The Laguerre pseudospectral method for the radial Schrödinger equation

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1. Introduction

In this article, we consider the radial part of the Schrödinger equation in M dimensions

\[
\left[ -\frac{d^2}{dr^2} \frac{M-1}{r} + \frac{\ell(\ell + M - 2)}{r^2} + V(r) \right] R^{(M)}_{n,\ell}(r) = E^{(M)}_{n,\ell} R^{(M)}_{n,\ell}(r), \quad R^{(M)}_{n,\ell}(r) \in L^2(0, \infty)
\]

with a variety of quantum mechanical potentials of the form \(V(\sqrt{x_1^2 + x_2^2 + \ldots + x_M^2}) = V(r)\), where \(r\) denotes the M-dimensional spherical coordinates such that \(r^2 = \sum_{i=1}^{M} x_i^2\). In (1), \(L^2(0, \infty)\) is the Hilbert space of square integrable functions on the half line, \(n, \ell = 0, 1, \ldots\) stand, respectively, for the radial and angular quantum numbers of the energy eigenvalues \(E\) and the corresponding wavefunctions \(R(r)\). M-dimensional radial Schrödinger equation has been the subject of many computational methods. The most commonly studied form of (1) is the three-dimensional case with \(M = 3\)

\[
\left[ -\frac{d^2}{dr^2} \frac{1}{r^2} + \frac{\ell(\ell + 1)}{r^2} + V(r) \right] \Psi(r) = E\Psi(r)
\]

(2)

in which the first derivative term is removed by making use of the transformation \(\Psi(r) = rR(r)\) on the dependent variable.

It is interesting to notice that the last equation can still be derived from (1) without any transformation. To be specific, in (1), regarding \(M\) as a parameter with the value \(M = 1\) and replacing \(\ell\) with \(\ell + 1\) we obtain (2). Therefore the link between the eigenpairs \(\{E_{n,\ell}, \Psi_{n,\ell}(r)\}\) and \(\{E^{(M)}_{n,\ell}, R^{(M)}_{n,\ell}(r)\}\) of (2) and (1), respectively, is given by the relations

\[
E_{n,\ell} = E^{(1)}_{n,\ell + 1}, \quad \Psi_{n,\ell}(r) = R^{(1)}_{n,\ell + 1}(r).
\]

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Various approximation methods have been proposed for computing the eigenvalues of this problem by many authors. Among them we may recall variational methods [32–34,36,37,39], Hill determinant method [7], pseudospectral methods [2], constant perturbation methods [17,20–22], Prüfer transformation followed by a shooting procedure [4,3], Pekeris-type approximations [12,15,16,18,25,41], asymptotic iteration technique [5] and Hamiltonian hierarchy picture [10].

In particular, in [2], we have studied the Schrödinger equation by an equation of the form

$$\sigma(\xi)y'' + \tau(\xi)y' + Q(\xi)y = -\lambda y.$$  (4)

called the equation of hypergeometric type with a perturbation (EHTP), by means of transformations on both independent and dependent variables. Here $\sigma(\xi)$ and $\tau(\xi)$ are polynomials of degrees at most two and one, respectively, and $\lambda$ is a parameter. In fact, in the special case of $Q(\xi) \equiv 0$, (4) reduces to the well-known equation of the hypergeometric type whose suitable solutions are the classical orthogonal polynomials. Accordingly, in [2], we have converted the radial Schrödinger equation in (1) into an EHTP

$$\xi y'' + \left(\ell + 1 - M - \xi\right)y' + \frac{1}{4}(\xi - c^2 V(c^{-1}\sqrt{\xi}))y = \left(2\ell + M - \frac{1}{4}c^{-2}E\right)y,$$  (5)

first by introducing the scaled quadratic variable $\xi = (cr)^2$ where $c$ is a positive constant and then proposing a solution of the type $R(\xi) = \xi^{\ell/2}e^{-\xi/2}y(\xi)$ satisfying the asymptotic boundary condition at infinity and the regularity condition at the origin. However, the quadratic transformation, which was necessary to convert (1) into an EHTP, does not seem suitable for potentials that contain both odd and even powers of the variable $r$. For the sake of a form that is well suited for all potentials, we have to sacrifice the EHTP. Therefore, in this study, instead of the quadratic transformation we start with a more flexible one

$$\xi = (cr)^{\alpha}, \quad \alpha, c > 0, \xi \in (0, \infty)$$  (6)

where the parameters $\alpha$ and $c$ may be exploited to accelerate the convergence rate of the method. Then we suggest a solution of type

$$R(\xi) = \xi^{\ell/2}e^{-\xi/2}y(\xi)$$  (7)

which transforms the radial Schrödinger equation (1) into

$$\xi y'' + (\gamma + 1 - \xi)y' + Q(\xi)y = \lambda\xi^{\frac{\ell}{2}}y$$  (8)

where

$$Q = Q(\xi; \alpha, c, \gamma) = \frac{1}{4} - \frac{1}{2}(\gamma + 1) - \frac{1}{(\alpha c)^2}\xi^{\frac{\ell}{2}}V(\xi^{1/\alpha}/c)$$  (9)

represents the modified potential, $\gamma$ is the parameter

$$\gamma = \gamma(\alpha, \ell, M) = \frac{1}{\alpha}(2\ell + M - 2),$$  (10)

and

$$\lambda = \lambda_n(\alpha, c, \gamma) = -\frac{1}{(\alpha c)^2}\xi^{(M)}E_{n,\ell}$$  (11)

the rescaled energy eigenvalues.

The positive nonconstant term $\xi^{\frac{\ell}{2}}$ on the right hand side of (8) can be seen as a weight function, and hence, the new form may be considered as a weighted and perturbed Laguerre (WPL) equation. Now the EHTP in (5) is a special case of (8) with $\alpha = 2$. Both (5) and (8) resemble the Laguerre differential equation

$$\xi y'' + (\gamma + 1 - \xi)y' = -ny, \quad \xi \in (0, \infty)$$  (12)

where $\gamma$ is a real parameter and $n$ a non-negative integer. In the next section, we construct the pseudospectral formulation of the WPL equation based on the associated Laguerre polynomials $L_n^{\gamma}(\xi)$ which are the polynomial solutions of (12). Section 3 introduces the numerical examples. Section 4 concerns with the implementation notes and the last section concludes the paper with some remarks.
2. The Laguerre pseudospectral method (LPM) for the WPL equation

A pseudospectral method, also known as spectral collocation method, is based on the $N$-th degree polynomial interpolation of a function $y(\xi)$ denoted by $P_N(\xi)$.

\[
P_N(\xi) = \sum_{n=0}^{N} \ell_n(\xi) y_n, \tag{13}
\]

where the $y_n = y(\xi_n)$ are the actual values of $y(\xi)$ at the specified nodes $\xi = \xi_n$ for $n = 0, 1, \ldots, N$. Such a pseudospectral scheme in which the $N$-th degree Lagrange polynomials

\[
\ell_n(\xi) = \frac{\psi_{N+1}(\xi)}{(\xi - \xi_n) \psi'_{N+1}(\xi_n)} = \frac{L_N^\gamma(\xi)}{(\xi - \xi_n)[d \psi_{N+1}(\xi)]/d \xi} \bigg|_{\xi = \xi_n}, \quad n = 0, 1, \ldots, N \tag{14}
\]

are defined by the normalized

\[
\psi_n(\xi) = \frac{1}{h_n} L_n^\gamma(\xi), \quad h_n = \sqrt{\frac{\Gamma(n + \gamma + 1)}{n!}}, \quad \gamma > -1 \tag{15}
\]

or standard Laguerre polynomials $L_n^\gamma(\xi)$ is called a LPM, where the nodes $\xi_n$ are the real, distinct and positive roots of $L_{N+1}^\gamma(\xi)$. Approximating the solutions of differential equations by Laguerre polynomials are usually not stable for large $N$ due to their wild behaviors at infinity, and hence, one usually works with the Laguerre functions $\psi_n(\xi) = e^{-\xi/2}L_n^\gamma(\xi)/h_n$ instead. This situation is theoretically investigated, for example in [11,24,28,29], and it is shown that the Laguerre functions have better stability properties than Laguerre polynomials. On the other hand, it is stated in [29] on p. 214 that the generalized Laguerre polynomials are useful for the approximation of functions which decay at infinity. Therefore, in this study, we continue with the normalized Laguerre polynomials in (15) since we search for the square integrable solutions of (1) which behave suitably at the origin and vanish exponentially at infinity.

Notice that, $y(\xi_n) = P_N(\xi_n)$ at least at the nodes since the Lagrange polynomials have the well-known property $\ell_n(\xi_n) = \delta_{nm}$ where $\delta_{nm}$ is Kronecker’s delta. In this article, the discretization procedure of (1) by the LPM for any arbitrary $\gamma$ parameter is presented keeping in mind that we will eventually take $\gamma$ as the parameter in (10).

It is also possible to approximate the derivatives of the function $y(\xi)$ by differentiating the interpolant $P_N(\xi)$. Furthermore, the derivative values at the nodes $\xi_n$ may be determined in terms of function values $y_n = P_N(\xi_n)$ by means of a differentiation matrix defined by

\[
D^{(k)} := [d_{mn}^{(k)}] = \frac{d^k}{d\xi^k}[\ell_n(\xi)] \bigg|_{\xi = \xi_m}, \quad k = 1, 2, \ldots, N \tag{16}
\]

for $m, n = 0, 1, \ldots, N$. The approximate derivative values $y^{(k)} = [P^{(k)}_N(\xi_0), P^{(k)}_N(\xi_1), \ldots, P^{(k)}_N(\xi_N)]^T$ may therefore be written in matrix–vector form

\[
y^{(k)} = D^{(k)} y \tag{17}
\]

where $y = [y_0, y_1, \ldots, y_N]^T$ is the vector of function values at the nodes. In particular, the entries of the first and the second order differentiation matrices can be obtained as

\[
d_{mn}^{(1)} = \begin{cases} 
\frac{2}{\xi_m - \xi_n} \frac{\psi_{N+1}'(\xi_m)}{\psi_{N+1}'(\xi_n)} & \text{if } m \neq n \\
\frac{1}{\psi_{N+1}'(\xi_n)} (\xi_n - \gamma - 1) & \text{if } m = n
\end{cases} \tag{18}
\]

and

\[
d_{mn}^{(2)} = \begin{cases} 
\frac{2}{\xi_m - \xi_n} \frac{1}{\psi_{N+1}'(\xi_n)} (\xi_n - \gamma - 1) - \frac{2}{\xi_m - \xi_n} \frac{\psi_{N+1}'(\xi_m)}{\psi_{N+1}'(\xi_n)} & \text{if } m \neq n \\
\frac{1}{\psi_{N+1}'(\xi_n)} (\xi_n - \gamma - 1) (\xi_n - \gamma - 2) - N & \text{if } m = n
\end{cases} \tag{19}
\]

by making use of (14) and (16) [35].

On the other hand, the three-term recursion [35]

\[
\sqrt{(n+\gamma)}\psi_{n-1}(\xi) - (2n + \gamma + 1 - \xi)\psi_n(\xi) - \sqrt{(n+1)(n+\gamma+1)}\psi_{n+1}(\xi) = 0 \tag{20}
\]

for the normalized Laguerre polynomials may be used to determine the zeros of $\psi_n(\xi)$ and therefore those of $L_n^\gamma(\xi)$. Actually, running the above recursion over the range $n = 0, 1, \ldots, N$ we obtain an inhomogeneous linear algebraic system $(W - \xi I)\mathbf{t} = \mathbf{b}$, or in matrix-vector form
\[
\begin{bmatrix}
\gamma + 1 - \xi & -\sqrt{\gamma + 1} & 0 & \cdots & 0 \\
-\sqrt{\gamma + 1} & \gamma + 3 - \xi & -\sqrt{2(\gamma + 2)} & \ddots & \vdots \\
0 & -\sqrt{2(\gamma + 2)} & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \cdots & \gamma + 2N - 1 - \xi & -\sqrt{N(\gamma + N)} \\
0 & \cdots & \cdots & 0 & \gamma + 2N + 1 - \xi
\end{bmatrix}
\begin{bmatrix}
\psi_0 \\
\psi_1 \\
\vdots \\
\psi_N
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
\psi_1 \\
\vdots \\
\psi_N
\end{bmatrix}
\]

(21)

where \( \psi_i = \psi_i(\xi) \) and the right-hand side is a vector with only one nonzero component \( b_{N+1} = \sqrt{(N + 1)(N + \gamma + 1)} \psi_{N+1}(\xi) \). Therefore, if we require \( \psi_{N+1}(\xi) = 0 \) or, equivalently, \( L_{N+1}^\gamma(\xi) = 0 \) then the system reduces to a standard eigenvalue problem \( W t = \xi t \) with the eigenvalue parameter \( \xi \), which provides us the roots \( \xi_i, i = 0, 1, \ldots, N \) of \( L_{N+1}^\gamma(\xi) \) as required [2,35].

Since the eigenvector associated to each eigenvalue of \( W \) is unique up to a constant factor, the \( m \)-th computed eigenvector

\[
v_m = [v_{0,m}, v_{1,m}, \ldots, v_{N-1,m}, v_{N,m}]^T
\]

of the matrix \( W \) associated to the eigenvalue \( \xi_m \) is a constant multiple of \( t_m = [\psi_0(\xi_m), \psi_1(\xi_m), \ldots, \psi_{N-1}(\xi_m), \psi_N(\xi_m)]^T \), that is \( v_m = \alpha t_m \). The value of \( \alpha \) can be determined by considering the first entries \( v_{0,m} \) and \( \psi_0(\xi_m) \) of the eigenvectors \( v_m \) and \( t_m \), respectively, since \( \psi_0(\xi) = 1/h_0 = 1/\sqrt{T(\gamma + 1)} \) is a constant polynomial we obtain \( \alpha = \sqrt{T(\gamma + 1)v_{0,m}} \).

Therefore, for \( n = 0, 1, \ldots, N \), the values \( \psi_n(\xi_m) \) of the orthonormal Laguerre polynomials at the zeros of \( \psi_{N+1}(\xi) \) may be computed as

\[
\begin{bmatrix}
\psi_0(\xi_m) \\
\psi_1(\xi_m) \\
\vdots \\
\psi_{N-1}(\xi_m) \\
\psi_N(\xi_m)
\end{bmatrix} = \frac{1}{\sqrt{T(\gamma + 1)v_{0,m}}}
\begin{bmatrix}
v_{0,m} \\
v_{1,m} \\
\vdots \\
v_{N-1,m} \\
v_{N,m}
\end{bmatrix}
\]

(23)

in terms of the computed eigenvector \( v_m \) of tridiagonal symmetric matrix \( W \).

Then we put the interpolant (13) into (8)

\[
\sum_{n=0}^{N} \left[ \xi \ell_n'(\xi) + (\gamma + 1 - \xi)\ell_n''(\xi) + Q(\xi)\ell_n(\xi) \right] y_n = \lambda \sum_{n=0}^{N} \xi^{\frac{d}{2}-1} \ell_n(\xi) y_n
\]

(24)

and demand its satisfaction at the grid points \( \xi_m \) for \( m = 0, 1, \ldots, N \), to get the discrete representation

\[
A y = \lambda B y
\]

(25)

of the WPL. The general entries \( A_{mn} \) and \( B_{mn} \) of the resulting matrices \( A \) and \( B \) are given by

\[
A_{mn} = \xi_m a_{mn}^{(2)} + (\gamma + 1 - \xi_m) a_{mn}^{(1)} + Q(\xi_m; \alpha, \gamma) \delta_{mn}
\]

(26)

and

\[
B_{mn} = \xi_m^{\frac{d}{2}-1} \delta_{mn}
\]

(27)

respectively. Since \( B \) is a diagonal matrix, the generalized matrix–eigenvalue problem in (25) can be replaced with the standard one

\[
\tilde{T} y = \lambda y
\]

(28)

where \( \tilde{T} = B^{-1} A \) and its general entry reads as

\[
\tilde{T}_{mn} = \xi_m^{1-\frac{d}{2}} \left[ \xi_m a_{mn}^{(2)} + (\gamma + 1 - \xi_m) a_{mn}^{(1)} + Q(\xi_m; \alpha, \gamma) \delta_{mn} \right]
\]

(29)

where \( m, n = 0, 1, \ldots, N \). Here, the vector \( y_n = [y_{0,n}, y_{1,n}, \ldots, y_{N,n}]^T \) involves the values of the \( n \)-th eigenfunction of (8) associated with the eigenvalue \( \lambda_n \) at the nodal points.
By using (18) and (19) the first two terms in (29) can be incorporated to define
\[
\tilde{K}_{mn} = -\frac{1}{6} \begin{cases} 
\frac{12\xi_n}{(\xi_m - \xi_n)^2} \psi'_{N+1}(\xi_m) \psi_{N+1}(\xi_n) & \text{if } m \neq n \\
\xi_n^{1-\frac{\alpha}{2}} [2N + \frac{1}{\xi_n} (\gamma - \xi_n)^2 - 1] & \text{if } m = n
\end{cases}
\]
which represents the effect of kinetic energy terms independent of a specified potential.

It seems that the evaluation of \(\tilde{K}_{mn}\) requires the computation of the derivatives \(\psi'_{N+1}(\xi_m)\) of the normalized Laguerre polynomials at the nodes. Fortunately, a nice similarity transformation \(T = S^{-1} \tilde{T} S\) in which
\[
S = s_m \delta_{mn} = \xi_m^{1-\frac{\alpha}{2}} \psi'_{N+1}(\xi_m) \delta_{mn}
\]
is a diagonal matrix, makes it possible to get rid of such a cumbersome labor. Furthermore, the matrix in (28) reduces to a symmetric one, say \(T = S^{-1}(K + Q)S\), whose entries are given by
\[
T_{mn} = K_{mn} + Q_{mn}
\]
where
\[
K_{mn} = -\frac{1}{6} \begin{cases} 
\frac{12\xi_m \xi_n^{1-\frac{\alpha}{2}}}{(\xi_m - \xi_n)^2} & \text{if } m \neq n \\
\xi_n^{1-\frac{\alpha}{2}} [2N + \frac{1}{\xi_n} (\gamma - \xi_n)^2 - 1] & \text{if } m = n
\end{cases}
\]
and
\[
Q_{mn} = \xi_m^{1-\frac{\alpha}{2}} Q(\xi_m; \alpha, c, \gamma) \delta_{mn} = \xi_m^{1-\frac{\alpha}{2}} \left[ \frac{1}{4} \xi_m - \frac{1}{2} (\gamma + 1) \right] \xi_m^{\frac{\alpha}{2} - 1} V(\xi_m^{\frac{1}{\alpha} / c}) \delta_{mn}.
\]

Thus, the eigenvalues of (28), and, hence, the approximate eigenvalues of the WPL can be determined by the symmetric matrix eigenvalue problem
\[
Tu = \lambda u
\]
since the similar matrices share the same spectrum. Note that, the Laguerre pseudospectral formulation of the WPL leads to the symmetric matrix eigenvalue problem whose construction requires only the knowledge of the roots of the Laguerre polynomial \(L_{N+1}^{\alpha}(\xi)\).

On the other hand, the \(n\)-th eigenvector \(y_n\) of (28) is given by the formula
\[
y_n = Su_n
\]
in terms of the \(n\)-th eigenvector \(u_n = [u_{0,n}, u_{1,n}, \ldots, u_{N,n}]^T\) of the symmetric matrix \(T = S^{-1} \tilde{T} S\) since \(S^{-1} \tilde{T} Su_n = \lambda u_n\) implies that \(\tilde{T}(Su_n) = \lambda (Su_n)\). Thus, the \(m\)-th entry \(m_{n,m} = y_{n}(\xi_m)\) of the \(n\)-th eigenvector \(y_n\) may be written as \(y_{m,n} = s_m u_{m,n}\), or in nodal notation we have
\[
y_n(\xi_m) = \xi_m^{1-\frac{\alpha}{2}} \psi'_n(\xi_m) u_{m,n}
\]
upon using (31). Then (7) determines the original wavefunction
\[
\mathcal{K}_{n,l}(\xi_m) = \psi'_{N+1}(\xi_m) \xi_m^{1+\frac{\alpha}{2}} e^{-\xi_m/2} u_{m,n}
\]
at a collocation point \(\xi_m\). Turning back to the original variable \(r\) via (6), the last equation reads as
\[
\mathcal{K}_{n,l}(r_m) = \psi'_{N+1}(r_m) \xi_m^{1+\frac{\alpha}{2}} e^{-r_m/2} u_{m,n}.
\]
Thus, we may state the following theorem.

**Theorem 2.1.** The approximate eigenvalues \(E_{n,l}^{(M)}\) of the radial Schrödinger equation in (1) are connected with the eigenvalues of the linear system in (35) by the formula
\[
E_{n,l}^{(M)} = -\frac{(\alpha c)^2}{\lambda_n(\alpha, c, \gamma)}, \quad n = 0, 1, \ldots
\]
and the values of the corresponding normalized eigenfunctions \(\mathcal{Y}_{n,l}^{(M)}(r_m)\) in \(L^2_\rho\) sense at the points \(r_m = \xi_m^{1/\alpha} / c\) are given by
\[
\mathcal{Y}_{n,l}^{(M)}(r_m) = \sqrt{\frac{\alpha c^M}{\Gamma(\alpha + 1)}} \xi_m^{1+\frac{\alpha}{2}} e^{-r_m/2} u_{m,n}
\]
whenever \(u_n\) is the normalized (in Euclidean 2-norm) eigenvector of (35). The \(v_{0,m}\) and \(v_{N,m}\) are the first and the last entries of (22), respectively.
Proof. The first part follows from (11). When written in the Sturm–Liouville form, it is not difficult to see that the weight functions of (1) and (8) are given by \( \rho(r) = r^{M-1} \) and \( \rho(\xi) = \xi^{\gamma + \frac{2}{\sigma} - 1}e^{-\xi} \), respectively. First using the scaling transformation in (6) we write

\[
\|p_n^{(M)}(r)\|^2_{L^2(\rho)} = \int_0^\infty [p_n^{(1,\ell)}(r)]^2 r^{M-1} dr = \int_0^\infty \left[ \sqrt{\alpha e^M} T_n^{(M)}(r) \right]^2 r^{M-1} dr = \int_0^\infty \left[ T_n^{(1,\ell)}(\xi) \right]^2 \xi^{\frac{M}{2} - 1} d\xi
\]

which, upon the use of (7), reads as

\[
\|p_n^{(M)}(r)\|^2_{L^2(\rho)} = \int_0^\infty y_n^2(\xi)\xi^{\gamma + \frac{2}{\sigma} - 1}e^{-\xi} d\xi.
\]

Applying the \( N + 1 \) point Laguerre–Gauss quadrature to the function \( \xi^{\frac{2}{\sigma} - 1}y_n^2(\xi) \), we obtain, in the limiting case when \( N \to \infty \)

\[
\|p_n^{(M)}(r)\|^2_{L^2(\rho)} = \int_0^\infty \xi^{\frac{2}{\sigma} - 1}y_n^2(\xi)\xi^{\gamma}e^{-\xi} d\xi = \lim_{N \to \infty} \sum_{m=0}^N \xi_m^{\frac{2}{\sigma} - 1}y_n^2(\xi_m)\omega_m
\]

where

\[
\omega_m = \frac{1}{(N+1)(N+\gamma+1)} \xi_m, \quad m = 0, 1, \ldots, N
\]

are known as the Christoffel numbers or weights of the quadrature in terms of the normalized Laguerre polynomials [13]. Now, the differential–difference relation [35]

\[
\xi \psi_n'(\xi) = n\psi_n(\xi) - \sqrt{n(n+\gamma)}\psi_{n-1}(\xi)
\]

of the normalized Laguerre polynomials with \( n = N + 1 \) and \( \xi = \xi_m \) leads to

\[
\psi_{n+1}(\xi_m) = -\frac{1}{\xi_m} \sqrt{(N+1)(N+\gamma+1)}\psi_{N}(\xi_m)
\]

since \( \psi_{N+1}(\xi_m) = 0 \) for \( m = 0, 1, \ldots, N \) and hence, (37) rewritten as

\[
y_n(\xi_m) = -\sqrt{(N+1)(N+\gamma+1)}\psi_{N}(\xi_m)\xi_m^{\frac{1}{\sigma}} u_{m,n}.
\]

Inserting (45) and (48) into the right hand side of (44) we obtain

\[
\|p_n^{(M)}(r)\|^2_{L^2(\rho)} = \lim_{N \to \infty} \sum_{m=0}^N u_{m,n}^2 = \lim_{N \to \infty} \|u_n\|_2^2 = \lim_{N \to \infty} 1 = 1.
\]

On the other hand, (39) together with (47) and (23) gives (41) which completes the proof. It is clear from (43) and (49) that

\[
\|y_n(\xi)\|^2_{L^2(\rho)} = 1
\]

is also true under the same assumption where \( \rho(\xi) = \xi^{\gamma + \frac{2}{\sigma} - 1}e^{-\xi} \).

3. Numerical examples

It is clear from (8) and (10) that the spectrum of the eigenvalue problem remains unchanged for a prescribed value of the sum \( 2\ell + M \). Hence the eigenvalues in \( M \) dimensions denoted by \( E_{n,\ell}^{(M)} \) are degenerate in such a way that

\[
E_{n,1}^{(2)} = E_{n,0}^{(4)}
E_{n,2}^{(2)} = E_{n,1}^{(4)} = E_{n,0}^{(6)}
\vdots
E_{n,\ell}^{(2)} = E_{n,\ell-1}^{(4)} = E_{n,\ell-2}^{(6)} = \ldots = E_{n,2}^{(2\ell-2)} = E_{n,1}^{(2\ell)} = E_{n,0}^{(2\ell+2)}
\]

(51)
The energy eigenvalues \( E_{n,0}^{(3)} \) of the potential, \( V(r) = r^2 + v_4 r^4 \), as a function of \( v_4 \) where \( a_{opt} = 2 \).

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<td>2</td>
<td>160</td>
<td>100</td>
<td>0</td>
<td>2604.432 483 714 639 307 459 405 681 55</td>
</tr>
<tr>
<td>10^4</td>
<td>9</td>
<td>30</td>
<td>0</td>
<td>0</td>
<td>81.903 316 953 284 467 567 471 308 555</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>80</td>
<td>25</td>
<td>1</td>
<td>9.253 923 499 415 499 714 821 586 373 98</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>100</td>
<td>50</td>
<td>5</td>
<td>23756.533 983 690 976 108 458 514 955 3</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>162</td>
<td>100</td>
<td>10</td>
<td>59302.060 316 455 519 491 294 154 604 9</td>
</tr>
</tbody>
</table>

\[\text{Reference [36]: } E_{n,0}^{(3)} = 5.4.184 984 610 454 439 924 123 480 175 7.\]

Table 2

The effect of second optimization parameter \( \alpha \) on the accuracy of ground state energies of isotropic quartic oscillator when \( v_4 = 10^{-4} \) and the Airy equation.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( E_{n,0}^{(3)} ) of isotropic quartic oscillator ((N = 8, c_{opt} = 1))</th>
<th>( E_{n,0}^{(3)} ) of Airy equation ((N = 66, c_{opt} = 6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3.066 750</td>
<td>9.111 969</td>
</tr>
<tr>
<td>2.5</td>
<td>3.026 398</td>
<td>4.842 756</td>
</tr>
<tr>
<td>2</td>
<td>3.003 874 896 936 121 098 337 846 829 9</td>
<td>2.632 534</td>
</tr>
<tr>
<td>1.5</td>
<td>2.993 411</td>
<td>2.338 107 893</td>
</tr>
<tr>
<td>1</td>
<td>2.946 460</td>
<td>2.338 107 410 459 767 038 489 197 252 4</td>
</tr>
<tr>
<td>0.5</td>
<td>3.027 127</td>
<td>2.338 111</td>
</tr>
</tbody>
</table>

for even values of space dimension \( M \) where \( E_{n,0}^{(2)} \) is single in the system. Similarly, if \( M \) is odd, then

\[
\begin{align*}
E_{n,0}^{(3)} &= E_{n,1}^{(1)} = \epsilon_{n,0} \\
E_{n,1}^{(3)} &= E_{n,0}^{(5)} \\
E_{n,2}^{(3)} &= E_{n,1}^{(7)} \\
&\vdots \\
E_{n,l}^{(3)} &= E_{n,l-1}^{(5)} = E_{n,l-2}^{(7)} = \cdots = E_{n,2}^{(2l-1)} = E_{n,1}^{(2l+1)} = E_{n,0}^{(2l+3)}
\end{align*}
\]

(52)

where \( \epsilon_{n,0} \) are the eigenvalues of the Schrödinger equation in (2). The degenerate structure of the spectrum of (1) now suggests evidently that we may consider only two- and three-dimensional cases, without any loss of generality.

As a first example we consider the \( M \)-dimensional isotropic quartic oscillator

\[
V(r) = r^2 + v_4 r^4
\]

(53)

where \( v_4 > 0 \). Taşeli and Zafer [36] expanded the wave function into a Fourier–Bessel series to solve the radial Schrödinger equation with isotropic polynomial potentials and Taşeli [32] proposed an alternative series solution to the isotropic quartic oscillator in \( M \) dimensions. It seems that the transformation (6) with \( \alpha = 2 \) is the most suitable one since the potential contains even powers of \( r \) only. In Table 1, we present eigenvalues of isotropic quartic oscillator in 3-dimensions for some pairs of \( (n, l) \). In all tables, \( n \) and \( l \) stand for the quantum numbers of the state, \( N \) the truncation order for which the desired (machine) accuracy of the corresponding eigenvalue is obtained, and \( c \) and \( \alpha \) denote some scaling or optimization parameters which may be used to accelerate the convergence rate of the method. The accuracy of the results in all tables reported here has been checked by inspecting the number of stable digits between two consecutive truncation orders. For comparison, at the bottom right of Table 1 we included a result from [36] when \( v_4 = 1 \).

On the other hand, the effect of the second optimization parameter \( \alpha \) is reported in Table 2. In order to regain the machine accuracy for \( E_{n,0}^{(3)} \) when, for example, \( \alpha = 1 \) we should choose \( N = 50 \) and \( c = 15 \) at the same time. Therefore, we may say that our prediction of \( \alpha \) is experimentally justified by Table 2. If further \( c = 1 \), that is, in the absence of scaling factors, the truncation order \( N \) increases dramatically. For unbounded domains scaling factors are crucial to obtain the desired accuracy with the possible smallest truncation order.

The second example is an odd polynomial potential
\[ V(r) = r, \quad r \in (0, \infty) \] (54)

for which the Schrödinger equation reduces to the Airy equation \(-y'' + ry = \lambda y\) when we set \(M = 1\) and \(\ell = 0\) or \(\ell = 1\) in (1). In this case, eigenvalues are given implicitly by \(\text{Ai}(-\lambda) = 0\) where \(\text{Ai}(x)\) is the Airy function [8]. Several states of the Airy equation in one dimension is reported in Table 3. The last column includes the negatives of zeros of the Airy function taken from [1]. It is clear from Table 2 that for the Airy equation the optimum value of the second scaling factor is \(\alpha_{opt} = 1\).

As a third example, we consider the exponential cosine partially screened Coulomb potential (ECPSC)

\[ V(r) = -2ZV_{ec}(r, \nu, \mu) - 2Z_{as}\left[\frac{1}{r} - V_{ec}(r, \nu, \mu)\right], \quad Z > 0, \quad Z_{as} > 0 \] (55)

where

\[ V_{ec}(r, \nu, \mu) = \frac{1}{r}e^{-\nu r} \cos(\mu r) \] (56)

with the two screening parameters \(\nu\) and \(\mu\) [17]. In particular, when \(Z_{as} = 0\) the potential reduces to the exponential cosine screened Coulomb potential (ECSC) \(V(r) = -2Z \exp(-\nu r) \cos(\mu r)/r\). If further, \(\mu = 0\) at the same time, it is known as the Yukawa potential \(V(r) = -2Z \exp(-\nu r)/r\). On the other hand, \(Z_{as} = Z\) corresponds to the pure attractive Coulomb potential \(V(r) = -2Z/r\) which has countably many discrete states given by

\[ E_{n,\ell}^{(M)} = \frac{-4Z^2}{(2n + 2\ell + M - 1)^2}, \quad n = 0, 1, \ldots \] (57)

together with the continuous spectrum over the entire positive real axis.

These potentials have been subject of several studies. For example, Lai [19] determined several states of ECSC within the framework of the hypervirial Padé scheme. Taşeli [33] used modified Laguerre basis for the ECSC and Yukawa potentials. Ixaru and co-workers [17] developed accurate, robust and safe approach for ECPSC.

Several eigenvalues of the ECPSC potential in three dimensions are reported in Table 4 for the parameter values \(Z = 50, Z_{as} = 1\) and \(\nu = \mu = 0.025\) when \(\ell = 0, 10\). It is clear from Table 4 that if we keep \(\alpha = 1\), higher levels become expensive or even impossible to obtain. In this stage, transformations (6) and (7) together with the decreasing character of \(c\) suggests that we should take smaller \(\alpha\) values. Indeed, when we take \(\alpha = 0.7\) while keeping \(c = 1\), it is possible to obtain higher states with relatively small truncation orders.

Table 5 demonstrates the bound states of the ECSC potential. In all computations we used quadruple-precision arithmetic on a main frame computer with machine accuracy of 32 digits, by truncating the results to 27–28 significant figures. For comparison, at the bottom right of the table, we attached results from [33] and [21] which are in good agreement with those of the present study to the accuracy quoted.

Fig. 1 illustrates the two normalized eigenfunctions \(\Psi_{30,0}(r)\) and \(\Psi_{4,0}(r)\) of the ECPSC and ECSC potentials, respectively, for the specified parameter values. Our results are in good agreement with those of MATSLISE, which is typical for all eigenfunctions considered in this study.

The present method works well also for the pure attractive Coulomb potential. For instance, in three dimensions when \(Z_{as} = Z = 1\), \(\ell = 0\), \(\alpha = 1\) and \(N = 500\), the eigenvalues \(E_{n,0}^{(3)}\) with \(2 \leq n \leq 125\) are obtained within the machine accuracy by taking \(c = 0.05\) while \(c = 0.005\) leads to the same accuracy for \(E_{n,0}^{(3)}\) with \(130 \leq n \leq 430\). That is, the optimization parameters may be seen as the position identifier of a flash lamp which illuminates the specific part of the eigenvalue.
Table 4
Several states of the ECPSC potential in three dimensions when $Z = 50$, $Z_a = 1$ and $\nu = \mu = 0.025$ as $\ell$ varies.

<table>
<thead>
<tr>
<th>$\alpha_{opt}$</th>
<th>$c_{opt}$</th>
<th>$N$</th>
<th>$n$</th>
<th>$\ell$</th>
<th>$E_{\alpha,\ell}^{(3)}$ = $E_{\alpha,\ell+1}^{(3)}$ = $E_{\alpha,\ell}$</th>
<th>$E_{\alpha,\ell}$ (Reference [17])</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>90</td>
<td>20</td>
<td>0</td>
<td>0</td>
<td>$-2497.550000612117302611994770$</td>
<td>$-2497.5500006120$</td>
</tr>
<tr>
<td>60</td>
<td>20</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>$-622.5500008558171070243163513285$</td>
<td>$-622.5500008557$</td>
</tr>
<tr>
<td>30</td>
<td>20</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$-275.32781986485534764663097500$</td>
<td>$-275.327819864$</td>
</tr>
<tr>
<td>8</td>
<td>30</td>
<td>10</td>
<td></td>
<td>0</td>
<td>$-18.218254845294488912506539439$</td>
<td>$-18.218254846$</td>
</tr>
<tr>
<td>5</td>
<td>20</td>
<td>30</td>
<td></td>
<td>0</td>
<td>$-3.3012939234749879462850075666$</td>
<td>Not reported</td>
</tr>
<tr>
<td>3</td>
<td>62</td>
<td>30</td>
<td>0</td>
<td>0</td>
<td>$-4.77979939510803625235770389$</td>
<td>Not reported</td>
</tr>
<tr>
<td>0.5</td>
<td>325</td>
<td>50</td>
<td></td>
<td>0</td>
<td>$-0.001531333745151369647958064$</td>
<td>$-0.00153133374$</td>
</tr>
<tr>
<td>0.7</td>
<td>1</td>
<td>350</td>
<td>100</td>
<td>0</td>
<td>$-0.00017430705849151$</td>
<td>$-0.00017430705849$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\alpha_{opt}$</th>
<th>$c_{opt}$</th>
<th>$N$</th>
<th>$n$</th>
<th>$\ell$</th>
<th>$E_{\alpha,\ell}^{(3)}$ = $E_{\alpha,\ell+1}^{(3)}$ = $E_{\alpha,\ell}$</th>
<th>$E_{\alpha,\ell}$ (Reference [17])</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8</td>
<td>25</td>
<td>0</td>
<td>10</td>
<td>$-18.21445124040845952916633118$</td>
<td>$-18.2144512404$</td>
</tr>
<tr>
<td>8</td>
<td>25</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>$-14.916599484348436359598723652512$</td>
<td>$-14.9165994843$</td>
</tr>
<tr>
<td>8</td>
<td>25</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>$-12.3512992295081145310345160781$</td>
<td>$-12.3512992294$</td>
</tr>
<tr>
<td>5</td>
<td>40</td>
<td>10</td>
<td></td>
<td>0</td>
<td>$-3.289943284017899972361084807$</td>
<td>$-3.28994328401$</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td>20</td>
<td></td>
<td>0</td>
<td>$-0.460117420637774647219316168$</td>
<td>Not reported</td>
</tr>
<tr>
<td>0.7</td>
<td>200</td>
<td>30</td>
<td></td>
<td>0</td>
<td>$-0.00036808642351318446880809$</td>
<td>Not reported</td>
</tr>
<tr>
<td>.3</td>
<td>355</td>
<td>50</td>
<td></td>
<td>0</td>
<td>$-0.00069963109266464508$</td>
<td>$-0.0006996310$</td>
</tr>
</tbody>
</table>

Table 5
Bound energy eigenvalues of the ECSC potential in three dimensions when $Z = 1$ and $\nu = 0.05$, as $\mu$ varies. The case, $\mu = 0$ corresponds to the Yukawa potential.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$c_{opt}$</th>
<th>$\alpha_{opt}$</th>
<th>$N$</th>
<th>$n$</th>
<th>$\ell$</th>
<th>$E_{\alpha,\ell}^{(3)}$ = $E_{\alpha,\ell+1}^{(3)}$ = $E_{\alpha,\ell}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.6</td>
<td>1</td>
<td>65</td>
<td>0</td>
<td>0</td>
<td>$-0.90363285704901108771243151$</td>
</tr>
<tr>
<td>1</td>
<td>1.0</td>
<td>1</td>
<td>56</td>
<td>0</td>
<td>1</td>
<td>$-0.163542391590506248346987285$</td>
</tr>
<tr>
<td>2</td>
<td>2.0</td>
<td>1</td>
<td>56</td>
<td>0</td>
<td>2</td>
<td>$-0.0387051096295046845907959536$</td>
</tr>
<tr>
<td>3</td>
<td>3.0</td>
<td>1</td>
<td>56</td>
<td>0</td>
<td>3</td>
<td>$-0.006183319800322642969317006$</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5</td>
<td>250</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>$-0.161480774075656912420254872$</td>
</tr>
<tr>
<td>0.4</td>
<td>1.0</td>
<td>56</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>$-0.03711503766811993209778988$</td>
</tr>
<tr>
<td>0.4</td>
<td>1.0</td>
<td>51</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>$-0.0051961170750143709355223825$</td>
</tr>
<tr>
<td>0.05</td>
<td>1.0</td>
<td>55</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$-0.9902349328413753366905524618$</td>
</tr>
<tr>
<td>0.05</td>
<td>1.0</td>
<td>55</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>$-0.1528991925004945878681337617$</td>
</tr>
<tr>
<td>0.05</td>
<td>1.0</td>
<td>55</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>$-0.02315128414215916951132233$</td>
</tr>
</tbody>
</table>

\* Appropriately scaled result from Reference [33]: $E_{0,0}^{(3)} = -0.903632857049011087712434$.
\* MATSLISE [21]: $E_{4,0}^{(1)} = E_{4,1}^{(1)} = E_{4,0} = -0.00000313898337$.

Fig. 1. Normalized eigenfunction $\psi_{0,0}(r) = R_{00}^{(1)}(r)$ of the ECPSC potential corresponding to $E_{0,0}^{(1)} = E_{0,0}$ when $Z = 50$, $Z_a = 1$, $\nu = \mu = 0.025$ (left).
Normalized eigenfunction $\psi_{4,0}(r) = R_{40}^{(1)}(r)$ of the ECSC potential corresponding to $E_{4,0}^{(1)} = E_{4,0}$ when $Z = 1$, $\nu = 0.05$, $\mu = 0$ (right).
column. Therefore, adjusting the position of the flashlight, it is possible to lightening the whole set of eigenvalues for a prescribed truncation order \( N \).

The next potential we consider is the partially screening Hulthén potential

\[
V(r) = -2ZV_H(r, \nu) - 2Z_{\text{as}} \left(\frac{1}{r} - V_H(r, \nu)\right), \quad Z > 0, \quad Z_{\text{as}} > 0
\]

(58)

where

\[
V_H(r, \nu) = \frac{ve^{-\nu r}}{1 - e^{-\nu r}}
\]

(59)

in which \( \nu \) is the screening parameter. It reduces to the Hulthén screening potential \([14]\) when \( Z_{\text{as}} = 0 \) which is exactly solvable when \( M = \ell = 1 \) (or \( \ell = 0 \)). In this case, bound states are given by

\[
E^{(1)}_{n,1} = E_{n,0} = -\left(\frac{Z}{n + 1} - \frac{(n + 1)\nu}{2}\right)^2, \quad n = 0, 1, \ldots, k
\]

(60)

where \( k = \lfloor \sqrt{2Z/\nu} \rfloor - 1 \) \([8]\). Here \( \lfloor a \rfloor \) denotes the integer part of a real number \( a \).

The partially screening Hulthén potential is considered by Ixaru, De Meyer and Vanden Berghe \([17]\). Hulthén potential is studied by many authors. For instance, Roy \([26]\) applied the generalized pseudospectral approach to approximate the bound states, Stubbins \([30]\) used the generalized variational method to compute the eigenvalues for \( n \leq 6 \), Bayrak and Boztosun \([5]\) used asymptotic iteration method for any \( \ell \) state and Gönül and co-workers \([10]\) considered the potential in the Hamiltonian hierarchy picture to approximate the eigenvalues when \( \ell \neq 0 \).

Table 6 illustrates the bound states of the Hulthén screening potential in three dimensions when \( Z = 50 \) and \( \nu = 0.025 \). For \( \ell = 0 \) the results are in good agreement with the exact eigenvalues. The last column includes results from \([17]\) when \( \ell = 10 \), which are also in good agreement to the accuracy quoted.

Finally, we take into account the Woods–Saxon potential defined by

\[
V(r) = -\frac{50}{1 + \frac{5t}{3(1 + t)}}
\]

(61)

where \( t = \exp[3/5(r - 7)] \). The potential has been considered by several authors; Zakrzewski \([40]\) used a power series method, Lo and Shizgal \([23]\) applied quadrature discretization method, Shao and Wang \([27]\) considered Obrechkoff one-step method to approximate the eigenvalues of the problem.

Bound states of the Woods–Saxon potential in two dimensions when \( \ell = 2 \) and in three dimensions when \( \ell = 0 \) are reported in Table 7. In both cases, there exist 14 discrete states before the start of continuous spectrum over the entire positive real axis.

Fig. 2 shows the first eigenfunction \( \Psi_{1,0}(r) = R_{1,1}^{(1)}(r) \) of the Woods–Saxon potential by using \( N = 120 \) points for different values of the optimization parameter \( c \) while keeping \( \alpha = 1 \). At this truncation order, the optimum \( c \) value is \( c_{\text{opt}} = 45 \). Notice that, \( c_{\text{opt}} \) collects the grid points to the region where the eigenfunction is nonzero. Neither the points are wasted in the region where the wavefunction is too close to zero, nor they are insufficient to recover the shape of the eigenfunction. In this way, it reduces the number \( N \) of collocation points used to get the desired accuracy. Here, for \( c = 15 \) and \( c = 45 \), the energy \( E_{1,0} = E_{1,1}^{(1)} \) is correct to 20 and 27 digits respectively, but no convergence occurs when \( c = 100 \) for the same truncation order of \( N = 120 \).
Table 7
Some bound states $E_{n,l}^{(M)}$ of Woods-Saxon potential.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E_{n,0}^{(2)}(N = 240, \alpha_{opt} = 20, \alpha_{opt} = 1)$</th>
<th>$E_{n,0}^{(3)} = E_{n,1}(N = 200, \alpha_{opt} = 30, \alpha_{opt} = 1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$-46.910$ $642$ $653$ $128$ $173$ $651$ $964$ $836$ $840$</td>
<td>$-48.148$ $430$ $420$ $006$ $361$ $035$ $971$ $245$ $463$</td>
</tr>
<tr>
<td>2</td>
<td>$-44.887$ $033$ $738$ $125$ $528$ $658$ $859$ $863$ $126$</td>
<td>$-46.290$ $753$ $954$ $466$ $087$ $580$ $582$ $890$ $228$</td>
</tr>
<tr>
<td>3</td>
<td>$-42.042$ $376$ $344$ $470$ $092$ $293$ $963$ $820$ $182$</td>
<td>$-43.968$ $318$ $431$ $814$ $233$ $002$ $577$ $289$ $254$</td>
</tr>
<tr>
<td>4</td>
<td>$-39.016$ $331$ $198$ $417$ $396$ $568$ $441$ $736$ $596$</td>
<td>$-41.232$ $607$ $772$ $180$ $218$ $479$ $078$ $577$ $843$</td>
</tr>
<tr>
<td>5</td>
<td>$-35.642$ $628$ $458$ $099$ $764$ $174$ $547$ $675$ $506$</td>
<td>$-38.122$ $785$ $096$ $727$ $919$ $755$ $861$ $765$ $839$</td>
</tr>
<tr>
<td>6</td>
<td>$-31.952$ $271$ $277$ $351$ $562$ $240$ $663$ $822$ $155$</td>
<td>$-34.672$ $313$ $205$ $699$ $650$ $691$ $489$ $091$ $456$</td>
</tr>
<tr>
<td>7</td>
<td>$-27.975$ $710$ $623$ $790$ $707$ $492$ $150$ $511$ $028$</td>
<td>$-30.912$ $247$ $487$ $908$ $848$ $263$ $645$ $899$ $252$</td>
</tr>
<tr>
<td>8</td>
<td>$-23.744$ $764$ $117$ $789$ $411$ $159$ $214$ $855$ $577$</td>
<td>$-26.873$ $448$ $916$ $059$ $872$ $462$ $417$ $696$ $632$</td>
</tr>
<tr>
<td>9</td>
<td>$-19.294$ $545$ $287$ $177$ $598$ $192$ $875$ $999$ $744$</td>
<td>$-22.588$ $602$ $257$ $693$ $219$ $572$ $212$ $411$ $689$</td>
</tr>
<tr>
<td>11</td>
<td>$-9.920$ $787$ $813$ $040$ $383$ $111$ $510$ $031$ $236$</td>
<td>$-13.436$ $869$ $040$ $250$ $076$ $995$ $975$ $578$ $733$</td>
</tr>
<tr>
<td>12</td>
<td>$-5.135$ $296$ $289$ $270$ $774$ $002$ $472$ $610$ $815$</td>
<td>$-8.676$ $081$ $670$ $736$ $545$ $808$ $091$ $349$ $527$</td>
</tr>
<tr>
<td>13</td>
<td>$-0.473$ $351$ $957$ $855$ $431$ $951$ $969$ $001$ $641$</td>
<td>$-3.908$ $232$ $481$ $206$ $230$ $174$ $049$ $698$ $348$</td>
</tr>
</tbody>
</table>

$^a$ Reference [40]: $E_{0,0} = -49.457$ $788$ $728$ $082$ $579$ $670$ $330$ $458$ $705$ $16$; $E_{1,0} = -48.148$ $430$ $420$ $006$ $361$ $035$ $971$ $245$ $461$ $716$.

4. Some remarks on the numerical implementations

A main frame computer is employed for the computations, where the computer code in FORTRAN programming language is executed in quadruple precision arithmetic (30 digits) by truncating the results to 27–28 significant figures. Regardless of which potential function is in question, the diagonalization of an $8 \times 8$ matrix with the specified accuracy requires no more than a second whereas it consumes approximately 15 seconds when $N = 350$ which is the highest truncation size appearing in our tables.

By the transformation $\xi = (cr)^\alpha$ in (6), we have introduced two optimization parameters $c$ and $\alpha$, which considerably decrease the number of points $N$ used to obtain the desired accuracy. Actually, the first optimization parameter $c$ rescales the points on the half line while the second one $\alpha$ determines the behavior of the eigenfunction at big distances $r$. When the grid points are collected in the interval where the eigenfunction is nonzero by means of $c$ or the correct behavior of the eigenfunction is caught by the help of $\alpha$, the desired accuracy can be obtained with the smallest possible truncation order $N$.

Notice that an eigenfunction of the radial Schrödinger equation is a Gaussian type function. The procedure for choosing the optimum value of $c$ for Gaussian type functions is described in [31]. In short, it is based on the collection of grid points into an interval ($0, K$) so that none of them are wasted in the interval where the wavefunction is almost zero (see Fig. 2). So the optimum value of $c$ may be determined by the formula $c_{opt} \approx r_N / K$, where $r_N$ is the maximum zero of the $L^{(N+1)}_N(r)$, and $K$ is a point after which the eigenfunction is very close to zero. As a typical example, consider the potential $V(r) = r^2 + v_4 r^4$, where $v_4 > 0$. Clearly the required solution will be a function of $r^2$ (not $r$) so that we choose $\alpha = 2$ to this end. On the other hand, the selection of the parameter $c$ is closely related to the asymptotic behavior of the solution. To be specific, as $r \to \infty$ the solution behaves like $\exp(-r^2/2)$ when $v_4 \ll 1$ and $\exp(-\sqrt{v_4} r^{3/2})$ when $v_4 \gg 1$, respectively. Since the trial solution we propose in (7) decays like $\exp(-\xi/2) = \exp(-c^2 r^2/2)$ in this case where $\alpha = 2$, we choose $c = 1$.
for sufficiently small coupling constants such as $\nu A = 10^{-4}$ (see the first row of Table 1). However, when $\nu A = 10^4$, in order to imitate the true asymptotic behavior $\exp(-100r^2/3)$ of the exact solution, we choose $c = 9$ where we have employed the rule suggested by Tang in [31]. That is, we first observe that $\exp(-100r^2/3) \approx 10^{-20}$ when $r = K \approx 1.1$. On the other hand, the largest zero of the corresponding Laguerre polynomial $L_{10}^{(1/2)}(\xi)$ is $\xi_N \approx 105.1$ in terms of the transformed variable $\xi$, or we have $\tau_N \approx 10.2$ in terms of the original variable $r$. Therefore, we get $c_{\text{opt}} \approx \tau_N / K \approx 10.2/1.1 \approx 9.3 \approx 9$ (see the ninth row of Table 1).

On the other hand, in general, the optimum value of the second optimization parameter is $0 < \alpha_{\text{opt}} < 1$. For the lower states of the potentials having countably infinite discrete states besides continuous spectrum, such as ECP potential, $\alpha_{\text{opt}} = 1$. In contrast, for the higher states of such potentials we have $0 < \alpha_{\text{opt}} < 1$ since the first optimization parameter $c$ remains incapable to reflect the correct behavior of the eigenfunction. While $0 < \alpha_{\text{opt}} < 1$ we have $c_{\text{opt}} = 1$. Therefore, in any case, we do not have to chose two optimization parameters at the same time. Particularly, for the isotropic polynomial potentials in $r^2$, $\alpha_{\text{opt}} = 2$.

5. Conclusion

In this article, we basically employ the Laguerre polynomials $L_y^\nu(\xi)$ satisfying the equation $\xi y'' + (\gamma + 1 - \xi)y' = -\nu y$, as the trial solutions in (13) and (14) to approximate the solutions of the WPL equation of the form $\xi y'' + (\nu + 1 - \xi)y' + Q(\xi)y = 2\nu \frac{e}{\alpha} \xi^{-1} y$ in a pseudospectral picture, which is an alternative representation of the radial Schrödinger equation in (1). It is important to note that the appropriate $\gamma$ values in the Laguerre polynomials $L_y^\nu(\xi)$ is not selected arbitrarily, but appears naturally in the WPL equation as the parameter $\gamma = (2\nu + M - 2)/\alpha$ in (10).

Recall, in particular, that if $\alpha = 2$ the weight function $\xi^{-1}$ reduces to unity and we may view the WPL equation as the perturbed Laguerre equation, which allows us to cope with the radial Schrödinger equation for potentials $V(r)$ containing only the even powers of $r$. This type of problems were discussed in our previous article [2] so that just one specific example is presented here, i.e. $V(r) = r^2 + v_3 r^4$ in (53). More generally, the present algorithm with $\alpha \neq 2$ for the WPL equation is now suitable for a larger class of potentials illustrated in Section 3, whose Taylor series expansions contain both even and odd powers of $r$.

The method is quite general in the sense that many other quantum mechanical eigenvalue problems, for example, with Gaussian, Morse, Deng–Fan, Manning–Rosen and Rosen–Morse potentials, can be handled without any modification. However, we do not include numerical results for these potentials in order not to overfill the content of the paper with tabular material anymore.

References