

Ladder Operators for Quantum Systems Confined by Dihedral Angles^{*}

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Abstract. We report the identification and construction of raising and lowering operators for the complete eigenfunctions of isotropic harmonic oscillators confined by dihedral angles, in circular cylindrical and spherical coordinates; as well as for the hydrogen atom in the same situation of confinement, in spherical, parabolic and prolate spheroidal coordinates. The actions of such operators on any eigenfunction are examined in the respective coordinates, illustrating the possibility of generating the complete bases of eigenfunctions in the respective coordinates for both physical systems. The relationships between the eigenfunctions in each pair of coordinates, and with the same eigenenergies are also illustrated.

Key words: Ladder operators; harmonic oscillator; hydrogen atom; confinement in dihedral angles

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1 Introduction

In this section, we provide the background information on our investigations on the hydrogen atom in diverse situations of confinement motivated by a variety of physical and chemical situations, spanning a period of thirty-some years as reviewed in [15], and also our current work for confinement by a dihedral angle [23]. In each case the Schrödinger equation is separable in the chosen coordinate system, and its solutions differ from the familiar ones for the free hydrogen atom by the condition of vanishing at the position of the confining natural boundary, determined by the fixed value of one of the coordinates. Such “natural” boundaries allow for separable and integrable solutions, with non-integer eigenvalues for the constant of motion canonically conjugate to the confining coordinate. The presence of such eigenvalues in the differential equations for the other two degrees of freedom affects correspondingly their eigensolutions, which nevertheless maintain their respective integer quantum numbers and constants of motion. The following paragraphs contain a description of our motivation to search, identify and construct ladder operators for both the harmonic oscillator and the hydrogen atom confined by dihedral angles, in the different coordinate systems sharing the broken rotational symmetry around the edge of the angle.

The research reported in this article was motivated by the feedback on our contribution in the Symposium on Superintegrability, Exact Solvability, and Special Functions. In fact, that contribution with the title “Superintegrability in Confined Quantum Systems” was focused on the case of the hydrogen atom confined inside spheres, and prolate spheroids, and in semi-infinite spaces with paraboloidal, hyperboloidal and circular cone boundaries [15] as well as

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dihedral angles [23]. The successive boundary condition equations determining the eigenvalues of the respective constants of motion canonically conjugate to the confining coordinate are

$$M(-\nu_r, 2\ell + 2, 2r_0/\nu) = 0, \quad \nu = \nu_r + \ell + 1, \quad (1)$$

$$S_{\nu_u}(u_0) = 0, \quad \nu = \nu_u + n_v + m + 1, \quad (2)$$

$$M(-\nu_\xi, m + 1, \xi_0^2/\nu) = 0, \quad \nu = \nu_\xi + n_\eta + m + 1, \quad (3)$$

$$S_{\nu_v}(v_0) = 0, \quad \nu = n_u + \nu_v + m + 1, \quad (4)$$

$$P_\lambda^m(\cos \vartheta_0) = 0, \quad \nu = n_r + \lambda + 1, \quad (5)$$

$$\sin \mu \varphi_0 = 0, \quad \nu = n_r + n_\theta + \mu + 1 = n_u + n_v + \mu + 1 = n_\xi + n_\eta + \mu + 1, \quad (6)$$

involving confluent hypergeometric functions $M(a, b, z)$, prolate spheroidal functions S in the spheroidal $1 < u_0 < \infty$ and hyperboloidal $-1 \leq v_0 \leq 1$ coordinates, associated Legendre P_λ^m functions, and trigonometric sine functions. Their respective quantum labels ν_r , ν_u , ν_ξ , ν_v , λ and μ are no longer integer. Consequently, the functions themselves are no longer polynomials as in the free hydrogen atom, and the principal quantum label ν is no longer an integer, either. The energy eigenvalues $E_\nu = -e^2/2a_0\nu^2$ and their degeneracies are also changed accordingly.

Since exact solvability requires polynomial solutions and raising and lowering operators connecting them, the first five types of confinement do not belong to this category. Nevertheless, their solutions can be accurately evaluated for practical applications [15] and original references therein.

Concerning the confinement by dihedral angles, the solutions in the other degrees of freedom maintain their polynomial character in spherical, spheroidal and parabolic coordinates. In order to establish whether they belong or not to the exactly solvable category, we must search for the respective raising and lowering operators.

From the known connection of the solutions of the free hydrogen atom in parabolic coordinates with the solutions of the harmonic oscillator in circular coordinates as implied in equation (3), we have decided to search first for the corresponding operators in the isotropic harmonic oscillator confined by dihedral angles, in circular cylindrical and spherical coordinates. Correspondingly, in Section 2 we identify the eigenfunctions and energy eigenvalues in the respective coordinates. In Section 3 the starting point is the familiar raising and lowering operators for the free harmonic oscillator in cartesian coordinates, followed by the identification of their forms in circular cylindrical and spherical coordinates; the next step is to incorporate the restrictions associated with the eigenfunctions in the confining angle, and finally examine its consequences on the other degrees of freedom. For the latter we make full use of the results of Section 2 establishing by mathematical induction the explicit and general forms of the raising and lowering operators for the circular, spherical radial and polar angle coordinate eigenfunctions. In Section 4 the relationships between the sets of degenerate circular cylindrical and spherical eigenfunctions are explicitly illustrated. The corresponding results for the hydrogen atom confined by dihedral angles are presented in the successive Sections 5–7. The discussion in Section 8 revolves around the superintegrability, exact solvability and special functions for both confined-by-dihedral-angle quantum systems, and others.

2 Eigenfunctions and eigenenergies of the isotropic harmonic oscillator confined by dihedral angles

The Schrödinger equation for the harmonic oscillator is known to be separable in cartesian, circular cylindrical and spherical coordinates [7, 19]:

$$x = \rho \cos \varphi = r \sin \vartheta \cos \varphi, \quad y = \rho \sin \varphi = r \sin \vartheta \sin \varphi, \quad z = r \cos \vartheta. \quad (7)$$

For the system confined by a dihedral angle defined by the meridian half-planes $\varphi = 0$ and $\varphi = \varphi_0$, the boundary conditions on the respective eigenfunctions are

$$\psi(\rho, \varphi = 0, z) = 0, \quad \psi(\rho, \varphi = \varphi_0, z) = 0, \quad (8)$$

$$\psi(r, \vartheta, \varphi = 0) = 0, \quad \psi(r, \vartheta, \varphi = \varphi_0) = 0. \quad (9)$$

The separability of the Schrödinger equation leads to the common eigenvalue equation for the square of the z -component of the angular momentum

$$\frac{d^2}{d\varphi^2} \Phi(\varphi) = -\mu^2 \Phi(\varphi). \quad (10)$$

As well as the eigenvalue equations for the circular radial and longitudinal cartesian Hamiltonians

$$\left[-\frac{\hbar^2}{2m} \left(\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{\mu^2}{\rho^2} \right) + \frac{1}{2} m \omega^2 \rho^2 \right] R(\rho) = E_{n_\rho \mu} R(\rho), \quad (11)$$

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \frac{1}{2} m \omega^2 z^2 \right] Z(z) = E_{n_z} Z(z),$$

and the counterparts for the square of the angular momentum and spherical radial Hamiltonian, respectively,

$$\left(-\frac{1}{\sin \theta} \frac{d}{d\theta} \sin \theta \frac{d}{d\theta} + \frac{\mu^2}{\sin^2 \theta} \right) \Theta(\theta) = \lambda(\lambda + 1) \Theta(\theta),$$

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{\lambda(\lambda + 1)}{r^2} \right] + \frac{1}{2} m \omega^2 r^2 \right\} R(\eta) = E_{n_\rho \lambda} R(r).$$

The boundary conditions of equations (8), (9) lead to the eigenfunctions and eigenvalues:

$$\Phi(\varphi) = \sqrt{\frac{2}{\varphi_0}} \sin \mu \varphi, \quad \mu = \frac{n_\varphi \pi}{\varphi_0}, \quad n_\varphi = 1, 2, 3, \dots \quad (12)$$

We write first its circular radial and axial coordinate companion factors in the cylindrical case, with length units $\sqrt{\hbar/m\omega}$,

$$R_{n_\rho, \mu}(\rho) = N_{n_\rho, \mu} \rho^\mu e^{-\rho^2/2} M(-n_\rho, \mu + 1, \rho^2), \quad (13)$$

$$Z_{n_z}(z) = N_{n_z} e^{-z^2/2} H_{n_z}(z) \quad (14)$$

in terms of singularity removing factors for $\rho \rightarrow 0$, $\rho \rightarrow \infty$ and $z \rightarrow \infty$, and the confluent hypergeometric polynomial of degree $2n_\rho$ and the Hermite polynomials, respectively. The latter correspond to the free harmonic oscillator in the cartesian axial coordinate, with parity $(-)^{n_z}$. The radial eigenfunction has the same form as in the free harmonic oscillator with the integer magnetic quantum number m replaced by the μ eigenvalues of equation (12). The respective energy eigenvalues in units $\hbar\omega$ become

$$E_{n_\rho n_z \mu} = 2n_\rho + \mu + n_z + \frac{3}{2}. \quad (15)$$

Next, we go on to the spherical radial and polar angle coordinate eigenfunctions:

$$R_{n_r n_\theta \mu}(r) = N_{n_r n_\theta \mu} r^{n_\theta + \mu} e^{-r^2/2} M\left(-n_r, n_\theta + \mu + \frac{3}{2}, r^2\right), \quad (16)$$

$$\Theta_{n_\theta + \mu}^\mu(\cos \theta) = N_{n_\theta + \mu} \frac{\sin^\mu \theta}{2} \left[{}_2F_1\left(-n_\theta, n_\theta + 2\mu + 1; \mu + 1; \frac{1 - \cos \theta}{2}\right) \right]$$

Table 1. Polynomial confluent hypergeometric functions.

n_ρ	$M(-n_\rho, \mu + 1, \rho^2)$
0	1
1	$1 - \frac{\rho^2}{\mu+1}$
2	$1 - \frac{2\rho^2}{\mu+1} + \frac{\rho^4}{(\mu+1)(\mu+2)}$
3	$1 - \frac{3\rho^2}{\mu+1} + \frac{3\rho^4}{(\mu+1)(\mu+2)} - \frac{\rho^6}{(\mu+1)(\mu+2)(\mu+3)}$

Table 2. Hermite polynomials.

n_z	Hermite(n_z, z)
0	1
1	$2z$
2	$-2 + 4z^2$
3	$-12z + 8z^3$
4	$12 - 48z^2 + 16z^4$
5	$120z - 160z^3 + 32z^5$
6	$-120 + 720z^2 - 480z^4 + 64z^6$

$$+ (-)^{n_\theta} {}_2F_1 \left(-n_\theta, n_\theta + 2\mu + 1; \mu + 1; \frac{1 + \cos \theta}{2} \right), \quad (17)$$

where the identification of the angular momentum label $\lambda = n_\theta + \mu$ is in order. The remarks about the radial eigenfunction are the same as for its cylindrical counterpart of equation (13). Concerning the polar angle eigenfunction, several remarks are necessary: *i*) each of the terms inside the brackets corresponds to a hypergeometric function representation of the associated Legendre polynomials, *ii*) for integer values of $\mu \rightarrow m$ they are equal to each other for n_θ even or odd, containing only even or odd powers of $\cos \theta$, *iii*) for the values of μ in equation (12), both contain even and odd powers of $\cos \theta$ and do not have a well defined parity, *iv*) their linear combination in equation (17) ensures that its parity $(-)^{n_\theta}$ is well-defined. While, the confining in the dihedral angle breaks the rotational symmetry around the z -axis, the μ values in each of the terms in equation (17) also break the $z \rightarrow -z$ parity; restoration of such a parity requires the chosen superposition. The corresponding energy eigenvalues are

$$E_{n_r n_\theta \mu} = 2n_r + n_\theta + \mu + \frac{3}{2}. \quad (18)$$

For a chosen value of μ , the states with $2n_\rho + n_z = 2n_r + n_\theta$ share the same energy. Notice that the Gaussian exponential factors in equation (13) and (14) reproduce the corresponding factor in equation (16); while the μ powers of r and $\sin \theta$ in equations (16) and (17) reproduce the μ power of ρ in equation (13). Consequently, the eigenfunctions with $n_\rho = n_z = 0$ and $n_r = n_\theta = 0$ are the same in both coordinate systems for all their common values of μ , or n_φ for each confining angle φ_0 , equation (12).

Tables 1–4 illustrate the polynomial factors in the lower excited radial and axial, and radial and polar angle polynomials equations (13), (14) and (16), (17) in the eigenfunctions for the respective coordinate systems. Each one of them serves as a guide in the identification of their respective raising and lowering operators; and the comparison of their products leads to the relationships between the complete sets of degenerate eigenfunctions in the alternative coordinates.

Table 3. Polynomial confluent hypergeometric functions.

n_r	$M(-n_r, \lambda + \frac{3}{2}, r^2)$
0	1
1	$1 - \frac{r^2}{\lambda + \frac{3}{2}}$
2	$1 - \frac{2r^2}{\lambda + \frac{3}{2}} + \frac{r^4}{(\lambda + \frac{3}{2})(\lambda + \frac{5}{2})}$
3	$1 - \frac{3r^2}{\lambda + \frac{3}{2}} + \frac{3r^4}{(\lambda + \frac{3}{2})(\lambda + \frac{5}{2})} - \frac{r^6}{(\lambda + \frac{3}{2})(\lambda + \frac{5}{2})(\lambda + \frac{7}{2})}$

Table 4. Associated Legendre polynomials with definite parity $(-)^{n_\theta}$.

n_θ	Even or odd powers of ${}_2F_1(-n_\theta, n_\theta + 2\mu + 1; \mu + 1; \frac{1 - \cos \theta}{2})$
0	1
1	$\cos \theta$
2	$\frac{-1 + (2\mu + 3)\cos^2 \theta}{2(\mu + 1)}$
3	$\frac{-3 \cos \theta + (2\mu + 5)\cos^3 \theta}{2(\mu + 1)}$
4	$\frac{3 - 6(2\mu + 5)\cos^2 \theta + (2\mu + 5)(2\mu + 7)\cos^4 \theta}{4(\mu + 1)(\mu + 2)}$
5	$\frac{15 \cos \theta - 10(2\mu + 7)\cos^3 \theta + (2\mu + 7)(2\mu + 9)\cos^5 \theta}{4(\mu + 1)(\mu + 2)}$
6	$\frac{-15 + 45((2\mu + 7)\cos^2 \theta - 15(2\mu + 7)(2\mu + 9)\cos^4 \theta + (2\mu + 7)(2\mu + 9)(2\mu + 11)\cos^6 \theta)}{8(\mu + 1)(\mu + 2)(\mu + 3)}$

3 Raising and lowering operators for the successive degrees of freedom

The creation and annihilation operators for the free harmonic oscillator in each cartesian coordinate constitute our starting point and immediate bridge to their circular cylindrical and spherical counterparts:

$$\hat{i} \left(x \pm \frac{\partial}{\partial x} \right) + \hat{j} \left(y \pm \frac{\partial}{\partial y} \right) + \hat{k} \left(z \pm \frac{\partial}{\partial z} \right) = (\vec{\rho} \pm \nabla_{\vec{\rho}}) + \hat{k} \left(z \pm \frac{\partial}{\partial z} \right) = (\vec{r} \pm \nabla_{\vec{r}}). \quad (19)$$

Let us consider the circular coordinate components rewritten in terms of the cartesian unit vectors \hat{i} and \hat{j} :

$$\begin{aligned} (\vec{\rho} \pm \nabla_{\vec{\rho}}) &= \hat{\rho} \left(\rho \pm \frac{\partial}{\partial \rho} \right) \pm \frac{\hat{\varphi}}{\rho} \frac{\partial}{\partial \varphi} \\ &= (\hat{i} \cos \varphi + \hat{j} \sin \varphi) \left(\rho \pm \frac{\partial}{\partial \rho} \right) \pm (-\hat{i} \sin \varphi + \hat{j} \cos \varphi) \frac{1}{\rho} \frac{\partial}{\partial \varphi}. \end{aligned} \quad (20)$$

The application of the operators in the \hat{i} direction on the eigenfunctions of equation (12), with the idea of raising and lowering the quantum number n_φ , suggests the change of φ by $\pi\varphi/\varphi_0$ in the respective trigonometric functions. In fact, for the angular factor of the radial operator term the result is

$$\cos \frac{\pi\varphi}{\varphi_0} \sin \frac{n_\varphi \pi\varphi}{\varphi_0} = \frac{1}{2} \left[\sin \frac{(n_\varphi + 1)\pi\varphi}{\varphi_0} + \sin \frac{(n_\varphi - 1)\pi\varphi}{\varphi_0} \right] \quad (21)$$

achieving the desired raising and lowering actions in the eigenfunctions. For the angular derivative term, the corresponding result is similar,

$$-\sin \frac{\pi\varphi}{\varphi_0} \frac{d}{d\varphi} \sin \frac{n_\varphi \pi\varphi}{\varphi_0} = -\frac{n_\varphi \pi}{\varphi_0} \sin \frac{\pi\varphi}{\varphi_0} \cos \frac{n_\varphi \pi\varphi}{\varphi_0}$$

$$= -\frac{n_\varphi\pi}{\varphi_0} \frac{1}{2} \left[\sin \frac{(n_\varphi+1)\pi\varphi}{\varphi_0} - \sin \frac{(n_\varphi-1)\pi\varphi}{\varphi_0} \right]. \quad (22)$$

The appropriate linear combinations of equations (21) and (22) allow the identification of the respective raising and lowering operators:

$$\left[\cos \frac{\pi\varphi}{\varphi_0} + \frac{\varphi_0}{n_\varphi\pi} \sin \frac{\pi\varphi}{\varphi_0} \frac{d}{d\varphi} \right] \sin \frac{n_\varphi\pi\varphi}{\varphi_0} = \sin \frac{(n_\varphi+1)\pi\varphi}{\varphi_0}, \quad (23)$$

$$\left[\cos \frac{\pi\varphi}{\varphi_0} - \frac{\varphi_0}{n_\varphi\pi} \sin \frac{\pi\varphi}{\varphi_0} \frac{d}{d\varphi} \right] \sin \frac{n_\varphi\pi\varphi}{\varphi_0} = \sin \frac{(n_\varphi-1)\pi\varphi}{\varphi_0}. \quad (24)$$

They have the same structure as the corresponding operators for the particle confined in the one-dimensional infinite square well [9], and are also connected with the two-dimensional harmonic oscillator in a sector operators [16].

The reader may also examine the actions of the corresponding operators in the \hat{j} direction recognizing that they lead to the companion cosine functions satisfying the Neumann boundary condition instead of the Dirichlet one of equations (8), (9).

For a fixed value of μ , the radial dependent operators in the combinations

$$\rho \pm \frac{d}{d\rho} \mp \frac{\mu}{\rho}$$

guarantee the removal of the singularities at $\rho \rightarrow 0$ and $\rho \rightarrow \infty$, including the annihilation of the eigenstates $\rho^\mu e^{-\rho^2/2}$ when the upper signs are chosen. For the states with radial excitations, we adapt the recurrence relations for the confluent hypergeometric functions (13.4.10) and (13.4.11) in [1]:

$$\left(a + z \frac{d}{dz} \right) M(a, b, z) = aM(a+1, b, z), \quad (25)$$

$$\left(b - a - z + z \frac{d}{dz} \right) M(a, b, z) = (b-a)M(a-1, b, z) \quad (26)$$

with the correspondences $a = -n_\rho$, $b = \mu + 1$ and $z = \rho^2$ in equation (13). The first one with $a+1 = -(n_\rho-1)$ is the lowering operator, while the second one with $a-1 = -(n_\rho+1)$ is the raising operator. The interested readers can check these actions between the consecutive entries in Table 1.

Since the harmonic oscillator in the z -direction is free, the actions of the corresponding operators in equation (19) on the Hermite polynomials of Table 2 are the familiar ones.

In the spherical coordinates, the raising and lowering operators in the φ angle are those in equations (23), (24), while those in the radial coordinate are also given by equations (25), (26) with the correspondences $a = -n_r$, $b = \lambda + \frac{3}{2}$, and $z = r^2$ in equation (16). Their actions can be verified by applying them in the entries of Table 3. For the polar angle the recurrence relations for the associated Legendre functions (8.5.3), (8.5.4) in [1]

$$\left[\lambda z - (z^2 - 1) \frac{d}{dz} \right] P_\lambda^\mu(z) = (\lambda + \mu) P_{\lambda-1}^\mu(z), \quad (27)$$

$$\left[(\lambda + 1)z + (\lambda^2 - 1) \frac{d}{dz} \right] P_\lambda^\mu(z) = (\lambda - \mu + 1) P_{\lambda+1}^\mu(z) \quad (28)$$

can not be applied directly to the eigenfunctions in equation (17) due to some of the remarks in that paragraph.

Nevertheless, equations (27), (28) suggest the structure of the correct lowering and raising operators for the polar angle eigenfunctions with parity $\pi = (-)^{n_\theta}$:

$$\begin{aligned} & \left[A_-^{(n_\theta)} z + (B_-^{(n_\theta)} z^2 + C_-^{(n_\theta)}) \frac{d}{dz} \right] {}_2F_1 \left(-n_\theta, 2\mu + n_\theta + 1; \mu + 1; \frac{1-z}{2} \right) \Big|_{\pi=(-1)^{n_\theta}} \\ &= {}_2F_1 \left(-(n_\theta - 1), 2\mu + n_\theta; \mu + 1; \frac{1-z}{2} \right) \Big|_{\pi=(-1)^{n_\theta-1}}, \end{aligned} \quad (29)$$

$$\begin{aligned} & \left[A_+^{(n_\theta)} z + (B_+^{(n_\theta)} z^2 + C_+^{(n_\theta)}) \frac{d}{dz} \right] {}_2F_1 \left(-n_\theta, 2\mu + n_\theta + 1; \mu + 1; \frac{1-z}{2} \right) \Big|_{\pi=(-)^{n_\theta}} \\ &= {}_2F_1 \left(-(n_\theta + 1), 2\mu + n_\theta + 2; \mu + 1; \frac{1-z}{2} \right) \Big|_{\pi=(-)^{n_\theta+1}}. \end{aligned} \quad (30)$$

Their applications to the entries in Table 4 lead by mathematical induction to the general results:

$$A_-^{(n_\theta)} = 1, \quad B_-^{(n_\theta)} = -\frac{1}{n_\theta}, \quad C_-^{(n_\theta)} = \frac{1}{n_\theta}, \quad (31)$$

$$A_+^{(n_\theta)} = 1, \quad B_+^{(n_\theta)} = \frac{1}{2\mu + n_\theta + 1}, \quad C_+^{(n_\theta)} = -\frac{1}{2\mu + n_\theta + 1}, \quad (32)$$

and in particular, $A_-^{(0)} = 0$ for annihilation of the eigenfunction with $n_\theta = 0$, which is 1 and also has a vanishing derivative, making the values of $B_-^{(0)}$ and $C_-^{(0)}$ irrelevant; also $A_+^{(0)} = 1$, and $B_+^{(0)}$ and $C_+^{(0)}$ irrelevant. Notice also the equal magnitudes and opposite signs of the respective B and C coefficients leading to the common factors $\mp(z^2 - 1)$ of the derivative terms in equations (29) and (30), respectively. The values of $A_-^{(n_\theta)}$ and $B_-^{(n_\theta)}$ guarantee the vanishing of the term with the n_θ power of z , while the values of $A_+^{(n_\theta)}$ and $B_+^{(n_\theta)}$ guarantee the highest power ($n_\theta + 1$) of z and its correct coefficient in the r.h.s. eigenfunction in equation (30).

The energy eigenvalues in equations (15) and (18) contain the same zero-point, radial and axial or polar angle contributions as in the free harmonic oscillator. The difference for the oscillator confined by dihedral angles corresponds to the μ contribution which according to equation (12) is quantized with integer values of n_φ and spacings inversely proportional to the confining angle φ_0 .

Let us start with the case of $\varphi_0 = \pi$, for which the dihedral angle becomes a plane and μ becomes n_φ ; consequently, its contributions to the energy are on the same footing as those of the other degrees of freedom. Next, let us consider the confining angles in the interval $\pi \leq \varphi_0 \leq 2\pi$ for which the μ energy contribution is less than those for the other degrees of freedom, taking its lowest value of one half for $\varphi_0 = 2\pi$; this is the quasi-free limit for the harmonic oscillator, being excluded from the xz half plane ($0 < x < \infty, y = 0, -\infty < z < \infty$), and definitely different from the free harmonic oscillator. On the other hand, for the interval $\pi \geq \varphi_0 > 0$, as the dihedral angle is closing starting from the plane, the μ contribution to the energy becomes larger than the contributions from the other degrees of freedom, tending to infinity as $\varphi_0 \rightarrow 0$ when the moving meridian half-plane of the confining angle approaches the position of the xz half plane.

4 Interbasis expansions of degenerate eigenfunctions in circular cylindrical and spherical coordinates

In this section the complete eigenfunctions of the harmonic oscillator confined by dihedral angles in circular cylindrical and spherical coordinates are compared, illustrating explicitly the relationships of their sets with the same energy, as counterparts of [8, 12, 14] for the free oscillator.

The complete eigenfunctions are the products of the common factor of equation (12), and the respective companions of equations (13), (14) and equations (16), (17):

$$\psi_{n_\rho n_\mu n_z}(\rho, \varphi, z) = R_{n_\rho \mu}(\rho) \Phi_\mu(\varphi) Z_{n_z}(z), \quad \psi_{n_r n_\theta \mu}(r, \theta, \varphi) = R_{n_r n_\theta \mu}(r) \Theta_{n_\theta + \mu}^\mu(\theta) \Phi_\mu(\varphi).$$

For a chosen value of μ , the eigenstates without excitations in the other degrees of freedom are the same in both coordinate systems, which is expressed as

$$|n_\rho = 0, \mu, n_z = 0\rangle = |n_r = 0, n_\theta = 0, \mu\rangle$$

using the ket notation. The eigenstates with excitations in the other degrees of freedom share the common factors in equations (13), (14) and (16), (17) as already discussed in the paragraph after equation (18). Correspondingly, their comparison can be restricted to that of the products of the polynomials in Tables 1 and 2 and in Tables 3 and 4, respectively. Such a comparison will be implemented for the eigenstates involving the successive rows in those tables, and making use of the connections between the respective coordinates, equation (7).

The lowest excitation eigenstates, with negative z -parity and energy $(\mu + 5/2)$ are also the same:

$$|n_\rho = 0, \mu, n_z = 1\rangle = |n_r = 0, n_\theta = 1, \mu\rangle$$

since $z = r \cos \theta$.

The next sets of excited states with positive z -parity and energy $(\mu + \frac{7}{2})$, $|n_\rho = 1, \mu, n_z = 0\rangle$, $|n_\rho = 0, \mu, n_z = 2\rangle$ and $|n_r = 1, n_\theta = 0, \mu\rangle$, $|n_r = 0, n_\theta = 2, \mu\rangle$ involve the products of the respective polynomials:

$$\begin{aligned} \left(1 - \frac{1}{\mu+1} \rho^2\right) \cdot 1, & \quad 1 \cdot (2z^2 - 1), \\ \left(1 - \frac{1}{\mu + \frac{3}{2}} r^2\right) \cdot 1, & \quad r^2 \cdot \frac{(2\mu + 3) \cos^2 \theta - 1}{2(\mu + 1)}. \end{aligned}$$

By using $r^2 \cos^2 \theta = z^2$ and $r^2 = \rho^2 + z^2$, the last pair can be written as the linear combinations of the first pair:

$$\left(1 - \frac{2(\rho^2 + z^2)}{2\mu + 3}\right) = \frac{2(\mu + 1)}{2\mu + 3} \left(1 - \frac{\rho^2}{\mu + 1}\right) - \frac{1}{2\mu + 3} (2z^2 - 1), \quad (33)$$

$$\frac{(2\mu + 3)z^2 - \rho^2 - z^2}{2(\mu + 1)} = \frac{1}{2\mu + 3} \left(1 - \frac{\rho^2}{\mu + 1}\right) + \frac{2(\mu + 1)}{2\mu + 3} (2z^2 - 1). \quad (34)$$

The relationships between the normalized eigenfunctions follows from these relationships between the polynomials

$$\begin{pmatrix} |n_r = 1, n_\theta = 0, \mu\rangle \\ |n_r = 0, n_\theta = 2, \mu\rangle \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{2(\mu+1)}{2\mu+3}} & -\sqrt{\frac{1}{2\mu+3}} \\ \sqrt{\frac{1}{2\mu+3}} & +\sqrt{\frac{2(\mu+1)}{2\mu+3}} \end{pmatrix} \begin{pmatrix} |n_\rho = 1, \mu, n_z = 0\rangle \\ |n_\rho = 0, \mu, n_z = 2\rangle \end{pmatrix}.$$

In the same way we have also obtained the following results for the successive eigenstates with higher excitations and energies $E = \mu + \frac{9}{2}, \mu + \frac{11}{2}, \mu + \frac{13}{2}$, respectively,

$$\begin{pmatrix} |n_r = 1, n_\theta = 1, \mu\rangle \\ |n_r = 0, n_\theta = 3, \mu\rangle \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2(\mu+1)}{2\mu+5}} & -\sqrt{\frac{3}{2\mu+5}} \\ \sqrt{\frac{3}{2\mu+5}} & +\sqrt{\frac{2(\mu+1)}{2\mu+5}} \end{pmatrix} \begin{pmatrix} |n_\rho = 1, \mu, n_z = 1\rangle \\ |n_\rho = 0, \mu, n_z = 3\rangle \end{pmatrix},$$

$$\begin{pmatrix} |20\mu\rangle \\ |12\mu\rangle \\ |04\mu\rangle \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{4(\mu+1)(\mu+2)}{(2\mu+3)(2\mu+5)}} & -\sqrt{\frac{4(\mu+1)}{(2\mu+3)(2\mu+5)}} & -\sqrt{\frac{3}{(2\mu+3)(2\mu+5)}} \\ \sqrt{\frac{4(\mu+2)}{(2\mu+3)(2\mu+7)}} & \frac{2\mu+1}{\sqrt{(2\mu+3)(2\mu+7)}} & \sqrt{\frac{12(\mu+1)}{(2\mu+3)(2\mu+7)}} \\ \sqrt{\frac{3}{(2\mu+5)(2\mu+7)}} & \sqrt{\frac{12(\mu+2)}{(2\mu+5)(2\mu+7)}} & -\sqrt{\frac{4(\mu+1)(\mu+2)}{(2\mu+5)(2\mu+7)}} \end{pmatrix} \begin{pmatrix} |2\mu 0\rangle \\ |1\mu 2\rangle \\ |0\mu 4\rangle \end{pmatrix},$$

$$\begin{pmatrix} |21\mu\rangle \\ |13\mu\rangle \\ |05\mu\rangle \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{4(\mu+1)(\mu+2)}{(2\mu+5)(2\mu+7)}} & -\sqrt{\frac{12(\mu+1)}{(2\mu+5)(2\mu+7)}} & \sqrt{\frac{15}{(2\mu+5)(2\mu+7)}} \\ \sqrt{\frac{12(\mu+2)}{(2\mu+5)(2\mu+9)}} & \frac{2\mu-1}{\sqrt{(2\mu+5)(2\mu+9)}} & -\sqrt{\frac{20(\mu+1)}{(2\mu+5)(2\mu+9)}} \\ \sqrt{\frac{15}{(2\mu+7)(2\mu+9)}} & \sqrt{\frac{20(\mu+2)}{(2\mu+7)(2\mu+9)}} & \sqrt{\frac{4(\mu+1)(\mu+2)}{(2\mu+7)(2\mu+9)}} \end{pmatrix} \begin{pmatrix} |2\mu 1\rangle \\ |1\mu 3\rangle \\ |0\mu 5\rangle \end{pmatrix}.$$

Notice the orthonormality of the transformation matrices, implying the Solomonian distribution of the coefficients in equations (33), (34) and their counterparts between the entries in the matrices and the normalization constants of the respective eigenfunctions. The sets of eigenstates come by pairs of singlets, doublets, triplets, and in general multiplets of order $(2n_\rho + n_z^e + 2)/2 = (2n_\rho + n_z^0 + 1)/2$ with $n_z^0 = n_z^e + 1$, etc., of positive and negative z -parity, and with equal successive energy spacings of $\hbar\omega$, for fixed values of μ . The relationships in this section are valid for any chosen values of μ from equation (12), for any n_φ excitation and for each angle of confinement φ_0 .

5 Eigenstates and eigenenergies of the hydrogen atom confined by dihedral angles

The Schrödinger equation for the hydrogen atom is separable in spherical coordinates, equations (7), as well as in parabolic and prolate spheroidal coordinates [2, 3, 4, 6, 10, 13, 21, 22, 24]:

$$\begin{aligned} x &= \xi\eta \cos \varphi = f\sqrt{(u^2-1)(1-v^2)} \cos \varphi, & y &= \xi\eta \sin \varphi = f\sqrt{(u^2-1)(1-v^2)} \sin \varphi, \\ z &= \frac{\xi^2 - \eta^2}{2} = fuv. \end{aligned} \tag{35}$$

The eigenfunctions of the hydrogen atom confined by dihedral angles in the respective coordinates must satisfy the equations (9) and their counterparts

$$\psi^P(\xi, \eta, \varphi = 0) = 0, \quad \psi^P(\xi, \eta, \varphi = \varphi_0) = 0, \tag{36}$$

$$\psi^{PS}(u, v, \varphi = 0) = 0, \quad \psi^{PS}(u, v, \varphi = \varphi_0) = 0. \tag{37}$$

They also share the eigenvalue equation and its solutions in equations (10), (12). In spherical coordinates, the eigenvalue equation for the square of the angular momentum is also the same as in Section 2, and for the spherical radial Hamiltonian:

$$\left\{ -\frac{\hbar^2}{2m_e} \left[\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{\lambda(\lambda+1)}{r^2} \right] - \frac{e^2}{r} \right\} R(r) = ER(r).$$

In parabolic coordinates, the z -component of the Runge–Lenz vector is the constant of motion leading to the separated ordinary differential equations:

$$\left[-\frac{\hbar^2}{2m_e} \left(\frac{1}{\xi} \frac{d}{d\xi} \xi \frac{d}{d\xi} - \frac{\mu^2}{\xi^2} \right) - E\xi^2 \right] \Xi(\xi) = A_\xi \Xi(\xi), \tag{38}$$

$$\left[-\frac{\hbar^2}{2m_e} \left(\frac{1}{\eta} \frac{d}{d\eta} \eta \frac{d}{d\eta} - \frac{\mu^2}{\eta^2} \right) - E\eta^2 \right] H(\eta) = A_\eta H(\eta), \tag{39}$$

where the separation constants must satisfy the condition

$$A_\xi + A_\eta = 2e^2. \quad (40)$$

For the bound states with negative energy of the hydrogen atom, these equations are equivalent to that of the two-dimensional harmonic oscillator in two dimensions in the circular radial coordinate, equation (11).

The constant of motion in prolate spheroidal coordinates is a linear combination of the square of the angular momentum, the z -component of the Runge–Lenz vector and the Hamiltonian [15], leading to the separated ordinary differential equations

$$\left\{ - \left[\frac{d}{du} (u^2 - 1) \frac{d}{du} - \frac{\mu^2}{u^2 - 1} \right] - \frac{2me^2 fu}{\hbar^2} - \frac{2me^2 E f^2 u^2}{\hbar^2} \right\} U(u) = -AU(u),$$

$$\left\{ - \left[\frac{d}{dv} (1 - v^2) \frac{d}{dv} - \frac{\mu^2}{1 - v^2} \right] + \frac{2me^2 fv}{\hbar^2} + \frac{2me^2 E f^2 v^2}{\hbar^2} \right\} V(v) = AV(v).$$

These two equations are the same in the respective domains $1 \leq u < \infty \leq$ and $-1 \leq v \leq 1$.

Their remaining radial and angular solutions have the same forms as those of the free hydrogen with the substitution of the integer magnetic quantum number m with the eigenvalue μ in equation (12).

In spherical coordinates, the polar angle eigenfunction of the square angular momentum is the one in equation (17), and the radial eigenfunction of the energy becomes

$$R_{n_r \lambda}^S(r) = N_{n_r \lambda} r^\lambda e^{-r/\nu a_0} M(-n_r, 2\lambda + 2, 2r/\nu a_0), \quad (41)$$

with $\lambda = n_\theta + \mu$. The energy eigenvalue $E = -e^2/2a_0\nu^2$ involves the non-integer principal quantum label

$$\nu = n_r + n_\theta + \mu + 1. \quad (42)$$

In parabolic coordinates, by adopting the harmonic oscillator parametrization in equations (11) and (15)

$$E = -\frac{1}{2}m\omega^2 = -\frac{e^2}{2\nu^2 a_0}, \quad A_\xi = \hbar\omega(2n_\xi + \mu + 1), \quad A_\eta = \hbar\omega(2n_\eta + \mu + 1),$$

the identification of their frequency $\omega = e^2/\hbar\nu$, length unit $\hbar/m\omega = \nu a_0$, and the connection between the quantum labels follow immediately:

$$\nu = n_\xi + n_\eta + \mu + 1, \quad (43)$$

as the counterpart of equation (42), and consistent with equation (40).

The respective eigenfunctions share the same forms

$$\Xi_{n_\xi \mu} = N_{n_\xi \mu} \xi^\mu e^{-\xi^2/2\nu a_0} M(-n_\xi, \mu + 1, \xi^2/\nu a_0), \quad (44)$$

$$H_{n_\eta \mu} = N_{n_\eta \mu} \eta^\mu e^{-\eta^2/2\nu a_0} M(-n_\eta, \mu + 1, \eta^2/\nu a_0), \quad (45)$$

which coincide with that of equation (13) for the harmonic oscillator in the circular radial coordinate. Notice also that $\xi\eta$ in equations (35) coincides with $\rho = r \sin\theta$ in equations (7), and that $(\xi^2 + \eta^2)/2 = r$ using equations (35) ensuring that the products of the factors in equations (44), (45) and equations (41), (17) share the same factors removing the singularities at the z -axis and at infinity.

Table 5. Confluent hypergeometric polynomials.

n_r	$M(-n_r, 2\lambda + 2, 2r)$
0	1
1	$1 - \frac{2r}{2\lambda+2}$
2	$1 - \frac{2(2r)}{2\lambda+2} + \frac{(2r)^2}{(2\lambda+2)(2\lambda+3)}$
3	$1 - \frac{3(2r)}{2\lambda+2} + \frac{3(2r)^2}{(2\lambda+2)(2\lambda+3)} - \frac{(2r)^3}{(2\lambda+2)(2\lambda+3)(2\lambda+4)}$

In prolate spheroidal coordinates the spheroidal and hyperboloidal eigenfunctions also share the same differential equation and forms:

$$U_{n_u\mu}(u) = N_{n_u\mu}(u^2 - 1)^{\mu/2} e^{-fu/\nu a_0} S_{n_u}^\mu(u), \quad (46)$$

$$V_{n_v\mu}(v) = N_{n_v\mu}(1 - v^2)^{\mu/2} e^{-fv/\nu a_0} S_{n_v}^\mu(v), \quad (47)$$

with polynomials

$$S_{n_u}^\mu(u) = \sum_{s=0}^{n_u+n_v} c_s(u-1)^s, \quad S_{n_v}^\mu(v) = \sum_{s=0}^{n_u+n_v} c_s(v-1)^s, \quad (48)$$

with common coefficients satisfying three-term recurrence relations [6, 15]

$$\begin{aligned} \frac{2f}{a_0\nu}(n_u + n_v + 1 - s)c_{s-1} + \left[s \left(s + 2\mu + 1 - \frac{2f}{a_0\nu} \right) - A \right] c_s \\ + 2(s+1)(s+\mu+1)c_{s+1} = 0, \end{aligned} \quad (49)$$

and in different ranges of their variables $1 \leq u < \infty$, $-1 \leq v \leq 1$. Now, equations (35) and (7) lead to the identification of $f\sqrt{(u^2-1)(1-v^2)} = r_1 \sin\theta_1$ and $f(u+v) = r_1$, where the subindex 1 indicates that the spherical coordinates are referred to the position of the nucleus as the origin and located at the focus ($x = 0$, $y = 0$, $z = -f$). Correspondingly, the products of equations (46), (47) and equations (41), (17) also share the same factors removing the singularities at the z -axis and at infinity.

The principal quantum label becomes

$$\nu = n_u + n_v + \mu + 1. \quad (50)$$

Comparison of equations (42), (43) and (50) with a common value of μ lead us to recognize the common value of their energy for the states with

$$n_r + n_\theta = n_\xi + n_\eta = n_u + n_v,$$

and with a degeneracy one unit above such sums.

Table 5 illustrates the explicit expressions of the polynomial confluent hypergeometric functions of equation (41). Their polar angle companions are those in Table 4.

The parabolic coordinate confluent hypergeometric polynomials of equations (44), (45) coincide with those in Table 1 with the respective replacement of ρ with ξ and η , as already discussed.

Table 6 illustrates directly the ratio of normalization constants and polynomial factors for excited states in spherical and parabolic coordinates, respectively.

The products of the spheroidal polynomials in equations (48) for the excited states with $n_1 + n_2 = 1, 2$, obtained from the recurrence relation of equation (49), have the same forms

$$\left[1 + \frac{A_i(u-1)}{2(1+\mu)} \right] \left[1 + \frac{A_i(v-1)}{2(1+\mu)} \right] \quad (51)$$

Table 6. The ratios of normalization constants $N_{n_1 n_2 \mu} // N_{00\mu}$ and polynomial factors for excited states.

States	Spherical coordinates	Parabolic coordinates
01 μ	$\frac{2}{\sqrt{2+\mu}} \frac{r \cos \theta}{a_0 \nu}$	$\frac{1+\mu}{\sqrt{2+\mu}} \left(1 - \frac{\eta^2}{a_0 \nu(1+\mu)}\right)$
10 μ	$\frac{2(1+\mu)}{\sqrt{2+\mu}} \left(1 - \frac{r}{a_0 \nu(1+\mu)}\right)$	$\frac{1+\mu}{\sqrt{2+\mu}} \left(1 - \frac{\xi^2}{a_0 \nu(1+\mu)}\right)$
02 μ	$\sqrt{\frac{4(1+\mu)}{(2+\mu)(3+\mu)(3+2\mu)}} \frac{r^2 [-1+(3+2\mu) \cos^2 \theta]}{(a_0 \nu)^2 (1+\mu)}$	$\frac{(1+\mu)\sqrt{2+\mu}}{\sqrt{3+\mu}} \left(1 - \frac{2\eta^2}{a_0 \nu(1+\mu)} + \frac{\eta^4}{a_0^2 \nu^2 (2+\mu)(1+\mu)}\right)$
11 μ	$\frac{\sqrt{8r \cos \theta}}{a_0 \nu} \left(1 - \frac{r}{a_0 \nu(2+\mu)}\right)$	$\frac{(1+\mu)\sqrt{2(1+\mu)}}{\sqrt{3+\mu}} \left(1 - \frac{\eta^2}{a_0 \nu(1+\mu)}\right) \left(1 - \frac{\xi^2}{a_0 \nu(1+\mu)}\right)$
20 μ	$\sqrt{\frac{2(1+\mu)^3(3+2\mu)}{3+\mu}} \times \left(1 - \frac{2r}{a_0 \nu(1+\mu)} + \frac{2r^2}{a_0^2 \nu^2 (1+\mu)(3+2\mu)}\right)$	$\frac{(1+\mu)\sqrt{2+\mu}}{\sqrt{3+\mu}} \left(1 - \frac{2\xi^2}{a_0 \nu(1+\mu)} + \frac{\xi^4}{a_0^2 \nu^2 (2+\mu)(1+\mu)}\right)$

for the states $|n_u = 0, n_v = 1, \mu\rangle$ and $|n_u = 1, n_v = 0, \mu\rangle$ where A_i with $i = 1, 2$ are the ordered roots of the quadratic equation

$$A^2 - \left(2\mu + 2 - \frac{4f}{a_0 \mu}\right) A - \frac{4f}{a_0 \mu} (\mu + 1) = 0. \quad (52)$$

Similarly, the states $|n_u = 0, n_v = 2, \mu\rangle$, $|n_u = 1, n_v = 1, \mu\rangle$ and $|n_u = 2, n_v = 0, \mu\rangle$ share the products

$$\left[1 + \frac{A_i(u-1)}{2(1+\mu)} - \frac{[A_i - 2(1+\mu)](4f + A_i \nu)(u-1)^2}{8(1+\mu)(2+\mu)\nu}\right] \times \left[1 + \frac{A_i(v-1)}{2(1+\mu)} - \frac{[A_i - 2(1+\mu)](4f + A_i \nu)(v-1)^2}{8(1+\mu)(2+\mu)\nu}\right], \quad (53)$$

where A_i with $i = 1, 2, 3$ are the ordered roots of the cubic equation

$$A^3 + \left(-8 - 6\mu + \frac{12f}{a_0 \nu}\right) A^2 + \left[12 + 20\mu + 8\mu^2 - \frac{16f(3\mu + 4)}{a_0 \mu} + \frac{12f^2}{(a_0 \mu)^2}\right] A + \frac{16f(1+\mu)(2\mu + 3)}{a_0 \mu} - \frac{64f^2(\mu + 1)}{(a_0 \mu)^2} = 0. \quad (54)$$

The generalization for any fixed value of $n_u + n_v$ involves the tridiagonal matrix representation of equation (49) of dimension $(n_u + n_v + 1) \times (n_u + n_v + 1)$. The corresponding secular determinant generalizing equations (52) and (54) is an algebraic equation for the eigenvalues A_i of degree $n_u + n_v + 1$. The diagonalization of the matrix yields the numerical values of A_i 's and the coefficients $c_s(A_i)$ for the respective polynomials in equations (48).

6 Raising and lowering operators

On the basis of the equivalence of the hydrogen atom eigenfunctions in parabolic coordinates, equations (44), (45), and the harmonic oscillator eigenfunctions in the circular radial coordinates, equation (13), they also share the same kind of raising and lowering operators of equations (25) and (26) with the correspondences $a = -n_\xi, -n_\eta, b = \mu + 1, z = \xi^2/\nu a_0 \xi, \eta^2/\nu a_0$,

$$\left(\mu + 1 + n_\xi - z + z \frac{d}{dz}\right) M(-n_\xi, \mu + 1, z) = (\mu + 1 + n_\xi) M(-(n_\xi + 1), \mu + 1, z),$$

$$\left(-n_\xi + z \frac{d}{dz}\right) M(-n_\xi, \mu + 1, z) = -n_\xi M(-(n_\xi - 1), \mu + 1, z).$$

In spherical coordinates, both the hydrogen atom and the harmonic oscillator share the same polar angle eigenfunctions of the square of the angular momentum and z -parity, equation (17), as well as their raising and lowering operators, in equations (29)–(32). For the hydrogen atom radial eigenfunctions of equation (41), the corresponding operators also follow from equations (25), (26) using the correspondences $a = -n_r$, $b = 2\lambda + 2$, $z = 2r/\nu a_0$:

$$\begin{aligned} \left(2\lambda + 2 + n_r - z + z \frac{d}{dz}\right) M(-n_r, 2\lambda + 2, z) &= (2\lambda + 2 + n_r) M(-(n_r + 1), 2\lambda + 2, z), \\ \left(-n_r + z \frac{d}{dz}\right) M(-n_r, 2\lambda + 2, z) &= -n_r M(-(n_r - 1), 2\lambda + 2, z). \end{aligned}$$

The interested readers can easily check their connecting actions between the successive entries in Table 5, including their extension.

Concerning the raising and lowering operators for the spheroidal polynomials of equations (48), the inspection of their explicit forms for the lowest excited states in equations (51)–(54) lead us to their respective identifications. In fact, for each fixed value of $n_u + n_v$, the $n_u + n_v + 1$ degenerate eigenfunctions share the same form differing in the associated eigenvalue A_i . Consequently, the successive changes in the neighboring eigenvalues $A_1 \rightarrow A_2 \rightarrow A_3 \rightarrow \dots \rightarrow A_{n_u+n_v} \rightarrow A_{n_u+n_v+1}$ translates into the raisings for the spheroidal quantum number $n_u = 0 \rightarrow n_u = 1 \rightarrow n_u = 2 \rightarrow \dots \rightarrow n_u = n_{u_{\max}} - 1 \rightarrow n_u = n_{u_{\max}}$ with the corresponding lowerings for the hyperboloidal quantum number $n_{v_{\max}} \rightarrow n_{v_{\max}} - 1 \rightarrow n_{v_{\max}} - 2 \rightarrow \dots \rightarrow n_v = 1 \rightarrow n_v = 0$, in such way that $n_{u_{\max}} = n_{v_{\max}} = n_u + n_v$.

On the other hand, for the polynomial solutions in equations (48), their common expansion coefficients depend on the respective eigenvalue $c_s(A_{n_u})$ where we replace the index $i = 1, 2, \dots, N_{\max} + 1$ ordering the eigenvalues with the quantum number $n_u = 0, 1, 2, \dots, N_{\max}$ counting the number of spheroidal nodes. Notice that both polynomials have the same form and are of degree $n_u + n_v$, their difference being associated with the distribution of their nodes in the spheroidal and hyperboloidal degrees of freedom, in a complementary way. Their total number is $n_u + n_v + 1$ associated with states of the same energy. The powers of $u - 1$ or $v - 1$ in which they are expanded appear in the same number in equations (48). Both finite sets of linearly independent sets of power functions can be expressed as linear superpositions of the corresponding sets $S_{n_u}(u)$ and $S_{n_v}(v)$, via the inverse transformation based on the inverse matrix of the coefficient $c_s(A_{n_u})$. These relationships have their counterparts for the familiar special functions, in polynomial and infinite series forms.

7 Interbasis expansions of degenerate eigenfunctions in spherical, parabolic and prolate spheroidal coordinates

Following the same order as in Section 4, the normalized eigenstates without excitations in the non-common degrees of freedom are the same in the three coordinates systems:

$$|n_r = 0, n_\theta = 0, \mu\rangle^S = |n_\xi = 0, n_\eta = 0, \mu\rangle^P = |n_u = 0, n_v = 0, \mu\rangle^{PS}.$$

From the entries in Table 6, the connections between the normalized eigenstates in spherical and parabolic coordinates become:

$$\begin{pmatrix} |01\mu\rangle^S \\ |01\mu\rangle^S \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} |01\mu\rangle^P \\ |01\mu\rangle^P \end{pmatrix}$$

and

$$\begin{pmatrix} |02\mu\rangle^S \\ |11\mu\rangle^S \\ |20\mu\rangle^S \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1+\mu}{2(3+2\mu)}} & -\sqrt{\frac{2+\mu}{3+2\mu}} & \sqrt{\frac{1+\mu}{2(3+2\mu)}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \sqrt{\frac{2+\mu}{2(3+2\mu)}} & \sqrt{\frac{1+\mu}{3+2\mu}} & \sqrt{\frac{2+\mu}{2(3+2\mu)}} \end{pmatrix} \begin{pmatrix} |02\mu\rangle^P \\ |11\mu\rangle^P \\ |20\mu\rangle^P \end{pmatrix},$$

where the orthonormality of the transformation matrices is obvious. These are the counterparts of the interbasis expansions for the free hydrogen atom [20].

Similarly, from the spherical entries in Table (6) and equations (48) for the prolate spheroidal polynomials, the transformation matrices between the respective products of polynomials are

$$\begin{pmatrix} \frac{2(1+\mu)}{f(A_2-A_1)} \left[A_2 - \frac{A_2^2}{2(1+\mu)} \right] & -\frac{2(1+\mu)}{f(A_2-A_1)} \left[A_1 - \frac{A_1^2}{2(1+\mu)} \right] \\ \frac{A_2^2}{2(1+\mu)(A_2-A_1)} & -\frac{A_1^2}{2(1+\mu)(A_2-A_1)} \end{pmatrix}$$

and

$$\begin{bmatrix} -\frac{8(1+\mu)\{2(1+\mu)[4+3\mu-(A_2+A_3)]+A_2A_3\}}{(A_1-A_2)(A_1-A_3)} & \frac{8(1+\mu)\{2(1+\mu)[4+3\mu-(A_3+A_1)]+A_3A_1\}}{(A_1-A_2)(A_1-A_3)} \\ -\frac{8f(1+\mu)[A_2-2(1+\mu)][A_3-2(1+\mu)]}{(A_1-A_2)(A_1-A_3)(A_1+2f)[A_1-2(1+\mu)]} & \frac{8f(1+\mu)[A_3-2(1+\mu)][A_1-2(1+\mu)]}{(A_1-A_2)(A_1-A_3)(A_1+2f)[A_1-2(1+\mu)]} \\ \frac{16f^2(2+\mu)[A_2A_3+4f(1+\mu)]}{(A_1-A_2)(A_1-A_3)(A_1+2f)(3+2\mu)[A_1-2(1+\mu)]} & \frac{16f^2(2+\mu)[A_1A_3+4f(1+\mu)]}{(A_1-A_2)(A_2-A_3)(A_2+2f)(3+2\mu)[A_2-2(1+\mu)]} \\ & \frac{8(1+\mu)\{2(1+\mu)[4+3\mu-(A_3+A_1)]+A_3A_1\}}{(A_1-A_2)(A_1-A_3)} \\ & \frac{8f(1+\mu)[A_1-2(1+\mu)][A_2-2(1+\mu)]}{(A_1-A_2)(A_3-A_2)(A_3+2f)[A_3-2(1+\mu)]} \\ & \frac{16f^2(2+\mu)[A_1A_2+4f(1+\mu)]}{(A_1-A_3)(A_2-A_3)(A_3+2f)(3+2\mu)[A_3-2(1+\mu)]} \end{bmatrix}.$$

These interbasis expansions are the counterparts of those for the free hydrogen atom [17, 18].

8 Discussion

The difference between the free harmonic oscillator and hydrogen atom and their confined by dihedral angle counterparts resides in the boundary conditions of equations (8), (9) and (36), (37) in the respective coordinate systems. The latter lead to the eigenfunctions and eigenvalues of the square of the z -component of angular momentum of equation (12), where μ replaces the familiar integer magnetic quantum number m .

Nevertheless, both the free and the confined-by-dihedral-angle quantum systems share their superintegrability and exact solvability. Admittedly, the separability and integrability is restricted to the coordinate systems sharing the dihedral angle coordinate: circular cylindrical and spherical for the harmonic oscillator, and spherical, parabolic and prolate spheroidal for the hydrogen atom. Sections 3 and 6 illustrated the identification and construction of the raising and lowering operators for the eigenfunctions of L_z^2 , the transverse and axial contributions to the Hamiltonian of the isotropic harmonic oscillator, its complete spherical radial Hamiltonian, the square of the angular momentum and z -parity operators; and their extensions and adaptations for the Hydrogen atom in the respective coordinates. These operators have their free harmonic oscillator and Coulomb potential counterparts in [5]. Concerning special functions, the reader is invited to recognize the roles of the fractional Fourier basis, equation (12), and the square of the angular momentum and z -parity eigenfunctions equation (17). Additionally, Sections 4 and 7 illustrate the relationships between the complete degenerate eigenfunctions of the confined quantum systems in pairs of the alternative coordinate systems.

Some of the eigenfunctions and their raising and lowering operators may also be adapted to other quantum or electromagnetic systems sharing the same constants of motion and confinement situations. As specific examples the free particle confined by dihedral angles, and nondiffracting vortex beams [11], can be mentioned.

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