge from above to the eigenvalues of the radial Schrödinger equation, when the potential is a polynomial.

In this work, we first prove a theorem in Section 2 which makes it possible to determine two-sided bounds for the eigenvalues E. In Section 3, expanding the solutions of two auxiliary eigenvalue problems, we obtain approximations to both upper and lower bound eigenvalues. The method is applied, in Section 4, to a general potential given by (1.4). Although we deal, in this paper, explicitly with a potential in the form of (1.4), the method can also be applied effectively to solve hydrogen-like systems in (1.5). In fact, the two classes of problems are related in higher-dimensional spaces, and there exists certain passage formulas between the anharmonic oscillators and the perturbed Coulomb problem [11, 14, 22]. The last section concludes the paper with a discussion of the results as usual.

2. The auxiliary eigenvalue problems

Transforming the dependent variable in (1.1) from Ψ to y, $y=r^{(N-2)/2}\Psi$, we shall consider the differential equation

$$\mathscr{L}y=E(\ell)y, \qquad \mathscr{L}=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{v^2}{r^2}+V(r), \quad v=l+\frac{1}{2}q-1 \tag{2.1}$$

and impose the condition that

$$ay(r)+bry'(r)=0 \quad \text{at } r=\ell, \tag{2.2}$$

where the prime stands for the derivative with respect to r, and a, b, and $\ell>0$ are real numbers. The regularity condition of a solution at the origin then becomes

$$y(r)=\mathcal{O}(r^v) \quad \text{as } r\to 0^+. \tag{2.3}$$

We should note that in this set up, the asymptotic boundary condition in (1.2) has been replaced by the condition in (2.2) on truncating the infinite interval of r to $[0,\ell]$. Note also that the eigenvalues $E(\ell)$ of $\mathscr{L}$ tends to E of the original Schrödinger operator in (1.1) as $\ell\to\infty$, when $a\neq 0$ and $b=0$.

For finite values of ℓ, a solution y is said to satisfy Dirichlet-type boundary condition if $a=1$ and $b=0$, and von-Neumann-type boundary condition if $a=0$ and $b=1$. We denote by $E^+(\ell)$ and $E^-(\ell)$ the corresponding eigenvalues of $\mathscr{L}$. In what follows, we make use of the inner product defined by

$$\langle f,g\rangle=\int_0^\ell rf(r)g(r)\,\mathrm{d}r \tag{2.4}$$

relative to which the eigenfunctions of $\mathscr{L}$ are orthogonal.

We may now state our theorem on which the main idea of this paper based.

Theorem 1. *If E denotes a bound state eigenvalue of the Schrödinger operator in* (1.1) *then the double inequality*

$$E^-(\ell)<E<E^+(\ell) \tag{2.5}$$

holds for all $\ell > 0$ *satisfying*

$$V(\ell) > E. \tag{2.6}$$

Condition (2.6) *is required only for the left-hand-side inequality* $E^-(\ell) < E$ *to be valid.*

Proof. It is clear that each eigenfunction y of $\mathscr{L}$ corresponding to the eigenvalue $E(\ell)$ depends on both r and ℓ. Without loss of generality, we may assume that $\langle y, y\rangle = 1$. Treating ℓ as a variable, and differentiating (2.1) with respect to ℓ, we obtain

$$\mathscr{L}\frac{\partial y}{\partial \ell} = \frac{\mathrm{d}E}{\mathrm{d}\ell} y + E\frac{\partial y}{\partial \ell}. \tag{2.7}$$

In view of (2.4) it follows from (2.7) that

$$\frac{\mathrm{d}E}{\mathrm{d}\ell} = \left\langle \mathscr{L}\frac{\partial y}{\partial \ell}, y \right\rangle - E\left\langle \frac{\partial y}{\partial \ell}, y \right\rangle. \tag{2.8}$$

Applying integration by parts formula to the first integral on the right-hand side of (2.8) we find that

$$\frac{\mathrm{d}E}{\mathrm{d}\ell} = -\ell\,[y_{r\ell}(\ell,\ell)y(\ell,\ell) - y_r(\ell,\ell)y_\ell(\ell,\ell)], \tag{2.9}$$

where subscripts denote partial derivatives. On the other hand, since

$$\left.\frac{\mathrm{d}y}{\mathrm{d}\ell}\right|_{r=\ell} = \left.\left(\frac{\partial y}{\partial \ell} + \frac{\partial y}{\partial r}\frac{\mathrm{d}r}{\mathrm{d}\ell}\right)\right|_{r=\ell} = y_\ell(\ell,\ell) + y_r(\ell,\ell), \tag{2.10}$$

differentiating (2.2) with respect to ℓ we have

$$a[y_\ell(\ell,\ell) + y_r(\ell,\ell)] + b\ell[y_{r\ell}(\ell,\ell) + y_{rr}(\ell,\ell)] + by_r(\ell,\ell) = 0. \tag{2.11}$$

The following two cases may be distinguished:

Case 1: *Dirichlet-type boundary condition*: Let $y^+(r,\ell)$ be an eigenfunction of $\mathscr{L}$ satisfying the condition that $y^+(\ell,\ell) = 0$. From (2.11) we write

$$y_r^+(\ell,\ell) = -y_\ell^+(\ell,\ell) \tag{2.12}$$

and, hence, (2.9) reduces to

$$\frac{\mathrm{d}E^+}{\mathrm{d}\ell} = -\ell[y_r^+(\ell,\ell)]^2 < 0, \tag{2.13}$$

implying that $E^+(\ell)$ decreases monotonically to its limit E as $\ell \to \infty$.

Case 2: *Neumann-type boundary condition*: Now, we deal with an eigenfunction $y^-(r,\ell)$ of $\mathscr{L}$ subject to $y_r^-(\ell,\ell) = 0$, in which case Eq. (2.11) leads to

$$y_{\ell r}^-(\ell,\ell) = -y_{rr}^-(\ell,\ell). \tag{2.14}$$

Setting $r = \ell$ and solving (2.1) for $y_{rr}^-(\ell,\ell)$ we see that

$$y_{\ell r}^-(\ell,\ell) = -\left[\frac{\nu^2}{\ell^2} + V(\ell) - E^-(\ell)\right] y^-(\ell,\ell), \tag{2.15}$$

upon substitution of which into (2.9) gives the relation

$$\frac{dE^-}{d\ell} = \ell\left[\frac{\nu^2}{\ell^2} + V(\ell) - E^-(\ell)\right][y^-(\ell,\ell)]^2. \tag{2.16}$$

Clearly, $E^-(\ell)$ has a minimum at $\ell = \ell_0$ for which

$$\frac{\nu^2}{\ell_0^2} + V(\ell_0) - E^-(\ell_0) = 0 \tag{2.17}$$

and increases monotonically for $\ell > \ell_0$, if $V(\ell) > E^-(\ell)$.

It is well known, from the classical oscillation and comparison theorems [3], that the Dirichlet eigenvalues $E_n^+(\ell)$ for any fixed quantum number n are always greater than the von Neumann eigenvalues $E_n^-(\ell)$ with the same quantum number n. As a result, the limiting value of $E_n^-(\ell)$ as $\ell \to \infty$ is bounded from above by E_n. Therefore, (2.13) and (2.16) now imply that

$$E < E^+(\ell) \tag{2.18}$$

for all $\ell > 0$, and that

$$E > E^-(\ell) \tag{2.19}$$

for all positive values of ℓ for which $V(\ell) > E^-(\ell)$. Note that $V(\ell) > E^-(\ell)$ can be replaced by $V(\ell) > E$, and it is a sufficient condition for (2.19). This suggests evidently that the boundary parameter ℓ should lie beyond the classical turning points of a specific state in question, which completes the proof.

Remark 1. The limit energy $E(\ell)$ in (2.1) as $\ell \to 0^+$ may be determined analytically. Indeed, by the use of the linear transformation $r = \ell\xi$ Eq. (2.1) becomes

$$\left[\frac{d^2}{d\xi^2} + \frac{1}{\xi}\frac{d}{d\xi} + \ell^2 E(\ell) - \frac{\nu^2}{\xi^2} - \ell^2 V(\ell\xi)\right] y = 0, \quad \xi \in [0,1] \tag{2.20}$$

with the boundary conditions

$$y(\xi) = \mathcal{O}(\xi^\nu) \text{ as } \xi \to 0^+ \quad \text{and} \quad ay(\xi) + by'(\xi) = 0 \text{ at } \xi = 1. \tag{2.21}$$

Apparently, the term $\ell^2 V(\ell\xi)$ vanishes as $\ell \to 0^+$ for the classes of potentials in (1.4) and (1.5), being considered in this work. Therefore, Eq. (2.20) reduces to the Bessel differential equation

$$\frac{d^2 y}{d\xi^2} + \frac{1}{\xi}\frac{dy}{d\xi} + \left(\beta^2 - \frac{\nu^2}{\xi^2}\right) y = 0, \quad \xi \in [0,1], \tag{2.22}$$

where $\beta^2 = \lim_{\ell \to 0^+} \ell^2 E(\ell)$. The Bessel functions of the first kind $J_\nu(\beta\xi)$ and the second kind $Y_\nu(\beta\xi)$ are the two linearly independent solutions of (2.22). The solution $Y_\nu(\beta\xi)$ is rejected, and any solution which behaves correctly at the origin should be a scalar multiple of $J_\nu(\beta\xi)$. Imposing the second condition in (2.21) we see that β can be determined as a positive root of $aJ_\nu(\beta) + bJ_\nu'(\beta) = 0$, and,

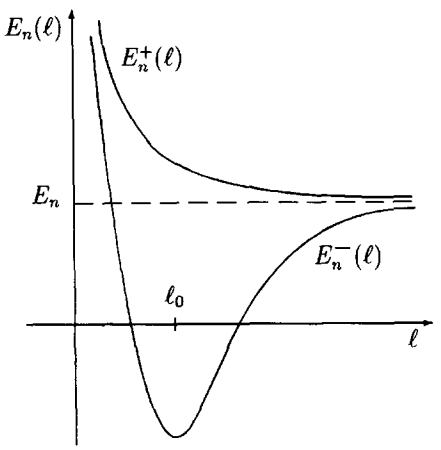

Fig. 1. Graphs of the Dirichlet and von Neumann eigenvalues.

therefore, $E(\ell)$ grows like ℓ^{-2} about the origin, i.e.

$$E(\ell)=\mathcal{O}(\ell^{-2}) \quad \text{as } \ell \to 0^+. \tag{2.23}$$

By means of Theorem 1 and Remark 1, we now completely deduce the qualitative behaviours of the Dirichlet and von Neumann eigenvalues for $\ell>0$. The sketches of the functions $E_n^+(\ell)$ and $E_n^-(\ell)$ are illustrated in Fig. 1.

In conclusion, the auxiliary eigenvalue problems produce upper and lower bounds to the eigenvalues E of the original non-confined system. Thus accurate calculation of E can be accomplished, provided that a method is developed for computing $E^+(\ell)$ and $E^-(\ell)$ to any desired accuracy for each fixed ℓ. The difference $|E^+(\ell)-E^-(\ell)|$ is then a rigorous measure of the error in the determination of E.

3. The Fourier–Bessel expansion

The Schrödinger equation (2.1) for which

$$V(r)=\begin{cases} 0 & \text{if } r\in[0,\ell), \\ \infty & \text{if } r\geqslant \ell, \end{cases} \tag{3.1}$$

reduces again to the Bessel differential equation

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}\phi}{\mathrm{d}r}+\left(\lambda^2-\frac{v^2}{r^2}\right)\phi=0, \quad r\in[0,\ell] \tag{3.2}$$

of form (2.22). This equation accompanied with the boundary conditions in (2.2) and (2.3) describes the motion of a free particle, which is regarded as the unperturbed eigenvalue problem in this work. The same approach was used in [19, 20] for solving two- and three-dimensional non-separable potentials, where the unperturbed problem similarly defined produces orthonormal basis sets in terms

of simple trigonometric functions. In the present case, we see that the sequence of the Bessel functions

$$\phi_n(r) = C_n J_\nu(\lambda_n r), \tag{3.3}$$

contains the required solution of the unperturbed eigenvalue problem for each natural number n, provided that λ_n is chosen in such a way that

$$\alpha_n = \lambda_n \ell \tag{3.4}$$

is a root of

$$aJ_\nu(x) + bxJ'_\nu(x) = 0, \tag{3.5}$$

where C_n stands for a normalization constant. It is a well-known fact that the functions J_ν and J'_ν each have an infinite number of zeros, all of which are simple with the possible exception of $x = 0$.

On the other hand, if $\alpha_1, \alpha_2, \ldots$ are the positive roots of (3.5), then

$$\langle J_\nu(\lambda_n r), J_\nu(\lambda_m r)\rangle = \begin{cases} 0 & \text{if } m \neq n \\ \frac{1}{2}\ell^2 J_{\nu+1}^2(\alpha_n) & \text{if } m = n \text{ and } (a,b) = (1,0), \\ \dfrac{\ell^2}{2\alpha_n^2}(\alpha_n^2 - \nu^2)J_\nu^2(\alpha_n) & \text{if } m = n \text{ and } (a,b) = (0,1), \end{cases} \tag{3.6}$$

which is referred to as the orthogonality property of Bessel functions [28]. Because of (3.6), the normalization constant C_n is taken as

$$C_n = \begin{cases} \dfrac{\sqrt{2}}{\ell J_{\nu+1}(\alpha_n)} & \text{when } (a,b) = (1,0), \\ \dfrac{\sqrt{2}\alpha_n}{\ell\sqrt{\alpha_n^2 - \nu^2}\, J_\nu(\alpha_n)} & \text{when } (a,b) = (0,1), \end{cases} \tag{3.7}$$

for which the sequence of eigenfunctions in (3.3), for $n = 1, 2, \ldots$, now constitutes an orthonormal set over the domain $[0, \ell]$ with respect to the weighting r, and, therefore,

$$\langle \phi_n, \phi_m \rangle = \delta_{nm}. \tag{3.8}$$

The orthonormality relation suggests evidently that the wave function of the perturbed problem formulated in (2.1)–(2.3) be expanded in terms of the eigenfunctions ϕ_n of the unperturbed problem. Hence, we may propose a solution of the form

$$y(r) = \sum_{n=1}^{\infty} a_n \phi_n(r), \tag{3.9}$$

which is the Fourier–Bessel expansion of the wave function with the linear combination coefficients a_n to be determined. The infinite series representation of $y(r)$ converge correctly to the exact solution since $\sqrt{r}\, y(r)$ is integrable on $[0, \ell]$. This follows directly from (2.3) since $\nu \geqslant 0$, and from the fact that the only singularity of the differential equation is located at the origin. A detailed discussion about the validity and convergence of such a series expansion, however, may be found in [28].

It should be noted that, if $(a,b)=(0,1)$ then $\alpha_1=0$ is a zero of $J_0'(x)$ with a non-zero contribution to (3.9) and yet (3.6) is assumed to hold for positive zeros. This fact does not create any problem, since we also have

$$\langle \phi_1, \phi_n \rangle = \left\langle \frac{\sqrt{2}}{\ell}, \frac{\sqrt{2}}{\ell J_0(\alpha_n)} J_0(\alpha_n r/\ell) \right\rangle = \delta_{n1}, \tag{3.10}$$

when $\nu=0$, for all n.

4. Truncated matrix eigenvalues for $E^+(\ell)$ and $E^-(\ell)$

The numerical implementation of the method can be accomplished by means of a truncated Fourier–Bessel series. Thus, we propose the trial solution

$$y(r)=\sum_{n=1}^{N} a_n \phi_n(r) \tag{4.1}$$

for the wave function, which converges to the exact solution as $N\to\infty$, and convert the Schrödinger differential equation to a matrix eigenvalue problem of the form

$$\sum_{n=1}^{N} [\mathscr{A}_{mn} - E(\ell)\delta_{mn}]a_n = 0, \tag{4.2}$$

where the matrix elements are given by

$$\mathscr{A}_{mn} = \lambda_n^2 \delta_{mn} + \langle V(r)\phi_m, \phi_n \rangle \tag{4.3}$$

for $m,n=1,2,\ldots,N$. As mentioned earlier, when the potential function is assumed to be analytic function of r^2, truncating (1.4) we have

$$V(r)=\sum_{k=1}^{M} v_{2k} r^{2k}, \tag{4.4}$$

where the constant term is deleted, as it can always be added to E. Therefore, the integrals of the type

$$\mathscr{J}_{mn}^{(\nu,k)} = C_{mn}^{(\nu)} \int_0^1 \xi^{2k+1} J_\nu(\alpha_n \xi) J_\nu(\alpha_m \xi)\, \mathrm{d}\xi \tag{4.5}$$

have to be evaluated for the construction of the matrix $[\mathscr{A}_{mn}]$, where $C_{mn}^{(\nu)} = C_n C_m$. The matrix elements may then be written in the compact form

$$\mathscr{A}_{mn} = \lambda_n^2 \delta_{mn} + \sum_{k=1}^{M} v_{2k} \ell^{2k+2} \mathscr{J}_{mn}^{(\nu,k)}. \tag{4.6}$$

It is noteworthy that evaluation of an integral of the form (4.5) even numerically is not an easy task due to the oscillatory behaviour of the integrand. Making use of some well-known properties

of Bessel functions we have, however, calculated these integrals analytically via recursive relations. The results are summarized as follows:

If $n \neq m$ then

$$\mathcal{J}_{mn}^{(\nu,k)} = \frac{C_{mn}^{(\nu)}}{\alpha_n^2 - \alpha_m^2}[\alpha_n J_{\nu+1}(\alpha_n)J_\nu(\alpha_m) - \alpha_m J_{\nu+1}(\alpha_m)J_\nu(\alpha_n)]$$
$$+\frac{2kC_{mn}^{(\nu)}}{(\alpha_n^2 - \alpha_m^2)^2}[(\alpha_n^2 + \alpha_m^2)J_\nu(\alpha_n)J_\nu(\alpha_m) + 2\alpha_n\alpha_m J_{\nu+1}(\alpha_n)J_{\nu+1}(\alpha_m)]$$
$$-\frac{4k}{(\alpha_n^2 - \alpha_m^2)^2}[(\alpha_n^2 + \alpha_m^2)^2(\nu + k)\mathcal{J}_{mn}^{(\nu,k-1)} + 2\alpha_n\alpha_m(k - \nu - 1)\mathcal{J}_{mn}^{(\nu+1,k-1)}] \tag{4.7}$$

with

$$\mathcal{J}_{mn}^{(\nu,0)} = \frac{C_{mn}^{(\nu)}}{\alpha_n^2 - \alpha_m^2}[\alpha_n J_{\nu+1}(\alpha_n)J_\nu(\alpha_m) - \alpha_m J_{\nu+1}(\alpha_m)J_\nu(\alpha_n)] \tag{4.8}$$

and if $n = m$ then

$$\mathcal{J}_{nn}^{(\nu,k)} = \frac{C_{nn}^{(\nu)}}{2(2k+1)\alpha_n^2}\{[\alpha_n^2 + 2k(k - \nu)]J_\nu^2(\alpha_n) + \alpha_n^2 J_{\nu+1}^2(\alpha_n)$$
$$+k(k - \nu)\alpha_n J_\nu(\alpha_n)J_{\nu+1}(\alpha_n)\} + \frac{2k(\nu^2 - k^2)}{(2k+1)\alpha_n^2}\mathcal{J}_{nn}^{(\nu,k-1)} \tag{4.9}$$

with

$$\mathcal{J}_{nn}^{(\nu,0)} = \tfrac{1}{2}C_{nn}^{(\nu)}[J_\nu^2(\alpha_n) + J_{\nu+1}^2(\alpha_n)], \tag{4.10}$$

where $k = 1, 2, \ldots, M$ and $\nu \geqslant 0$.

The derived expressions are very general in the sense that no assumption is made about α_n. If, however, α_n's are the zeros of either $J_\mu(x)$ or $J'_\mu(x)$ with a specific $\mu \geqslant 0$, then it can be shown that the integrals $\mathcal{J}_{mn}^{(\mu,k)}$ can be expressed in terms of the zeros α_n. Therefore, no evaluation of any Bessel function is required, which makes our method even more desirable.

Under the Dirichlet-type condition, we obtain a two-dimensional array $[M,N]$ of approximants for $E^+(\ell)$. Similarly, the use of the von Neumann-type boundary condition leads to the estimation of $E^-(\ell)$ for sufficiently large values of M and N. Clearly, Theorem 1 implies that $E^+(\ell) - E^-(\ell)$ with a given ℓ stands for the uncertainty in the eigenvalues E of the non-confined system. Despite the lack of a rigorous mathematical proof of

$$\lim_{\ell \to \infty} |E^+(\ell) - E^-(\ell)| = 0, \tag{4.11}$$

our numerical experiments show that there exists a critical value of ℓ for which

$$E^+(\ell_{\mathrm{cr}}) - E^-(\ell_{\mathrm{cr}}) < \varepsilon, \tag{4.12}$$

where $\varepsilon > 0$ can be made as small as we please. At the numerical side of this work, ε is prescribed to be 10^{-20} so that the bound state eigenvalues E will be computed to about 20 significant figures.

To illustrate the performance of our method, we deal explicitly with the harmonic oscillator

$$V(r)=r^2, \quad q=2, \tag{4.13}$$

the generalized anharmonic oscillators

$$V(r)=r^{2K}, \quad K=2,3,4,5,10, \quad q=2,3, \tag{4.14}$$

the two-well potential

$$V(r)=-Z^2r^2+r^4, \quad q=3, \tag{4.15}$$

the non-polynomial test potential

$$V(r)=\mathrm{e}^{\gamma r^2}, \quad \gamma>0, \quad q=3, \tag{4.16}$$

and with the Gaussian potential

$$V(r)=-\mathrm{e}^{-\gamma r^2}, \quad \gamma>0, \quad q=3. \tag{4.17}$$

Note that some examples of two- and three-dimensional problems are to be solved only without any loss of generality. In fact, as discussed in [9, 13, 18, 22] the spectrum of the eigenvalue problem remains unchanged for a prescribed value of $2l+q$. Hence, the eigenvalues in q dimensions, denoted by $E^{(q)}_{n_r,l}$ with the radial and angular quantum numbers n_r and l, respectively, are degenerate in such a way that

$$\begin{aligned}
&E^{(2)}_{n_r,1}\equiv E^{(4)}_{n_r,0},\\
&E^{(2)}_{n_r,2}\equiv E^{(4)}_{n_r,1}\equiv E^{(6)}_{n_r,0},\\
&\quad\vdots\\
&E^{(2)}_{n_r,l}\equiv E^{(4)}_{n_r,l-1}\equiv E^{(6)}_{n_r,l-2}\equiv\cdots\equiv E^{(2l-2)}_{n_r,2}\equiv E^{(2l)}_{n_r,1}\equiv E^{(2l+2)}_{n_r,0},
\end{aligned} \tag{4.18}$$

when q is even, and

$$\begin{aligned}
&E^{(3)}_{n_r,1}\equiv E^{(5)}_{n_r,0}\\
&E^{(3)}_{n_r,2}\equiv E^{(5)}_{n_r,1}\equiv E^{(7)}_{n_r,0}\\
&\vdots\\
&E^{(3)}_{n_r,l}\equiv E^{(5)}_{n_r,l-1}\equiv E^{(7)}_{n_r,l-2}\equiv\cdots\equiv E^{(2l-1)}_{n_r,2}\equiv E^{(2l+1)}_{n_r,1}\equiv E^{(2l+3)}_{n_r,0},
\end{aligned} \tag{4.19}$$

when q is odd, where $E^{(2)}_{n_r,0}$ and $E^{(3)}_{n_r,0}$ are single in the system. Thus, it suffices to handle the cases $q=2$ and 3 to cover the whole spectrum of the q-dimensional case. It is clear, from (2.1), that the parameter v is an integer and half an odd integer when $q=2$ and 3, respectively, so that the numerical algorithm requires the zeros α_n of either the Bessel functions of integer order or the spherical Bessel functions, which are calculated by making use of the *Mathematica* software.

Table 1
Convergence rates of the N-truncated bounds for several eigenvalues of the two-dimensional harmonic oscillator $V(r)=r^2$ as a function of ℓ. The numerical bounds are compared with the exact analytical eigenvalues $E_{\text{exact}}=2(1+2n_r+l)$ of the usual problem in the unbounded domain where $\ell\to\infty$

$l+2n_r$	ℓ	N	$E^-(\ell)$	$E^+(\ell)$	E_{exact}
0	4.5	5	2.000 128	2.000 011	
		8	1.999 999 862 392	2.000 000 123 248	
		10	1.999 999 862 391	2.000 000 123 233	2
	6.0	8	2.000 000 925	2.000 000 102	
		10	2.000 000 000 065	2.000 000 000 004	
		12	1.999 999 999 999 660	2.000 000 000 000 032	2
	7.5	10	2.000 001	2.000 000 182	
		15	2.000 000 000 000 556	2.000 000 000 000 000 039	
		20	1.999 999 999 999 999 999 999	2.000 000 000 000 000 000 001	2
1	4.5	5	4.000 167	4.000 016	
		8	3.999 997 331	4.000 002 357	
		10	3.999 997 331	4.000 002 357	4
	6.0	8	4.000 002	4.000 000 225	
		10	4.000 000 000 126	4.000 000 000 009	
		12	3.999 999 999 998 794	4.000 000 000 001 134	4
	7.5	10	4.000 003 512	4.000 000 621	
		15	4.000 000 000 000 002	4.000 000 000 000 000 117	
		20	3.999 999 999 999 999 999 995	4.000 000 000 000 000 000 001	4
2	5.0	5	6.002 100	6.000 028	
		8	5.999 999 579	6.000 000 379	
		10	5.999 999 578	6.000 000 379	6
	6.5	8	6.000 047	6.000 007	
		10	6.000 000 013	6.000 000 001	
		12	5.999 999 999 995	6.000 000 000 000 085	6
	8.0	10	6.000 062	6.000 014	
		15	6.000 000 000 000 471	6.000 000 000 000 045	
		20	5.999 999 999 999 999 999 999	6.000 000 000 000 000 000 001	6

Another remark is that the harmonic potential in (4.13) is an analytically solvable system in the unbounded domain, which provides a convenient testing ground to deduce the confidence in the accuracy of our two-sided bounds. It should also be noted that the polynomial potentials in (4.13)–(4.15) are exactly represented by the general form of $V(r)$ in (4.4), for special values of the parameters v_{2k} and the degree M. Therefore, in these cases the general approximation scheme for finding the eigenvalues reduces to a single sequence of N, the truncation size of the eigenfunctions.

Table 2
Lower and upper bounds to eigenvalues $E^{(2)}_{n_r,l}$, for several quantum numbers n_r and l, of the potentials $V(r)=r^{2K}$ as a function of K

K	n_r	l	$E^{(2)}_{n_r,l}$	ℓ_{cr}	N
2	0	0	2.344 829 072 744 275 2098/9	4.25	20
	0	5	21.590 048 138 799 549 056/7	4.50	22
	0	10	47.463 041 125 098 522 451/2	4.75	24
	5	0	53.486 335 321 438 145 046/7	4.75	26
	5	5	86.908 365 353 723 948 346/7	5.00	28
	10	0	126.617 561 998 884 379 41/2	5.25	34
3	0	0	2.609 388 463 253 714 0068/9	3.25	26
	0	5	28.315 788 118 458 607 808/9	3.25	26
	0	10	67.522 486 389 084 298 086/7	3.25	26
	5	0	82.731 043 892 681 375 353/4	3.50	30
	5	5	142.088 846 735 876 653 59/60	3.50	32
	10	0	218.046 930 963 991 478 84/5	3.50	36
4	0	0	2.828 786 159 942 523 3487/8	2.75	28
	0	5	33.197 966 996 834 368 041/2	2.75	28
	0	10	82.696 404 525 852 108 715/6	2.75	28
	5	0	107.282 578 642 816 534 63/4	2.75	32
	5	5	190.472 186 690 290 158 95/6	2.75	34
	10	0	301.521 948 561 541 444 73/4	2.75	40
5	0	0	3.015 327 587 033 583 9918/9	2.50	34
	0	5	36.924 381 678 647 102 740/1	2.50	34
	0	10	94.405 430 820 331 044 681/2	2.50	34
	5	0	127.504 074 561 749 428 33/4	2.50	36
	5	5	231.414 960 352 022 247 66/7	2.50	38
	10	0	373.990 476 786 330 620 79/80	2.50	44
10	0	0	3.651 024 848 669 465 8340/2	1.65	54
	0	5	47.670 123 913 763 695 184/5	1.65	54
	0	10	127.575 456 124 836 257 09/10	1.65	54
	5	0	188.701 155 665 025 386 16/7	1.65	56
	5	5	359.773 343 201 409 515 36/7	1.65	58
	10	0	609.215 685 752 278 184 12/67	1.65	64

5. Numerical results and discussion

In this article, an extensive numerical analysis of the aforementioned quantum mechanical potentials are presented. In Table 1, N-truncated eigenvalue bounds for the two-dimensional harmonic oscillator are tabulated and compared with the exact analytical results. It is shown that both lower and upper bounds converge from above as N increases, and their significant digits so determined provide indeed two-sided bounds on the eigenvalues of the unbounded system. Furthermore, more accurate bounds can be achieved by way of increasing ℓ, confirming the mathematical analysis in Section 2.

Table 3
Lower and upper bounds to eigenvalues $E^{(3)}_{n_r,l}$, for several quantum numbers n_r and l, of the potentials $V(r)=r^{2K}$ as a function of K

K	n_r	l	$E^{(3)}_{n_r,l}$	ℓ_{cr}	N
2	0	0	3.799 673 029 801 394 1687/8	4.25	20
	0	5	23.940 622 097 894 264 116/7	4.50	22
	0	10	50.305 736 167 707 034 998/9	4.75	24
	5	0	56.734 214 055 173 036 047/8	4.75	26
	5	5	90.373 823 037 450 379 389/90	5.00	28
	10	0	130.642 068 748 629 978 82/3	5.25	34
3	0	0	4.338 598 711 513 981 1916/7	3.25	26
	0	5	31.719 280 900 827 550 416/7	3.25	26
	0	10	72.020 071 790 814 934 528/9	3.25	26
	5	0	88.392 375 769 030 215 606/7	3.50	30
	5	5	148.364 911 801 181 853 86/7	3.50	32
	10	0	225.852 006 093 743 59399/400	3.50	36
4	0	0	4.755 874 413 960 759 8693/4	2.75	28
	0	5	37.386 714 985 516 424 289/90	2.75	28
	0	10	88.512 091 769 467 303 189/90	2.75	28
	5	0	115.120 801 108 759 852 45/6	2.75	32
	5	5	199.378 311 104 884 152 38/9	2.75	34
	10	0	313.042 006 220 240 519 65/6	2.75	40
5	0	0	5.097 876 529 203 380 5010/1	2.50	34
	0	5	41.712 628 607 015 919 880/1	2.50	34
	0	10	101.259 528 625 635 761 71/2	2.50	34
	5	0	137.212 594 251 523 159 95/6	2.50	36
	5	5	242.634 553 878 058 402 68/9	2.50	38
	10	0	388.880 652 178 954 556 31/2	2.50	44
10	0	0	6.219 360 528 618 843 7846/7	1.65	54
	0	5	54.133 868 954 795 890 507/8	1.65	54
	0	10	137.372 769 001 823 278 20/1	1.65	54
	5	0	204.369 762 904 256 022 06/7	1.65	56
	5	5	378.613 187 208 892 251 86/7	1.65	58
	10	0	635.690 810 800 680 389 16/7	1.65	64

Tables 2 and 3 list eigenvalue bounds for two- and three-dimensional potentials of the type r^{2K} in (4.14). To denote lower and upper bounds, we employ the notation in which, for example, 2.344...2098/9 in the first row of Table 2 implies that $2.344\ldots2098 < E^{(2)}_{00} < 2.344\ldots2099$. The distance ℓ_{cr} and the truncation order N of the eigenfunctions for which the prescribed accuracy is reached, are included in the tables as well. We see that the numerical characteristics of the algorithm remain unchanged in the two- and three-dimensional cases. It is also shown that the critical values ℓ_{cr} diminish as K increases due to the contraction of the potentials, whereas the truncation sizes N increase in getting at the required accuracy. In all cases, however, 20 significant figures are obtainable by diagonalizing matrices of reasonable orders N, typically ranging from 20 to 65. On

Table 4
Lower and upper bounds to eigenvalues $E^{(3)}_{n_r,l}$, for several quantum numbers n_r and l, of the potentials $V(r)=-Z^2r^2+r^4$ as a function of Z^2

Z^2	n_r	l	$E^{(3)}_{n_r,l}$	ℓ_{cr}	N
10^{-2}	0	0	3.790 651 217 036 336 2310/1	4.25	20
	0	5	23.914 001 559 449 152 939/40	4.25	22
	1	4	30.478 325 182 857 788 774/5	4.50	22
	2	3	37.007 326 015 166 163 848/9	4.50	22
	3	2	43.536 998 592 038 097 225/6	4.50	22
	4	1	50.094 565 169 438 444 671/2	4.50	24
	0	10	50.266 166 628 053 268 426/7	4.75	26
	5	0	56.699 794 400 050 696 524/5	4.75	28
	5	5	90.329 068 175 907 887 977/8	5.00	30
	10	0	130.589 837 047 920 667 72/3	5.25	34
1	0	0	2.834 536 202 119 304 2146/7	4.50	30
	0	5	21.200 285 583 288 184 523/4	4.50	30
	1	4	27.672 922 663 300 275 447/8	4.50	32
	2	3	34.072 567 888 029 424 131/2	4.75	32
	3	2	40.445 488 723 690 448 103/4	4.75	32
	0	10	46.268 329 155 506 282 178/9	5.00	36
	4	1	46.827 656 017 126 357 343/4	4.75	34
	5	0	53.245 474 927 626 236 240/1	5.00	38
	5	5	85.845 832 349 517 541 768/9	5.25	40
	10	0	125.372 316 850 633 525 48/9	5.50	44
10^2	0	0	−2485.867 880 342 075 2943/2	12.50	90
	0	5	−2485.265 353 438 290 8701/0	12.50	94
	0	10	−2483.658 974 985 381 4206/5	12.50	100
	1	4	−2457.238 673 069 606 8734/3	12.50	94
	2	3	−2429.235 105 951 154 0434/3	12.50	96
	3	2	−2401.254 041 926 095 0600/599	12.50	96
	4	1	−2373.294 839 731 257 6385/4	12.50	98
	5	0	−2345.356 825 499 765 3424/3	12.50	104
	5	5	−2344.727 370 853 291 7037/6	12.50	106
	10	0	−2206.397 933 085 838 6702/1	12.50	110

the other hand, slightly larger ℓ_{cr} and N values have been recorded for the eigenvalues with larger quantum numbers.

In Table 4, we report eigenvalues of the potential in (4.15) as a function of Z^2. This potential is interesting, because it stands for a two-well potential with two minima in Cartesian coordinate system. It is well known that many numerical difficulties are encountered in finding the eigenvalues for large values of Z^2. In fact, the system does not describe a physical phonemena since the discrete eigenvalue spectrum does not exist as $Z^2 \to \infty$. We see, from Table 4, that the eigenvalues for $Z^2 = 100$ stabilize to a 20 figure accuracy at a truncation size which is relatively very large.

Tables 5 and 6 are concerned with the non-polynomial potentials defined by (4.16) and (4.17). Clearly, the lower and upper bounds are estimated by a two-dimensional array $[M,N]$ of approximants in these cases. More specifically, N and M are increased simultaneously in a systematic manner to

Table 5
Convergence rates of the two-sided bounds for the lowest eigenvalue $E_{0,0}^{(3)}$ of the non-polynomial potential $e^{\gamma r^2}$ as a function of the degree M of polynomial approximations, when $\gamma = 0.001$ and $\gamma = 0.01$

γ	M	$E_{0,0}^{(3)}$	ℓ_{cr}	N
0.001	2	1.094/7	4.00	4
	4	1.096 67/8	4.00	6
	6	1.096 729/34	4.00	8
	8	1.096 731 17/25	5.00	8
	10	1.096 731 233/5	5.00	10
	12	1.096 731 2348/9	5.00	12
	14	1.096 731 234 877/9	6.00	14
	16	1.096 731 234 8788/9	6.00	16
	18	1.096 731 234 878 862/4	6.00	18
	20	1.096 731 234 878 8639/40	6.00	20
	22	1.096 731 234 878 863 917/9	7.00	22
	24	1.096 731 234 878 863 918 86/92	7.00	24
	26	1.096 731 234 878 863 918 904/6	7.00	26
	28	1.096 731 234 878 863 918 9052/4	7.00	28
	30	1.096 731 234 878 863 918 905 280/9	7.00	28
0.01	2	1.3/4	4.00	6
	4	1.317/19	4.00	6
	6	1.3182/4	4.00	10
	8	1.318 37/9	4.00	10
	10	1.318 3827/39	5.00	14
	12	1.318 3838/40	5.00	16
	14	1.318 383 90/3	5.00	16
	16	1.318 383 916/8	5.00	18
	18	1.318 383 917 14/20	6.00	22
	20	1.318 383 917 187/93	6.00	26
	22	1.318 383 917 190/2	6.00	28
	24	1.318 383 917 190 69/74	6.00	28
	26	1.318 383 917 190 713/7	6.00	28
	28	1.318 383 917 190 715/6	7.00	30
	32	1.318 383 917 190 715 449/52	7.00	30
	34	1.318 383 917 190 715 449 79/85	7.00	30
	36	1.318 383 917 190 715 449 834/8	7.00	30
	38	1.318 383 917 190 715 449 8367/8	7.00	30
	40	1.318 383 917 190 715 449 836 910/9	7.00	30

characterize the exact solution more precisely and to obtain a better approximation for the potential function, respectively. Thus, the conforming digits of consecutive approximants are regarded as significant digits. There is an important difference between the spectra of the two exponential-type potentials considered here. The potential in (4.16) with $\gamma > 0$ has solely a discrete positive spectrum in both the truncated and the original unbounded intervals. In contrast, the Gaussian potential in the unbounded domain possesses a finite number of discrete states located on the negative real axis together with a continuous spectrum which covers the entire positive real axis in the eigenvalue complex plane, for proper (small) values of γ. When γ exceeds a so-called threshold value, the discrete negative spectral points can not survive any more and merge fully into the continuous

Table 6
Convergence rates of the two-sided bounds for the lowest eigenvalue $E_{0,0}^{(3)}$ of the Gaussian potential $-\mathrm{e}^{-\gamma r^2}$ as a function of the degree M of polynomial approximations, when $\gamma = 0.001$ and $\gamma = 0.01$

γ	M	$E_{0,0}^{(3)}$	ℓ_{cr}	N
0.001	2	−0.91/0	4.00	6
	6	−0.907 02/1	4.00	8
	10	−0.907 01930/28	5.00	8
	14	−0.907 019 292 60/59	5.00	12
	18	−0.907 019 292 592 8123/0	6.00	16
	22	−0.907 019 292 592 812 10/07	6.00	20
	26	−0.907 019 292 592 812 0830/26	7.00	24
	30	−0.907 019 292 592 812 082 716/5	7.00	28
	34	−0.907 019 292 592 812 082 7155/0	7.00	28
0.01	2	−0.73/0	4.00	8
	6	−0.720/18	4.00	10
	10	−0.71917/5	4.00	14
	14	−0.719 168 93/60	5.00	16
	18	−0.719 168 935/33	5.00	20
	22	−0.719 168 934/3	5.00	20
	26	−0.719 168 933 45/3	5.00	24
	30	−0.719 168 933 446/5	6.00	26
	34	−0.719 168 933 445 09/6	6.00	26
	38	−0.719 168 933 445 091/88	6.00	26
	42	−0.719 168 933 445 0904/2	7.00	30
	46	−0.719 168 933 445 090 398/80	7.00	30
	50	−0.719 168 933 445 090 398/6	7.00	30
	54	−0.719 168 933 445 090 3975/0	7.00	30

spectrum. In the truncated interval, however, the spectrum of the Gaussian potential becomes a purely discrete one for all γ, since an infinite potential is assumed for $r \geqslant \ell$. We see, from Table 6, that this discrepancy in the spectral nature of the original and the confined Gaussian potentials does not affect at all the accuracy of our method in computing the discrete states. Only the number of terms M we should take in the series representation of the potential increases to this end.

We observe that the trivial eigenvalue ordering properties

$$E_{n_r,l_2}^{(q)} > E_{n_r,l_1}^{(q)} \quad \text{and} \quad E_{n_{r_2},l}^{(q)} > E_{n_{r_1},l}^{(q)} \tag{5.1}$$

hold for all $l_2 > l_1$ and $n_{r_2} > n_{r_1}$, respectively. These inequalities and (4.18) and (4.19) now suggest that

$$E_{n_r,l}^{(q_2)} > E_{n_r,l}^{(q_1)}, \tag{5.2}$$

when $q_2 > q_1$, which has been confirmed by our calculations. Moreover, if we characterize the spectral points as groups denoted by m, where $m = n_r + l$, then we infer that the eigenvalues in such a group may be ordered according to the rule

$$E_{0,m}^{(q)} < E_{1,m-1}^{(q)} < \cdots < E_{m-1,1}^{(q)} < E_{m,0}^{(q)}, \tag{5.3}$$

which is independent of the potential under consideration and the space dimension q.

To conclude, accurate numerical bounds for the discrete states of a wide class of Schrödinger potentials can be determined by the method developed in this paper. In principle, it may also be extended to a general Sturm–Liouville system defined on an infinite domain. The treatment of the eigenvalue spectrum of this more general problem along the same lines is in progress.

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