Lagrange-mesh solution of the Schrödinger equation in generalized spherical coordinates

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Abstract
The solution of the multi-dimensional Schrödinger equation in the generalized spherical coordinates is constructed in the Lagrange-mesh method. Laguerre and Jacobi meshes are used to construct matrix elements for the generalized Hamiltonian. The matrix elements are functions of quadrature abscissas and involve few free parameters for each angular dimension. A ring-shaped non-central separable potential, and a system of four linearly coupled anharmonic oscillators are used for illustrations of the efficiency and accuracy of the method. The numerical solutions involving eigenfunctions of the kinetic energy operator display the typical slow convergence with the accuracy improving as the Lagrange-mesh bases size increases. The Lagrange-mesh solutions converge to the exact solution when the parameters of the matrix elements are chosen appropriately.

1. Introduction
Theoretical studies of quantum mechanical systems rely on solutions to quantum mechanical equations for the systems to extract theoretical predictions of properties of the systems. Several numerical methods have been, and continue to be, developed to generate accurate solutions to the Schrödinger equation efficiently, see [1–4] for example. However, many of the methods become challenged when the dimensionality of the problem increases. The Lagrange-mesh method [5–7] was shown to have several advantages over many of the methods. This method is a variational method that employs the Lagrange basis functions defined on numerical quadratures to construct variational solutions to quantum mechanical equations. Compared to other numerical methods, the method was shown to generate simpler, faster and more accurate solutions for different quantum mechanical systems [8–11], and is not restricted to one-dimensional or separable problems. In the present work the Lagrange-mesh method is explored for the numerical solution of the Schrödinger equation in more than three dimensions, in spherical coordinates without directly using the usual spherical harmonics. The regularized Lagrange-Jacobi functions employed and, therefore, the associated kinetic energy matrix elements are characterized by free parameters that can be tuned to accelerate the convergence of the solution.
solution. In this work, the free parameters are chosen consistent with the eigenfunctions of the angular kinetic energy operator. The discussion of an effective procedure for tuning the free parameters is postponed to beyond this paper. Until now, these matrix elements had not been truly tested for efficiency and accuracy in practical applications.

This paper is organized as follows. Section 2 presents an outline of the \(D\)-dimensional Schrödinger equation in spherical coordinates. Principles of the Lagrange-mesh method and the associated matrix elements of the Hamiltonian for the Schrödinger equation are discussed in section 3. Illustrative applications of the matrix elements are discussed in section 4. The central harmonic oscillator and the Coulomb potential in six dimensions, four linearly coupled anharmonic oscillators, and a double ring-shaped non-central separable potential are considered for this purpose. Conclusions are given in section 5.

2. The Schrödinger equation in many dimensions

The Schrödinger equation in several dimensions is widely discussed in the literature, see for example [17, 18]. This equation, for a particle of mass \(m\) in a potential field \(V(\vec{r})\), in a \(D\)-dimensional configuration space, has the form (\(\hbar = m = 1\))

\[
-\frac{1}{2} \nabla_D^2 + V(\vec{r}) \Psi(\vec{r}) = E \Psi(\vec{r})
\]

where \(E\) is the energy, \(\Psi(\vec{r})\) the wave function, and \(\vec{r}\) the position vector in \(D\) dimensions of the particle. This vector is characterized by Cartesian components \([x_1, x_2, \ldots, x_D]\) and generalized spherical components \([r, \theta_1, \theta_2, \ldots, \theta_{D-1}]\), which are related by [17]

\[
\begin{align*}
x_1 &= r \cdot \cos \theta_1 \cdot \sin \theta_2 \cdots \sin \theta_{D-1} \\
x_2 &= r \cdot \sin \theta_1 \cdot \sin \theta_2 \cdots \sin \theta_{D-1} \\
x_3 &= r \cdot \cos \theta_2 \cdot \sin \theta_3 \cdots \sin \theta_{D-1} \\
x_4 &= r \cdot \cos \theta_3 \cdot \sin \theta_4 \cdots \sin \theta_{D-1} \\
&\vdots \\
x_{D-1} &= r \cdot \cos \theta_{D-2} \cdot \sin \theta_{D-1} \\
x_D &= r \cdot \cos \theta_{D-1},
\end{align*}
\]

for \(D \geq 2\). The generalized spherical coordinates are defined in the domain \(r \in [0, \infty), \theta_1 \in [0, 2\pi]\) and \(\theta_i \in [0, \pi]\) for \(i = 2, 3, \ldots, D - 1\). Equation (1) is solved for \(E\) and \(\Psi(\vec{r})\) in a domain determined mainly by the potential.

In the Cartesian coordinates and in the spherical coordinates, the Laplace operator has the form [17]

\[
\nabla_D^2 = \sum_{i=1}^{D} \frac{\partial^2}{\partial x_i^2} = \frac{\partial^2}{\partial r^2} + \frac{D-1}{r} \frac{\partial}{\partial r} - \frac{\hat{L}^2(\Omega_{D-1})}{r^2}
\]

where \(\hat{L}^2(\Omega_{D-1})\) is the general or total angular operator and \(\Omega_{D-1} = \{\theta_1, \theta_2, \ldots, \theta_{D-1}\}\). This angular operator is written in the compact iterative form [17]

\[
\hat{L}^2(\Omega_{D-1}) = -\frac{\partial^2}{\partial \theta^2_{D-1}} - (D-2) \cot \theta_{D-1} \frac{\partial}{\partial \theta_{D-1}} + \frac{\hat{L}^2(\Omega_{D-2})}{\sin^2 \theta_{D-1}},
\]

where \(\Omega_{D-2} = \{\theta_1, \theta_2, \ldots, \theta_{D-2}\}\). The iteration procedure, over \(k\), say, is carried out using the relation

\[
\hat{L}^2(\Omega_k) = -\frac{\partial^2}{\partial \theta^2_k} - (k-1) \cot \theta_k \frac{\partial}{\partial \theta_k} + \frac{\hat{L}^2(\Omega_{k-1})}{\sin^2 \theta_k},
\]

starting from \(k = 2\), with \(\hat{L}^2(\Omega_1) = -\partial^2/\partial \theta^2_1\). The operator (4) has known eigensolutions which, as shown later, are readily constructed. Based on the structure of the operators in (3) with (4), it may be argued that the Laplacian in Cartesian coordinates appears less involved, and seem easier to treat numerically, than in spherical coordinates.

The objective of this work is to solve (1) numerically in spherical coordinates. Bound-state solutions to this equation for a given potential \(V(\vec{r})\) are determined by the Dirichlet boundary conditions as well as the square-integrability condition.
\[
\int_\tau \Psi^*(\vec{r}) \Psi(\vec{r}) \, d\vec{r} < \infty, \tag{6}
\]
where \(\Psi^*\) denotes the complex conjugate of \(\Psi\) and \(\tau\) the volume of integration with
\[
d\vec{r} = r^{D-1} \, dr \prod_{k=1}^{D-1} (\sin \theta_k)^{k-1} \, d\theta_k \tag{7}
\]
as the volume element. The presence of the first order derivatives in the Laplacian (3) introduce non-unique non-zero initial conditions on the wave function. To eliminate such first order derivatives in the wave function, the factorization
\[
\Psi(\vec{r}) = r^{-(D-1)/2} \prod_{k=1}^{D-1} (\sin \theta_k)^{-(k-1)/2} \, \Phi(\vec{r}) \tag{8}
\]
is introduced, where the auxiliary function \(\Phi(\vec{r})\) satisfies the Dirichlet boundary conditions. This auxiliary function also satisfies the differential equation
\[
\left\{ -\frac{1}{2} \frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \left( \hat{L}^2(\Omega_{D-1}) + \frac{\rho_k}{4} \right) + V(\vec{r}) \right\} \Phi(\vec{r}) = E \, \Phi(\vec{r}) \tag{9}
\]
where the corresponding angular operator is constructed with
\[
\hat{L}^2(\Omega_k) = -\frac{\partial^2}{\partial \theta_k^2} - \frac{(k-1)^2}{4} + \frac{1}{\sin^2 \theta_k} \left[ \hat{L}^2(\Omega_{k-1}) + \frac{\rho_k}{4} \right], \tag{10}
\]
also from \(k = 2\) with \(\hat{L}^2(\Omega_2) = \hat{L}^2(\Omega_1)\), and \(\rho_k = (k-1)(k-3)\). Note that the constant terms in (10) at each iteration step for \(k < D - 1\) have the form \(\rho_k - (k - 2)^2/4 = -\frac{1}{4}\). The same finding holds at the final step \(k = D - 1\) only when the total Laplacian is considered. The eigenvalues of \(\hat{L}^2(\Omega_k)\) are readily constructed in terms of the Jacobi functions which are more advantageous when considering (9) with a general potential \(V(\vec{r})\). The eigenfunctions of the Laplace operator are readily developed from the iterative structure of the operator. Note that the operator is separable in all the coordinates, which justifies a factorization of the auxiliary wave function in the form
\[
\Phi(\vec{r}) = R(r) \prod_{j=1}^{D-1} \Theta_j(\theta_j) \tag{11}
\]
where \(R(r)\) is the radial function and \(\Theta_j(\theta_j)\) the angular functions. As a result, the differential equations for these functions, developed from (3) with \(V(\vec{r}) = 0\), are separable and have the form
\[
-\frac{\partial^2}{\partial \theta_1^2} \Theta_1(\theta_1) = \sigma_1^2 \Theta_1(\theta_1) \tag{12}
\]
\[
-\frac{\partial^2}{\partial \theta_k^2} + \frac{\sigma_{k-1}^2 - \frac{1}{4}}{\sin^2 \theta_k} \Theta_k(\theta_k) = \sigma_k^2 \Theta_k(\theta_k); \quad k \in [2, D - 1], \tag{13}
\]
\[
-\frac{1}{2} \frac{\partial^2}{\partial r^2} - \frac{\sigma_{D-1}^2 - \frac{1}{4}}{r^2} R(r) = E \, R(r), \tag{14}
\]
where \(\sigma_k^2\) are the separation constants. These three equations, the solutions of which are known, together describe the motion of a free particle. For a particle in a central potential only the radial equation (14), and its solution, differ from the free-particle case.

Focusing on the angular equations, the differential equation for \(\theta_1\) is immediately solved to obtain
\[
\Theta_1(\theta_1) = (2 \pi)^{-1/2} \exp (\pm i \sigma_1 \theta_1); \quad \sigma_1 = 0, 1, 2, \ldots \tag{15}
\]
All the differential equations (13) have a form that is consistent with the Pöschl-Teller Hamiltonian [19]. Such a Hamiltonian admits exact solutions that involve Gegenbauer functions, which are a special case of the Jacobi functions. For this reason, and noting that (13) have singularities at \(\theta_k = 0\) and \(\theta_k = \pi\), the solutions to (13) can be shown to have the form
\[
\Theta_k(\theta_k) = (\sin \theta_k)^{\alpha + \frac{1}{2}} \, C_{\alpha}^{\alpha + \frac{1}{2}}(\cos \theta_k) \tag{16}
\]
for all \(k > 1\), where \(C_{\alpha}^{\alpha + \frac{1}{2}}(\cos \theta_k)\) are Gegenbauer polynomials of order \(\ell_k\). It, then, follows that the corresponding eigenvalues are given by
\[ \sigma_k^2 = \left( \ell_k + \sigma_{k-1} + \frac{1}{2} \right)^2; \quad \ell_k = 0, 1, 2, \ldots, \] \tag{17}

which defines the separation constants. It can be inferred from this expression that the separation constants obey the recurrence relation

\[ \sigma_k = \ell_k + \sigma_{k-1} + \frac{1}{2} \] \tag{18}

with the corresponding integers \( \{ \ell_{k-1}, \ell_{k-2}, \ldots, \ell_1 \} \) restricted to the domains \( \ell_{k-1} \in [0, \ell_k] \) for \( k \in [3, D - 1] \), and \( \ell_1 = \sigma_1 \in [-\ell_2, +\ell_2] \) \[17\]. Note that \( C_\theta^{\alpha+\frac{1}{2}}(\cos \theta) \propto P_\ell^\alpha(\cos 2\theta) \) where the latter are Jacobi polynomials.

Other solutions to (13) can be derived by considering the symmetry of the equations about the centers of the angular domains. Because of this symmetry, the equations may be solved considering only one segment of each domain and then adapt the results to the entire domain. Such a treatment is also necessary when solving (13) with potentials that have singularities that segment the angular domains \[19, 20\]. This approach leads to general solutions of the form

\[ \Theta_k(\theta_i) = (\sin \theta_k)^{\alpha+\frac{1}{2}}(\cos \theta_i)^{\alpha+\frac{1}{2}} P_\ell^\alpha(\cos 2\theta_k) \] \tag{19}

where \( \sigma_k \) are constants. These constants are determined consistent with the general Pöschl-Teller Hamiltonian \[19\]. The eigenvalues corresponding to (19) are

\[ \sigma_k^2 = (2 \ell + \sigma_{k-1} + \sigma_k + 1)^2; \quad \ell_k = 0, 1, 2, \ldots, \] \tag{20}

with the applicable recurrence relations

\[ \sigma_k = 2 \ell + \sigma_{k-1} + \sigma_k + 1 \quad \text{and} \quad \ell_k = \ell_{k-1}, \] \tag{21}

for \( k \in [2, D - 1] \). Therefore, solutions to (1) with general potentials may involve combinations of (16) and (19). However, the relation (16) may be more suited for domains in which the potential is even. Note that the kinetic energy operator is an even function of all the angles \( \theta_i (i > 1) \).

Illustrative applications of the two solutions discussed above can be found in the literature. The \( D = 3 \) case, the solution of which involve \( \Theta_2(\theta_2)\Theta_1(\theta_1) \) usually referred to as the ring-shaped functions, is discussed in \[21\], while several \( D \geq 3 \) cases can be found in \[19, 20\]. The construction of the numerical solutions \( \Theta_k(\theta_k) \) to (13) in the Lagrange-mesh method is discussed in the next section. For this purpose, it should be noted that when \( V(r) = 0 \) or \( V(r) \) is separable, then (1) is also separable.

3. The Lagrange-mesh matrix elements

Lagrange-mesh bases functions are constructed so as to generate simple forms of matrix elements for common mathematical operators. A set of \( N \) Lagrange functions \( f_j(z) \) are defined on a mesh \( z_j (j = 1, 2, 3, \ldots, N) \) in a domain \( [a, b] \) by the properties \[6, 7\]

\[ \langle f_j(z) | V(z) | f_i(z) \rangle = V(z_i) \delta_{ij} \] \tag{22}

\[ \langle f_j(z) | f^{(k)}(z) \rangle = \lambda_j^{1/2} f_j^{(k)}(z_i) \] \tag{23}

\[ \langle f_j(z) | f_i(z) \rangle = \delta_{ij} \] \tag{24}

where the Dirac notation denoted integration (here Gauss approximated), \( V(z) \) a scalar function and \( f^{(k)} = d^k f dz^k \). For a quadrature rule defined by a weight function \( w(z) \), the mesh is given by the quadrature abscissas and weights \( [z_i, w_i] \) and \( \lambda_i = w_i / w(z) \). When the domain \( [a, b] \) is scaled by some factor \( h \), the properties will also depend on \( h \). These properties hold for all Lagrange functions \[2\].

Lagrange-Laguerre functions employed in this work are the modified Lagrange-Laguerre \[6\] and the Lagrange-Laguerre functions regularized by \( r^{1/2} \), both defined in the interval \( [0, \infty) \). The latter functions have the form

\[ R_M^\sigma(r) = \frac{(-1)^j}{\sqrt{h_M^\sigma}} \frac{L_M^\sigma(r)}{r^{(\sigma+1)/2}} \frac{e^{-r/2}}{r}, \] \tag{25}

where \( h_M^\sigma \) is the normalization coefficient of the Laguerre polynomials \( L_M^\sigma(r) \) of order \( M \). These functions are defined on the mesh \( \eta_j (j = 1, \ldots, M) \), which are the roots of the polynomial \( L_M^\sigma(r) \). The matrix elements of the operator \( -d^2 / dr^2 \) at the Gauss approximation have the exact form as those given in \[6\] for a regularization by \( r^{1/2} \). The Jacobi mesh is defined by \( N \) zeros \( z_i \) of the Jacobi polynomials \( P_M^{\alpha, \beta}(z) \) of order \( N \) and characterized by the weight function \( w(z) = (1 - z)^{\alpha}(1 + z)^{\beta} \) with parameters \( \{\alpha, \beta\} \geq -\frac{1}{2} \). This mesh is then used to construct regularized Lagrange-Jacobi functions \[7\].
\[ U_j(z) = (-1)^{N-j} \left[ \frac{w(z)(1-z^2)^\mu}{K_N^{a,b}(1-z^2)^{\mu-1}} \right]^{1/2} P_N^{a,b}(z) / (z - z_j) \]  

(26)

where \( \mu \) is the regularizing parameter, \( b^{a,b}_N \) the normalizing constant of the Jacobi polynomials and \( K_N^{a,b} = 2 N + \alpha + \beta + 1 \). These functions are defined in the interval [\(-1, 1\)]. Other regularized Lagrange functions defined on meshes based on other classical orthogonal polynomials that are related to the Jacobi polynomials can be deduced from (26). The matrix elements of the Jacobi differential operator, constructed with these approximations, are given in [7].

To use the Lagrange-Jacobi function (26) in the construction of the solution to (10), the angular domains are first mapped onto the domains \( u_k \in [-1, 1] \). This can be achieved through a number of transformations, such as \( u_k = \cos n_k \theta_k \) where \( n_k \) are constants related to the periodicity of the potential. The exact form of the transformations, or values of the \( n_k \), are determined by convenience, related mainly to the angular domain of the potential to be mapped. To simplify the discussion, without loss of generality, the transformations \( u_k = \cos n_k \theta_k \) are considered, and the more simple cases of \( n_k = 1 \) and \( n_k = 2 \) used. For these cases, one readily shows that

\[
\frac{d}{d\theta_k} = -n_k \sqrt{1 - u_k^2} \frac{d}{du_k} \quad \text{and} \quad \frac{d^2}{d\theta_k^2} = n_k^2 \left[ (1 - u_k^2) \frac{d^2}{du_k^2} - u_k \frac{d}{du_k} \right]
\]

(27)

and \( \sin^2 \theta_k = (1 - u_k^{2/n_k}) / n_k \). Applying this transformations on the operator (5) one obtains

\[
\hat{L}_k^2 = -n_k^2 \hat{T}_u + \frac{n_k \hat{T}_{k-1}^2}{1 - u_k^{2/n_k}}
\]

(28)

where \( \hat{T}_u \) are \( k \)-dependent. Using the same transformations on (10) leads to

\[
\hat{L}_k^2 = -n_k \hat{T}_u - \frac{(k - 1)^2}{4} + \frac{n_k}{1 - u_k^{2/n_k}} \left[ \hat{L}_{k-1}^2 + \frac{\hat{D}_k}{4} \right]
\]

(29)

with \( \hat{L}_k^2 = -n_k \hat{T}_u \), where the operators

\[
\hat{T}_u = (1 - u^2) \frac{\partial^2}{\partial u^2} - u \frac{\partial}{\partial u}
\]

(30)

are independent of \( k \). This paper focuses on the operator (29) because of its relative simplicity. The operator (30) is related to the Chebyshev polynomials of the first kind, which are a special case of the classical Jacobi polynomials [22]. Note that the transformation \( u = \cos \theta \) necessarily involve (16) and (18), whereas \( u = \cos 2\theta \) requires the use of (19) and (21).

Note that the differential operators in (29) are likely to have the same form at each iteration step. Therefore, the matrix elements of the operator (29) would involve similar, if not the same, \( T_u \) as, at result, may be calculated only once. The matrix elements \( T_u^m \) for the operator (30), constructed with the regularized Lagrange-Jacobi functions \( U_j(z) \), are given in [7]. Using any of the classical orthogonal polynomials related to the Jacobi polynomials as the Lagrange functions requires only the appropriate choice of the values for \( (\alpha, \beta) \) in (26). These matrix elements are then used to construct iteratively, from \( k = 1 \) to \( k = D - 1 \), the matrix elements of the operator (29).

The solution to (9) is constructed by expanding the reduced wave function \( \Phi(r, \vec{u}) \), \( \vec{u} = \{ u_1, u_2, \ldots, u_{D-1} \} \), in the Lagrange functions, of basis size \( N_k \), over each coordinate as

\[
\Phi(r, \vec{u}) = \sum_{i_1=1}^{N_1} \cdots \sum_{i_{D-1}=1}^{N_{D-1}} A_{i_1 \cdots i_{D-1}} R_{i_1}(r) \prod_{k=1}^{D-1} U_k(u_k)
\]

(31)

where \( R_{i_1}(r) \) are the Lagrange-Laguerre functions [6], \( U_j(u_k) \) the Lagrange-Jacobi functions (26) and \( A_{i_1 \cdots i_{D-1}} \) the variational parameters. Minimizing the functional \( \langle \Phi | [H - E] | \Phi \rangle \) with respect to the variational parameters leads to the eigenvalue problem

\[
\sum_{j_1=1}^{N_1} \cdots \sum_{j_{D-1}=1}^{N_{D-1}} \left[ H^0_{j_1 \cdots j_{D-1}} + V(r_{j_1}, \vec{u}_{j_1}) \prod_{k=0}^{D-1} \delta_{j_k l_k} \right] A_{j_1 \cdots j_{D-1}} = E A_{j_1 \cdots j_{D-1}}
\]

(32)

for the parameters, where the abbreviation \( \vec{j} = \{ j_1, j_2 \cdots j_{D-1} \} \) is used. The matrix elements for the kinetic energy operator are given by

\[
H^0_{j_1 \cdots j_{D-1}} = -\frac{1}{2} \left[ T^0_{j_1 \cdots j_{D-1}} \prod_{k=1}^{D-1} \delta_{j_k l_k} - \frac{1}{r^2} \left( \hat{L}^2_{D-1} \right)_{j_1 \cdots j_{D-1}} \right]
\]

(33)
where the angles-related elements have the form
\[
(L_k^{\theta})_{jj'} = -\left[n_k^2 T_{\theta_k}^{\theta_{jj'}} + \frac{(k - 1)^2}{4} \delta_{\theta_k^{\theta_{jj'}}} \right] \prod_{k=0}^{D-1} \delta_{\theta_k^{\theta_{jj'}}} + \frac{m_k}{1 - (u_k)^2/\rho^2} \left[(L_k^{\theta})_{jj'} + \frac{\rho_k}{4} \delta_{\theta_k^{\theta_{jj'}}} \right] \prod_{k=0}^{D-1} \delta_{\theta_k^{\theta_{jj'}}}\]
(34)

The symbol \( \prod' \) signifies the exclusion, from the product, of the delta function corresponding to the iteration step index. The elements \( T_{\theta_k}^{\theta_{jj'}} \) are given in [7] while \( T_{\theta_k}^{\theta_{jj'}} \) are given by a suitable Lagrange-Laguerre mesh [6]. It can be said that the elements \( H_{\theta_k}^{\theta_{jj'}} \) are simple and easy to construct. It must be emphasized that the elements \( H_{\theta_k}^{\theta_{jj'}} \) and \( V(\theta_k, u_j) \) are the Gauss quadrature approximations, respectively, of the kinetic and potential energy matrix elements. These approximations introduce inherent integration errors in the numerical results [23]. Instructive illustrations of the use and accuracy of the matrix elements (32) are presented in the next section.

4. Illustrations

The following illustrations of the application of the Lagrange-mesh matrix elements involve the instructive Coulomb and harmonic oscillator potentials. Only the Gauss approximations of the matrix elements for the Hamiltonian of the problems are used in all the calculations presented. All the Gaussian quadrature abscissas and weights used are determined with accuracy no better than 3 \( \times \) \( 10^{-14} \). It is noted that the matrix elements involve free parameters, three at each iteration step in the construction of the total Hamiltonian matrix. The values of these parameters are determined as follows. A closer look at (26), and comparing with (19), suggests that all the angular functions may be set to \( \frac{1}{2} \). As already indicated, all the \( \beta_k \) may be fixed depending on whether (16) or (19) is used. Note that the recurrence relations (18) and (21) also determine the parameter \( \sigma_{D-1} \) of the Laguerre mesh. Using the initial values \( \alpha_1 = \beta_1 = -\frac{1}{2} \), all the parameters are determined. These initial values correspond to the Chebyshev functions of the first kind, which are the eigenfunctions of (30) with eigenvalues corresponding to (15). However, the parameters \( (\alpha_k, \beta_k) \) may be optimized to accelerate the convergence of the bases expansions.

4.1. Central harmonic oscillator and Coulomb potentials

Simple, yet instructive, applications of the matrix elements presented are provided by the central harmonic oscillator and Coulomb potentials. The Schrödinger equations with these potentials can be solved exactly [20]. The central harmonic oscillator (ho) and Coulomb (C) potentials have the forms
\[
V_{ho}(r, \Omega_{D-1}) = \frac{1}{2} r^2; \quad r \in [0, \infty)
\]
(35)
\[
V_{C}(r, \Omega_{D-1}) = -\frac{\eta}{r}; \quad r \in (0, \infty)
\]
(36)
in \( D \)-dimensions, where \( \eta \) is a constant. The eigenvalues of the potentials are given by
\[
E_{\nu_0, \ldots, \nu_{D-1}}^{ho} = \sum_{i=0}^{D-1} \left(n_i + \frac{1}{2}\right), \quad E_{\nu_0, \ldots, \nu_{D-1}}^{C} = -\frac{2 \eta^2}{(2 \nu_0 + \sigma_{D-1} + 1)^2},
\]
(37)
where \( n_i = 0, 1, 2, \ldots \) for all \( i \) and \( \sigma_{D-1} \) is the parameter for the associated Laguerre polynomials which are part of the analytical solution to the central Coulomb problem [20]. This parameter coincides with that of the Laguerre mesh for this problem. The Schrödinger equations for these potentials are solved in six dimensions, as a one-dimensional radial problem considering only (14), and directly as a six-dimensional problem using (32). For the one-dimensional treatment, the exact eigenvalues of the five-dimensional angular equations (13) and (15) are used. The difference in the accuracy of the results from the two solutions may give an indication of the errors introduced by the matrix elements \( T_{\theta_k}^{\theta_{jj'}} \).

The modified Laguerre (in \( r^2 \)) [6] and the Jacobi meshes were used for the harmonic oscillator whereas the regularized (by \( r^{1/2} \)) Laguerre and the Jacobi meshes were used for the Coulomb potential. Since the angular kinetic energy operator is an even function of all the angles \( \theta_k (i > 1) \), the transformations \( u_k = \cos 2\theta_k \) was employed in both the harmonic oscillator and the Coulomb cases. The parameters of the Lagrange-Jacobi functions were chosen as explained earlier. The accuracy of the calculated energies \( E_{\nu}^{ho} \) is determined as the relative difference.
The error differences are, where $a_i$ are constants. This potential leads to a separable Schrödinger equation that admits exact solutions with eigenvalues $E_n \equiv \sqrt{n+1}$. It can be seen, in the table, that the energies for the two potentials are reproduced to machine accuracy in the oscillator and Coulomb potentials, obtained with bases sizes $N = N_0 \times N_0^{D-1}$ where $N_0 = 3$ for the oscillator and $N_0 = 30$ for the Coulomb potential. The radial domain for the Coulomb potential was scaled by a parameter $h = 1/(\sigma_D - 1 + 1)$ to focus on the ground state [6], while the domain for the oscillator was unscaled ($h = 1$). The same basis size $N_0$ for the radial functions was used in both the one-dimensional and the six-dimensional treatments.

It can be seen, in the table, that the energies for the two potentials are reproduced to machine accuracy in the one-dimensional treatment. In the six-dimensional treatment the results are reproduced to close to machine accuracy with the degeneracy of the states correctly determined. In general, the accuracy is the same for all the calculated states and appears to be independent of the bases size in the case of the oscillator. The maximum error in the results of the direct six-dimensional treatment is $\epsilon_n \sim 10^{-12}$ in the case of the oscillator potential, which is an order of magnitude greater that the error in the one-dimensional treatment. The error difference in the two treatments is two orders of magnitude in the case of the Coulomb potential. However, note that in the Coulomb case a larger radial basis was required to generate results of reasonable accuracy. This difference in the errors can be attributed to the use of the matrix elements $T^2_{ab}$ in the solution of the problems. The error differences are, however, very small considering the dimensional size of the problem. The results of the Coulomb potential display a similar trend in accuracy as the oscillator potential except that, in this case, the accuracy deteriorates as the level of the states increases. Errors in the results of problems involving only central potentials are expected to display a similar trend.

### 4.2. Ring-shaped potential

An interesting application is provided by a more practical problem of a non-central ring-shaped potential coupled to a central Coulomb potential in three-dimensions ($D = 3$). The potential has the form [24]

$$
V(r, \Omega_2) = \frac{1}{2} \frac{a_1 + a_2 \sin^2 \theta_2 + a_3 \sin^4 \theta_2}{r^2 \sin^2 \theta_2 \cos^2 \theta_2} \frac{a_0}{r},
$$

$$
r \in (0, \infty), \quad \theta_2 \in (0, \pi) \quad \text{and} \quad \theta_1 \in [0, 2 \pi]
$$

where $a_i$ are constants.
Table 2. The convergence of the calculated energies for the first two states of the potential in (42) with the basis size $N_2$ corresponding to $u_2$ ($N_0, N_1) = (30, 1)$.

| $N_2$ | $(\alpha_2, \beta_2)$ | $-E_{100}$ | $-E_{110}$ |
|-------|---------------------|------------|------------|
| 10    | $(0, -0.5)$         | 0.104 21   | 0.069 07   |
|       | $(1.5, 1.5)$        | 0.104 129  | 0.069 032  |
| 20    | $(0, -0.5)$         | 0.104 157  | 0.069 047  |
|       | $(1.5, 1.5)$        | 0.104 146  | 0.069 041  |
| 30    | $(0, -0.5)$         | 0.104 152  | 0.069 044  |
|       | $(1.5, 1.5)$        | 0.104 147  | 0.069 042  |
| 40    | $(0, -0.5)$         | 0.104 150  | 0.069 043  |
|       | $(1.5, 1.5)$        | 0.104 148  | 0.069 042  |
| Exact | $(\sqrt{2}, 1.5)$   | 0.104 149  | 0.069 042  |

$$E_{n_0, n_1} = -\frac{2a_0^2}{[2n_0 + 2\sqrt{\Lambda_{n_0 n_1}^2 - a_0} + 1]^2}$$

(40)

where

$$\Lambda_{n_0 n_1} = 2n_2 + \sqrt{n_1^2 + a_1 + \frac{1}{4} + a_1 + a_2 + a_3 + 1}.$$  

(41)

The Schrödinger Hamiltonian with this potential has singularities at 0, $\frac{\pi}{2}$ and $\pi$ in the $\theta_2$ domain. Therefore, the $\theta_2$ domain is mapped onto $[-1, +1]$ using the transformation $u_2 = \cos 2\theta_2$, which casts the potential in the form

$$V(r, u_1, u_2) = \frac{1}{2} \frac{4a_1 + 2a_2(1 - u_2) + a_3(1 - u_2)^2}{r^2(1 - u_2^2)} - \frac{a_0}{r},$$

(42)

$r \in (0, \infty)$, $u_2 \in (-1, +1)$ and $u_1 \in [-1, +1]$. The regularized Laguerre and the Jacobi meshes were used to solve the Schrödinger equation for this potential. The potential parameters were set to $a_0 = a_1 = 2$ and $a_2 = -a_3 = -\frac{1}{4}$ to generate a symmetric Pöschl-Teller potential.

The values of the parameters $(\alpha_3, \beta_3)$ for the elements $T_k^3$ and $\sigma_3D_{-1}$ must be specified. Noting that the potential is independent of $u_3$, one must have $\alpha_1 = \beta_1 = -\frac{1}{2}$, as explained earlier. The independence of the potential from $u_1$ also implies that the size of the basis corresponding to $u_1$ may not affect the results significantly. The optimal values of $(\alpha_2, \beta_2)$ are not readily deduced and are, as a result, determined by trial-and-error [7]. The trial values $(\alpha_2, \beta_2) = (0, -\frac{1}{2})$ and $(\alpha_2, \beta_2) = (\frac{1}{2}, \frac{3}{2})$ are tested for convergence. The former set of values corresponds to the case of central potentials while the latter corresponds to a symmetric Pöschl-Teller in $u_2$. The radial domain was treated as in the case of the central Coulomb potential, where the radial basis was set to $N_0 = 30$, however, here the scaling parameter is set to $\hbar = 1$. Since the basis size corresponding to $u_1$ could also be fixed, only the $u_2$ basis size $N_2$ was varied. The convergence of the energies, with increasing $N_2$, for the first two states of the potential are shown in table 2. As can be seen, in the table, the accuracy of the calculated energies change from relative errors of $\sim 10^{-4}$ involving $N_2 = 10$ basis functions to $\sim 10^{-6}$ with $N_2 = 40$ basis functions. This signifies slow convergence of the numerical solutions, which is characteristic of the eigenfunction expansion approach [25], determined with both sets of parameters. It also appears that the results for one set of the trial values of $(\alpha_2, \beta_2)$ converge from above while those of the other converge from below, though at comparable rates, to the exact energies. This trend can be used to tune the trial values of $(\alpha_2, \beta_2)$ to improve convergence. Recalling that the parameter $\sigma_3D_{-1}$ depends on $(\alpha_2, \beta_2)$, the variation of the radial basis size $N_0$ may affect the accuracy of the results.

4.3. Linearly coupled anharmonic oscillators

Another interesting application is offered by the non-central and non-separable system of four linearly coupled anharmonic oscillators. The potential for this system in the generalized spherical coordinates has the form

$$V(r, \Omega_3) = \frac{1}{2}r^2 + \frac{1}{3}r^3 \sin \theta_3 \cos \theta_3 \sin \theta_2 \cos \theta_2 g(\theta_1)$$

$$+ \frac{1}{7}r^2 \sin^2 \theta_3 \sin \theta_2 \sin \theta_1 \cos \theta_1 \cos \theta_2 g(\theta_1);$$

$$r \in [0, \infty), \quad \theta_3, \theta_2 \in [0, \pi] \quad \text{and} \quad \theta_1 \in [0, 2\pi],$$

(43)

where $g(\theta_1) = \sin \theta_1 + \cos \theta_1$. The Schrödinger equation for this potential is non-separable but has exact solutions with eigenvalues [26].
The Lagrange-mesh method was used to construct numerical solutions to the multi-dimensional Schrödinger equation in spherical coordinates. The Laguerre mesh was used to treat the radial domain while Jacobi meshes were used for all the parametrized angular domains. Standard Laguerre-mesh matrix elements were used for the radial component, while the newly developed Jacobi-mesh matrix elements were used for the parametrized angular components of the kinetic energy operator. Simple, yet instructive, applications involving central, non-central separable, and non-central non-separable Coulomb as well as harmonic oscillator-type potentials in three, four and six dimensions were treated. Results for the Lagrange-mesh solutions of the two central potentials are shown in Table 3. The variation of the calculated energies, with the bases size, for the first two excited states of the potential (45).

Table 3. Variation of the calculated energies, with the bases size, for the first two excited states of the potential (45).

| $N_i$ | Set | $E_0$ | $E_1$ | $E_2$ |
|------|-----|-------|-------|-------|
| 6    | a   | 1.919 | 2.708 | 3.503 |
|      | b   | 1.9319| 2.7355| 3.5061|
|      | c   | 1.9298| 2.7552| 3.3462|
| 8    | a   | 1.920 | 2.731 | 3.527 |
|      | b   | 1.9320| 2.7411| 3.5298|
|      | c   | 1.9318| 2.7489| 3.3462|
| 10   | a   | 1.921 | 2.727 | 3.537 |
|      | b   | 1.9319| 2.7435| 3.54010|
|      | c   | 1.931851| 2.748382| 3.346080|
| Exact|     | 1.931851| 2.748348| 3.346065|

\[ E_{n_1n_2n_3n_4} = \sum_{i=1}^{4} \sqrt{1 + a_i (n_i + \frac{1}{2})} \text{,} \quad n_i = 0, 1, 2, \ldots, \] (44)

where $a_1 = 1, a_2 = a_3 = a_4 = -1/3$. Since the angular kinetic energy operators have singularities at the boundaries and the potential has none, the transformations $u_i = \cos \beta_i$ are used to map the entire domain of each angular variable on $(-1, +1)$. With this transformation, the potential assumes the form

\[ V (r, u_1, u_2, u_3) = \frac{1}{2} r^2 + \frac{1}{2} r^2 u_3 \sqrt{1 - u_2^2} \left[ u_0 + \eta_0 \sqrt{1 - u_2^2} \right] \]

\[ + \frac{1}{3} r^2 (1 - u_2^2) \sqrt{1 - u_2^2} \left[ \eta_1 u_0 + \eta_0 \sqrt{1 - u_2^2} \right]; \quad r \in [0, \infty) \quad \text{and} \quad u_0 \in (-1, +1). \] (45)

where

\[ \eta_0 = u_0 \sqrt{1 - u_2^2} \quad \text{and} \quad \eta_1 = u_0 + \sqrt{1 - u_2^2}. \]

The modified Laguerre and the Jacobi meshes were used to solve the Schrödinger equation for this potential, and the radial domain was unscaled ($h = 1$).

The potential does not have symmetries that are as readily noticeable as in Cartesian coordinates. As a result, optimal values of all the parameters ($\alpha_2, \beta_1$) and $\sigma_{D-1}$ cannot be easily identified for trial. For this reason, the parameters are determined through trial-and-error. The first set of trial values of \{ $\alpha_1, \alpha_2, \sigma_2, \sigma_3$ \}, labelled set (a), are \{-0.5, 0, 0.5, 1\} which consists of values corresponding to eigenfunctions of the kinetic energy operator. The second set of trial values of \{-0.5, 0.01, 0.52, 1.03\}, labelled set (b), is chosen empirically by slightly adjusting the values of set (a). The variation of the calculated energies of the low-lying states of the potential with increasing bases sizes of each set was tested. The calculated energies for the first three states are shown in Table 3. The results are compared with those of a similar calculation in Cartesian coordinates [26], labelled (c) in the table.

It is observed, in the table, that the energies of the first two levels, calculated using parameter set (a), are obtained with relative errors of $\sim 10^{-3}$ with $N_i = 6$ by the current method, which are similar to the accuracy for the Cartesian treatment. A slight change in the parameter values, set (b), improved the accuracy of the calculated energy of the ground state energy by two orders of magnitude. Increasing the bases sizes to $N_i = 10$ does not improve the accuracy significantly. However, the results for the Cartesian treatment improved by four orders of magnitude. It is seen that the calculated energy $E_2 = 3.346$ of second excited state is not successfully located and, instead, the nearby third excited state $E_3 = 3.565$ is located, in the present treatment. Nonetheless, the rate of convergence with both bases sets is a lot slower than in the Cartesian-coordinate calculations. This is not surprising since, unlike in the present work, the results of [26] were generated with optimized bases. The rate of convergence of the results of this work is, therefore, expected to improve when the parameters ($\alpha_2, \beta_1$) and $\sigma_{D-1}$ are optimized. A systematic optimization procedure for this purpose still needs to be explored.

5. Conclusions

The Lagrange-mesh method was used to construct numerical solutions to the multi-dimensional Schrödinger equation in spherical coordinates. The Laguerre mesh was used to treat the radial domain while Jacobi meshes were used to treat all the parametrized angular domains. Standard Laguerre-mesh matrix elements were used for the radial component, while the newly developed Jacobi-mesh matrix elements were used for the parametrized angular components of the kinetic energy operator. Simple, yet instructive, applications involving central, non-central separable, and non-central non-separable Coulomb as well as harmonic oscillator-type potentials in three, four and six dimensions were treated. Results for the Lagrange-mesh solutions of the two central
potentials problems in six dimensions were reproduced within machine accuracy. These results showed practically no error contributions from the direct treatments involving the use of the parametrized angular kinetic energy matrix elements. Results for the solutions of the non-central potentials displayed the characteristic slow convergence of the eigenfunction expansion approach when the matrix elements corresponding to the eigenfunctions of the kinetic energy operator were used. However, the Lagrange-mesh results with smaller bases sizes for the anharmonic oscillator potential in four dimensions had the same accuracy as those of a Cartesian treatment of the same potential. The results also showed that Lagrange-mesh matrix elements with optimized free parameters may improve the convergence rate.

The numerical solution of the Schrödinger equation in generalized spherical coordinates, in more than three dimensions, is realized through the Lagrange-mesh method. The matrix elements of the Hamiltonian for the problem are simple and require no computer time to evaluate. The results of this work has demonstrated that the multi-dimensional Schrödinger equation in spherical coordinates can be numerically solved with the same simplicity as in Cartesian coordinates. However, a more rigorous optimization procedure for determining the free parameters, of the Lagrange-mesh matrix elements associated with the kinetic energy operators, needs to be investigated. Currently such parameters are optimized empirically through trial-and-error. The independence of the potential matrix elements from the free parameters renders many standard parameter optimization techniques inapplicable.

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