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ON A GENERALIZED KEPLER-COULOMB SYSTEM: INTERBASIS EXPANSIONS

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1. Introduction

The purpose of the present paper is to further study the nonrelativistic quantum mechanical system corresponding to the three-dimensional axially symmetric potential

$$V = \alpha \frac{1}{\sqrt{x^2+y^2+z^2}} + \beta \frac{z}{\sqrt{x^2+y^2+z^2}} \frac{1}{x^2+y^2} + \gamma \frac{1}{x^2+y^2} \tag{1}$$

(in Cartesian coordinates), where α, β and γ are constants such that $\alpha < 0$ and $\gamma \geq |\beta|$. If $\beta = \gamma = 0$, we have the ordinary (spherically symmetric) Kepler-Coulomb potential. In the case where $\beta = 0$ and $\gamma \neq 0$, the potential (1) reduces to the Hartmann potential that has been used for describing axially symmetric systems like ring-shaped molecules [1-3] and investigated from different points of view in the last decade [4-20]. The generalized Kepler-Coulomb system corresponding to $\beta \neq 0$ and $\gamma \neq 0$ has been worked out in Refs. [9, 14, 17-20]. In particular, the (quantum mechanical) discrete spectrum for the generalized Kepler-Coulomb system is well known [9, 14, 17], even for the so-called (q,p)-analogue of this system [17]. Furthermore, a path integral treatment of the potential (1) has been given in Refs. [14, 18]. Recently, the dynamical symmetry of the generalized Kepler-Coulomb system has been studied in Refs. [17, 19, 20], the classical motion of a particle moving in the potential (1) has been considered in Ref. [19], and the coefficients connecting the parabolic and spherical bases have been identified in Ref. [20] as Clebsch-Gordan coefficients of the pseudo-unitary group SU(1, 1).

The potential V [see Eq. (1)] belongs to a set of three-dimensional potentials systematically investigated in the 1960s (in connection with the question of accidental degeneracy) by the late Professor Smorodinsky and some of his students and/or collaborators [21-23] and revived, in recent years, by Evans [24-26].

The generalized Kepler-Coulomb system turns out to be interesting from both a classical-mechanical and a quantum-mechanical point of view. Indeed, not all the (bounded) classical trajectories are periodic and the quantum energy spectrum exhibits accidental degeneracies with respect to the geometrical group O(2). (The latter two points are probably connected.) The accidental degeneracy arises from the fact that the Schrödinger equation for the potential V is separable in more than one system of coordinates [21-23]. In addition, the potential V generalizes the Kepler-Coulomb potential, that is of central importance in quantum chemistry, and, like the Hartmann potential, may have applications [possibly in a (q,p)-deformed form or in a supersymmetric form] in chemical physics for systems presenting a line of singularity.

A further motivation for the present work is the following. It has been recognized for a long time that the Schrödinger equation and the Hamilton-Jacobi equation for the potential (1) can be separated in spherical polar and parabolic rotational coordinates [23]. However, to the best of our knowledge, it has never been questioned, even in the recent papers of Refs. [9, 14, 17-20], if these equations are also separable in an additional coordinate system as the system of prolated ellipsoidal and hyperboloidal coordinates. This is actually the case and the originality of our work is mainly concerned with this separability in prolate spheroidal coordinates.

The system of spheroidal coordinates constitute a natural system for investigating many problems in mathematical physics (see Ref. [27] and references cited therein). In quantum mechanics, the spheroidal coordinates play an important role because they are appropriate in describing the behavior of a charged particle in the field of two Coulomb centres. The distance R between the centres is a dimensional parameter characterizing the spheroidal coordinates. These coordinates are changed into spherical and parabolic coordinates as $R \to 0$ and $R \to \infty$, respectively, if the positions of one Coulomb centre and of the charged particle are fixed when taking the limits. In this sense, the spheroidal coordinates are more general than the spherical and parabolic ones. This explains the interest of spheroidal coordinates in various domains (astrophysics, plasma physics, theory of the chemical bond, etc.). Such an interest is well documented in quantum chemistry, for instance in the study of two-center systems like H_2^+ and H_2 (see Refs. [28-34] for a nonhexhaustive list of papers showing the interest of spheroidal coordinates in quantum chemistry).

The paper is organized as follows. In Sections 2 and 4, we describe the spherical and parabolic bases, for the generalized Kepler-Coulomb system, in a way adapted to the introduction of interbasis expansions. In Section 3, we prove an additional orthogonality property for the spherical radial wavefunctions of given orbital quantum number l. In Section 5, by using the property of bi-orthogonality of the spherical basis, we calculate the coefficients of interbasis expansions between spherical and parabolic bases. In Section 6, we construct the spheroidal basis of the potential (1) in terms of the superposition of the spherical and parabolic bases. Finally, we prove in the appendix that the bi-orthogonality property (discussed in Section 3) of the spherical radial wavefunctions is a consequence of the accidental degeneracy of the discrete spectrum for the generalized Kepler-Coulomb system.

2. Spherical Basis

By introducing the nonnegative constants c_i $(i = 1, 2)$ such that

$$\beta = c_2 - c_1, \qquad \gamma = c_1 + c_2, \tag{2}$$

the potential V [see Eq. (1)] can be rewritten in the Pöschl-Teller form

$$V = \alpha\frac{1}{r} + c_1\frac{1}{2r^2\cos^2\frac{\theta}{2}} + c_2\frac{1}{2r^2\sin^2\frac{\theta}{2}}, \tag{3}$$

in spherical coordinates ($x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$). The Schrödinger equation

$$H\Psi = E\Psi \tag{4}$$

for the potential (3) may be solved by searching for a wavefunction in the form

$$\Psi(r,\theta,\varphi) = R(r)Z(\theta,\varphi). \tag{5}$$

This leads to the two coupled differential equations

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Z}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Z}{\partial\varphi^2} - \left(\frac{c_1}{\cos^2\frac{\theta}{2}} + \frac{c_2}{\sin^2\frac{\theta}{2}}\right)Z = -AZ, \tag{6}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{A}{r^2}R + 2\left(E - \frac{\alpha}{r}\right)R = 0, \tag{7}$$

where A is a separation constant in spherical coordinates. [We use a system of units for which the reduced mass μ and the Planck constant h satisfy $\mu = h/(2\pi) = 1$.]

The solution of Eq. (6) is easily found to be

$$\begin{aligned} Z(\theta,\varphi) &\equiv Z_{lm}(\theta,\varphi;\delta_1,\delta_2) \\ &= N_{lm}(\delta_1,\delta_2)(1+\cos\theta)^{\frac{|m|+\delta_1}{2}}(1-\cos\theta)^{\frac{|m|+\delta_2}{2}} P_{l-|m|}^{(|m|+\delta_2,|m|+\delta_1)}(\cos\theta)e^{im\varphi}, \end{aligned} \tag{8}$$

where $l \in \mathbf{N}$, $m \in \mathbf{Z}$, $\delta_i = \sqrt{m^2+4c_i} - |m|$ (for $i = 1,2$) and $P_n^{(\alpha,\beta)}$ denotes a Jacobi polynomial. Furthermore, the separation constant A is quantized as

$$A = \left(l + \frac{\delta_1+\delta_2}{2}\right)\left(l + \frac{\delta_1+\delta_2}{2} + 1\right). \tag{9}$$

The normalization constant $N_{lm}(\delta_1,\delta_2)$ in (8) is given (up to a phase factor) by

$$N_{lm}(\delta_1,\delta_2) = \frac{(-1)^{\frac{m-|m|}{2}}}{2^{|m|}}\sqrt{\frac{(2l+\delta_1+\delta_2+1)(l-|m|)!\,\Gamma(l+|m|+\delta_1+\delta_2+1)}{2^{\delta_1+\delta_2+2}\,\pi\,\Gamma(l+\delta_1+1)\,\Gamma(l+\delta_2+1)}}. \tag{10}$$

The angular wavefunctions Z_{lm} [see Eq. (8)] shall be referred to as ring-shaped functions. These ring-shaped functions generalize the functions studied by Hartmann [1-3] in the case $\beta = 0$ (i.e., $\delta_1 = \delta_2$). Due to the connecting formula [35]

$$\left(\lambda + \frac{1}{2}\right)_n C_n^\lambda(x) = (2\lambda)_n P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x) \tag{11}$$

between the Jacobi polynomial $P_n^{(\alpha,\beta)}$ and the Gegenbauer polynomial C_n^λ, the case $\delta_1 = \delta_2 = \delta$ yields

$$Z_{lm}(\theta,\varphi;\delta,\delta) = (-1)^{\frac{m-|m|}{2}} 2^{|m|+\delta} \Gamma\left(|m| + \delta + \frac{1}{2}\right) \sqrt{\frac{(2l+2\delta+1)(l-|m|)!}{4\pi^2 \Gamma(l+|m|+2\delta+1)}}$$

$$\cdot \, (\sin\theta)^{|m|+\delta} C_{l-|m|}^{|m|+\delta+\frac{1}{2}}(\cos\theta) e^{im\varphi}, \tag{12}$$

a result already obtained in Ref. [36]. [In Eq. (11), $(x)_n$ stands for a Pochhammer symbol.] The case $\delta = 0$ (i.e., $\beta = \gamma = 0$) can be treated by using the connecting formula

$$P_l^{|m|}(x) = \frac{(-2)^{|m|}}{\sqrt{\pi}} \Gamma\left(|m| + \frac{1}{2}\right) (1-x^2)^{\frac{|m|}{2}} C_{l-|m|}^{|m|+\frac{1}{2}}(x) \tag{13}$$

between the Gegenbauer polynomial C_n^λ and the associated Legendre function $P_l^{|m|}$ [35]. In fact for $\delta = 0$, Eq. (12) can be reduced to

$$Z_{lm}(\theta,\varphi;0,0) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) e^{im\varphi}, \tag{14}$$

an expression that coincides with the usual (surface) spherical harmonic $Y_{lm}(\theta,\varphi)$ (e.g., see [37]). The surface spherical harmonics thus arise as particular cases of more general functions, viz., the ring-shaped functions.

Let us go now to the radial equation. The introduction of (9) into (7) leads to

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{1}{r^2}\left(l + \frac{\delta_1+\delta_2}{2}\right)\left(l + \frac{\delta_1+\delta_2}{2} + 1\right) R + 2\left(E - \frac{\alpha}{r}\right) R = 0, \tag{15}$$

which is *reminiscent of the radial equation for the hydrogen atom except that the orbital* quantum number l is replaced here by $l + (1/2)(\delta_1 + \delta_2)$. The solution of (15) for the discrete spectrum is

$$R(r) \equiv R_{nl}(r;\delta_1,\delta_2) = C_{nl}(\delta_1,\delta_2)(\varepsilon r)^{l+\frac{\delta_1+\delta_2}{2}} e^{-\frac{\varepsilon}{2}r} {}_1F_1(-n+l+1, 2l+\delta_1+\delta_2+2; \varepsilon r), \tag{16}$$

where $n \in \mathbf{N} - \{0\}$. In Eq. (16), the normalization factor $C_{nl}(\delta_1,\delta_2)$ reads

$$C_{nl}(\delta_1,\delta_2) = \frac{2(-\alpha)^{3/2}}{(n+\frac{\delta_1+\delta_2}{2})^2} \frac{1}{\Gamma(2l+\delta_1+\delta_2+2)} \sqrt{\frac{\Gamma(n+l+\delta_1+\delta_2+1)}{(n-l-1)!}} \tag{17}$$

and the parameter ε is defined by

$$\varepsilon = -\frac{2\alpha}{n+\frac{\delta_1+\delta_2}{2}}. \tag{18}$$

The eigenvalues E are then given by

$$E \equiv E_n = -\frac{\alpha^2}{2\left(n+\frac{\delta_1+\delta_2}{2}\right)^2}, \qquad n = 1, 2, 3, \cdots, \tag{19}$$

in agreement with Ref. [14] (see also Refs. [9, 17]). Equations (16) to (19) can be specialized to the cases $\delta_1 = \delta_2 = \delta$ (with $\delta \neq 0$ or $\delta = 0$). In the limiting case $\delta = 0$, we recover the familiar results for hydrogenlike atoms.

3. Bi-Orthogonality of the Radial Wavefunctions

The radial wavefunctions R_{nl} [see Eq. (16)] satisfy the orthogonality relation

$$I_{nn'} = \int_0^\infty R_{n'l}(r;\delta_1,\delta_2) R_{nl}(r;\delta_1,\delta_2) r^2 dr = \delta_{nn'}, \tag{20}$$

which is necessary for the normalization of the total wavefunction $\Psi_{nlm}(r,\theta,\varphi;\delta_1,\delta_2)$ given by Eqs. (5), (8), and (16). In addition to the condition (20), we have also the following orthogonality condition

$$J_{ll'} = \int_0^\infty R_{nl'}(r;\delta_1,\delta_2) R_{nl}(r;\delta_1,\delta_2) dr = \frac{2\alpha^2}{(n+\frac{\delta_1+\delta_2}{2})^3} \frac{1}{2l+\delta_1+\delta_2+1} \delta_{ll'}. \tag{21}$$

This new relation shall prove useful when dealing with the interbasis expansions in Section 5. The proof of Eq. (21) is as follows.

In the integral appearing in (21), we replace R_{nl} and $R_{nl'}$ by their expressions (16). Then, we take the hypergeometric function ${}_1F_1(-n+l+1, 2l+\delta_1+\delta_2+2; \varepsilon r)$ in (16) as the finite sum

$${}_1F_1(-n+l+1, 2l+\delta_1+\delta_2+2; \varepsilon r) = \sum_{s=0}^{n-l-1} \frac{(-n+l+1)_s}{(2l+\delta_1+\delta_2+2)_s} \frac{(\varepsilon r)^s}{s!} \tag{22}$$

and we perform the integration term by term with the help of the formula [38]

$$\int_0^\infty e^{-\lambda x} x^\nu {}_1F_1(\alpha,\gamma;kx)\, dx = \frac{\Gamma(\nu+1)}{\lambda^{\nu+1}} {}_2F_1\left(\alpha, \nu+1, \gamma; \frac{k}{\lambda}\right). \tag{23}$$

By using

$${}_2F_1(a,b,c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, \tag{24}$$

we arrive at

$$\begin{aligned} J_{ll'} &= \frac{2\alpha^2}{(n+\frac{\delta_1+\delta_2}{2})^3} \frac{\Gamma(l+l'+\delta_1+\delta_2+1)}{\Gamma(2l+\delta_1+\delta_2+2)} \sqrt{\frac{1}{(n-l-1)!(n-l'-1)!} \frac{\Gamma(n+l+\delta_1+\delta_2+1)}{\Gamma(n+l'+\delta_1+\delta_2+1)}} \\ &\cdot \sum_{s=0}^{n-l-1} \frac{(-n+l+1)_s}{s!} \frac{(l+l'+\delta_1+\delta_2+1)_s}{(2l+\delta_1+\delta_2+2)_s} \frac{\Gamma(n-l-s)}{\Gamma(l'-l-s+1)}. \end{aligned} \tag{25}$$

By introducing the formula [35]

$$\frac{\Gamma(z)}{\Gamma(z-n)} = (-1)^n \frac{\Gamma(-z+n+1)}{\Gamma(-z+1)} \tag{26}$$

into (25), the sum over s can be expressed in terms of the ${}_2F_1$ Gauss hypergeometric function of argument 1. We thus obtain

$$J_{ll'} = \frac{2\alpha^2}{(n+\frac{\delta_1+\delta_2}{2})^3} \frac{1}{l+l'+\delta_1+\delta_2+1}$$

$$\cdot\sqrt{\frac{(n-l-1)!}{(n-l'-1)!}\frac{\Gamma(n+l+\delta_1+\delta_2+1)}{\Gamma(n+l'+\delta_1+\delta_2+1)}}\frac{1}{\Gamma(l-l'+1)\Gamma(l'-l+1)}. \tag{27}$$

Equation (21) then easily follows from (27) since $[\Gamma(l-l'+1)\Gamma(l'-l+1)]^{-1}=\delta_{ll'}$.

The result provided by Eq. (21) generalizes the one for the hydrogen atom [39]. Indeed, orthogonality properties similar to (21) hold for the hydrogen atom system and the harmonic oscillator system in f-dimensional spaces ($f\geq 2$) [39]. Such unusual orthogonality properties are connected to the accidental degeneracies of the energy spectra for these systems. In this connection, the property (21) is a consequence of the accidental degeneracy (with respect to the orbital quantum number l) of the discrete energy spectrum for the generalized Kepler-Coulomb system under consideration ; this point is further studied in the appendix.

4. Parabolic Basis

In the parabolic coordinates

$$x=\sqrt{\mu\nu}\cos\varphi,\quad y=\sqrt{\mu\nu}\sin\varphi,\quad z=\frac{1}{2}(\mu-\nu),\quad 0\leq\mu,\nu<\infty,\quad 0\leq\varphi<2\pi, \tag{28}$$

the potential V reads

$$V=\alpha\frac{2}{\mu+\nu}+c_1\frac{2}{\mu(\mu+\nu)}+c_2\frac{2}{\nu(\mu+\nu)}. \tag{29}$$

By looking for a solution of the Schrödinger equation (4) for this potential in the form

$$\Psi(\mu,\nu,\varphi)=f_1(\mu)f_2(\nu)e^{im\varphi}, \tag{30}$$

we obtain the two coupled equations

$$\frac{d}{d\mu}\left(\mu\frac{df_1}{d\mu}\right)+\left[\frac{E}{2}\mu-\frac{(|m|+\delta_1)^2}{4\mu}+B_1\right]f_1=0, \tag{31}$$

$$\frac{d}{d\nu}\left(\nu\frac{df_2}{d\nu}\right)+\left[\frac{E}{2}\nu-\frac{(|m|+\delta_2)^2}{4\nu}+B_2\right]f_2=0, \tag{32}$$

where the two separation constants B_1 and B_2 obey $B_1+B_2=-\alpha$. (In the whole paper, we use Ψ to denote the total wavefunction whatsoever the coordinate system is. The wavefuctions Ψ in spherical, parabolic and prolate spheroidal coordinates are then distinguished by the corresponding quantum numbers.) By solving (31) and (32), we get the normalized wavefunction

$$\Psi(\mu,\nu,\varphi)\equiv\Psi_{n_1n_2m}(\mu,\nu,\varphi;\delta_1,\delta_2)=\frac{\varepsilon^2}{\sqrt{-8\alpha}}f_{n_1m}(\mu;\delta_1)f_{n_2m}(\nu;\delta_2)\frac{e^{im\varphi}}{\sqrt{2\pi}}, \tag{33}$$

where

$$f_i(t_i)\equiv f_{n_im}(t_i;\delta_i)=\frac{1}{\Gamma(|m|+\delta_i+1)}\sqrt{\frac{\Gamma(n_i+|m|+\delta_i+1)}{n_i!}}$$

$$\cdot \left(\frac{\varepsilon t_i}{2}\right)^{\frac{|m|+\delta_i}{2}} e^{-\frac{\varepsilon t_i}{4}} {}_1F_1\left(-n_i, |m|+\delta_i+1; \frac{\varepsilon t_i}{2}\right), \tag{34}$$

with $i = 1, 2$ ($t_1 \equiv \mu$ and $t_2 \equiv \nu$). In Eq. (34), we have

$$n_i = -\frac{|m|+\delta_i+1}{2} + \frac{2}{\varepsilon} B_i, \qquad (i = 1, 2). \tag{35}$$

Here again $m \in \mathbf{Z}$ in order to ensure the univaluedness of $\Psi_{n_1 n_2 m}$. In addition, $n_i \in \mathbf{N}$ (for $i = 1, 2$) in order that $\Psi_{n_1 n_2 m}$ be in $L^2(\mathbf{R}^3)$. Therefore, the quantized values of the energy E are given by (19) where now the quantum number n is $n = n_1 + n_2 + |m| + 1$, a number that parallels the principal quantum number of the hydrogen atom in parabolic coordinates.

The results (33) to (35) agree with the corresponding ones of Ref. [19] derived by making use of the Kustaanheimo-Stiefel transformation (see also Ref. [9]).

Following Kibler and Campigotto [19], we can obtain a further integral of motion besides E. In parabolic coordinates, this integral corresponds to the hermitean operator

$$X = \frac{2}{\mu+\nu}\left[\mu\frac{\partial}{\partial\nu}\left(\nu\frac{\partial}{\partial\nu}\right) - \nu\frac{\partial}{\partial\mu}\left(\mu\frac{\partial}{\partial\mu}\right)\right] + \frac{\mu-\nu}{2\mu\nu}\frac{\partial^2}{\partial\varphi^2} + \frac{2c_1\nu}{\mu(\mu+\nu)} - \frac{2c_2\mu}{\nu(\mu+\nu)} - \alpha\frac{\mu-\nu}{\mu+\nu}. \tag{36}$$

The eigenvalues of X are

$$B_1 - B_2 = -\alpha\frac{n_1 - n_2 + \frac{\delta_1-\delta_2}{2}}{n + \frac{\delta_1+\delta_2}{2}}. \tag{37}$$

In Cartesian coordinates, the operator X can be rewriten as

$$X = z\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - x\frac{\partial^2}{\partial x\partial z} - y\frac{\partial^2}{\partial y\partial z} - \frac{\partial}{\partial z} - \alpha\frac{z}{r} + c_1\frac{r-z}{r(r+z)} - c_2\frac{r+z}{r(r-z)}, \tag{38}$$

so that it immediately follows that X is connected to the z-component A_z of the Laplace-Runge-Lenz-Pauli vector via

$$X = A_z + c_1\frac{r-z}{r(r+z)} - c_2\frac{r+z}{r(r-z)} \tag{39}$$

and coincides with A_z when $\beta = \gamma = 0$.

5 . Interbasis Expansion between Parabolic and Spherical Bases

The connection between the spherical (r, θ, φ) and parabolic (μ, ν, φ) coordinates is

$$\mu = r(1-\cos\theta), \qquad \nu = r(1+\cos\theta), \qquad \varphi(\text{parabolic}) = \varphi(\text{spherical}). \tag{40}$$

For a given subspace corresponding to a fixed value of E_n, we can write the parabolic wavefunction (30) in terms of the spherical wavefunctions (5) as

$$\Psi_{n_1 n_2 m}(\mu, \nu, \varphi; \delta_1, \delta_2) = \sum_{l=|m|}^{n-1} W^l_{n_1 n_2 m}(\delta_1, \delta_2)\Psi_{nlm}(r, \theta, \varphi; \delta_1, \delta_2). \tag{41}$$

By virtue of Eq. (40), the left-hand side of (41) can be rewritten in spherical coordinates. Then, by substituting $\theta = 0$ in the so-obtained equation and by taking into account that

$$P_n^{(\alpha,\beta)}(1) = \frac{(\alpha+1)_n}{n!}, \tag{42}$$

we get an equation which depends only on the variable r. Thus, we can use the orthonormality relation (21) on the orbital quantum numbers l. This yields

$$W^l_{n_1 n_2 m}(\delta_1,\delta_2) = \frac{(-1)^{\frac{m-|m|}{2}}}{\Gamma(|m|+\delta_1+1)\Gamma(2l+\delta_1+\delta_2+2)}\, E^{lm}_{n_1 n_2}\, K^{lm}_{nn_1}, \tag{43}$$

where

$$E^{lm}_{n_1 n_2} = \sqrt{(2l+\delta_1+\delta_2+1)(l-|m|)!\Gamma(l+\delta_1+1)} \cdot \left[\frac{\Gamma(n_1+|m|+\delta_1+1)\Gamma(n_2+|m|+\delta_2+1)\Gamma(n+l+\delta_1+\delta_2+1)}{(n_1)!(n_2)!(n-l-1)!\Gamma(l+\delta_2+1)\Gamma(l+|m|+\delta_1+\delta_2+1)}\right]^{1/2} \tag{44}$$

and

$$K^{lm}_{nn_1} = \int_0^\infty x^{l+|m|+\delta_1+\delta_2} e^{-x}\, {}_1F_1(-n_1, |m|+\delta_1+1; x)\, {}_1F_1(-n+l+1, 2l+\delta_1+\delta_2+2; x)\, dx. \tag{45}$$

To calculate the integral $K^{lm}_{nn_1}$, it is sufficient to write the confluent hypergeometric function ${}_1F_1(-n_1, |m|+\delta_1+1; x)$ as a series, to integrate according to (23) and to use the formula (24) for the summation of the Gauss hypergeometric function ${}_2F_1(a,b,c;1)$. We thus obtain

$$K^{lm}_{nn_1} = \frac{(n-|m|-1)!\Gamma(2l+\delta_1+\delta_2+2)\Gamma(l+|m|+\delta_1+\delta_2+1)}{(l-|m|)!\Gamma(n+l+\delta_1+\delta_2+1)} \cdot {}_3F_2\left\{ \begin{matrix} -n_1, -l+|m|, l+|m|+\delta_1+\delta_2+1 \\ |m|+\delta_1+1, -n+|m|+1 \end{matrix} \middle| 1 \right\}. \tag{46}$$

The introduction of (46) into (43) gives

$$W^l_{n_1 n_2 m}(\delta_1,\delta_2) = \frac{(-1)^{\frac{m-|m|}{2}}(n-|m|-1)!\Gamma(l+|m|+\delta_1+\delta_2+1)}{(l-|m|)!\Gamma(|m|+\delta_1+1)\Gamma(n+l+\delta_1+\delta_2+1)} \cdot {}_3F_2\left\{ \begin{matrix} -n_1, -l+|m|, l+|m|+\delta_1+\delta_2+1 \\ |m|+\delta_1+1, -n+|m|+1 \end{matrix} \middle| 1 \right\} E^{lm}_{n_1 n_2} \tag{47}$$

and owing to (44) we end up with

$$W^l_{n_1 n_2 m}(\delta_1,\delta_2) = \sqrt{\frac{(2l+\delta_1+\delta_2+1)\Gamma(n_1+|m|+\delta_1+1)\Gamma(n_2+|m|+\delta_2+1)}{(n_1)!(n_2)!(n-l-1)!(l-|m|)!}} \cdot (-1)^{\frac{m-|m|}{2}} \frac{(n-|m|-1)!}{\Gamma(|m|+\delta_1+1)} \sqrt{\frac{\Gamma(l+\delta_1+1)\Gamma(l+|m|+\delta_1+\delta_2+1)}{\Gamma(l+\delta_2+1)\Gamma(n+l+\delta_1+\delta_2+1)}} \cdot {}_3F_2\left\{ \begin{matrix} -n_1, -l+|m|, l+|m|+\delta_1+\delta_2+1 \\ |m|+\delta_1+1, -n+|m|+1 \end{matrix} \middle| 1 \right\} \tag{48}$$

that constitutes a closed form expression for the interbasis coefficients.

The next step is to show that the interbasis coefficients (48) are indeed a continuation on the real line of the Clebsch-Gordan coefficients for the group SU(2). It is known that the Clebsch-Gordan coefficient $C_{a\alpha;b\beta}^{c\gamma} \equiv \langle a\alpha b\beta | abc\gamma \rangle$ can be written as [37]

$$C_{a\alpha;b\beta}^{c\gamma} = (-1)^{a-\alpha}\delta_{\gamma,\alpha+\beta}(a+b-\gamma)!(b+c-\alpha)!$$

$$\cdot \left[\frac{(2c+1)(a+\alpha)!(c+\gamma)!}{(a-\alpha)!(b-\beta)!(b+\beta)!(c-\gamma)!(a+b+c+1)!(a+b-c)!(a-b+c)!(b-a+c)!}\right]^{1/2}$$

$$\cdot \, {}_3F_2\left\{ \begin{matrix} -a-b-c-1, -a+\alpha, -c+\gamma \\ -a-b+\gamma, -b-c+\alpha \end{matrix} \middle| 1 \right\}. \tag{49}$$

In view of the formula [40]

$${}_3F_2\left\{ \begin{matrix} s, s', -N \\ t', 1-N-t \end{matrix} \middle| 1 \right\} = \frac{(t+s)_N}{(t)_N} \, {}_3F_2\left\{ \begin{matrix} s, t'-s', -N \\ t', t+s \end{matrix} \middle| 1 \right\}, \tag{50}$$

equation (49) can be rewritten in the form

$$C_{a\alpha;b\beta}^{c\gamma} = (-1)^{a-\alpha}\delta_{\gamma,\alpha+\beta}\left[\frac{(2c+1)(b-a+c)!(a+\alpha)!(b+\beta)!(c+\gamma)!}{(a-\alpha)!(b-\beta)!(c-\gamma)!(a+b-c)!(a-b+c)!(a+b+c+1)!}\right]^{1/2}$$

$$\cdot \frac{(a+b-\gamma)!}{(b-a+\gamma)!} \, {}_3F_2\left\{ \begin{matrix} -a+\alpha, c+\gamma+1, -c+\gamma \\ \gamma-a-b, b-a+\gamma+1 \end{matrix} \middle| 1 \right\}. \tag{51}$$

By comparing Eqs. (51) and (48), we finally obtain

$$W_{n_1 n_2 m}^{l}(\delta_1, \delta_2) = (-1)^{n_1 + \frac{m-|m|}{2}} C^{l+\frac{\delta_1+\delta_2}{2}, |m|+\frac{\delta_1+\delta_2}{2}}_{\frac{n+\delta_2-1}{2}, \frac{|m|+n_2-n_1+\delta_2}{2}; \frac{n+\delta_1-1}{2}, \frac{|m|+n_1-n_2+\delta_1}{2}}. \tag{52}$$

Equation (52) proves that the coefficients for the expansion of the parabolic basis in terms of the spherical basis are nothing but the analytic continuation, for real values of their arguments, of the SU(2) Clebsch-Gordan coefficients.

The inverse of Eq. (41), namely

$$\Psi_{nlm}(r, \theta, \varphi; \delta_1, \delta_2) = \sum_{n_1=0}^{n-|m|-1} \widetilde{W}_{nlm}^{n_1}(\delta_1, \delta_2) \Psi_{n_1 n_2 m}(\mu, \nu, \varphi; \delta_1, \delta_2), \tag{53}$$

is an immediate consequence of the orthonormality property of the SU(2) Clebsch-Gordan coefficients. The expansion coefficients in (53) are thus given by

$$\widetilde{W}_{nlm}^{n_1}(\delta_1, \delta_2) = (-1)^{n_1 + \frac{m-|m|}{2}} C^{l+\frac{\delta_1+\delta_2}{2}, |m|+\frac{\delta_1+\delta_2}{2}}_{\frac{n+\delta_2-1}{2}, \frac{n+\delta_2-1}{2}-n_1; \frac{n+\delta_1-1}{2}, n_1+|m|-\frac{n-\delta_1-1}{2}} \tag{54}$$

and may be expressed in terms of the ${}_3F_2$ function through (49) or (51).

To close this section, it should be mentioned that (52) and (54) generalize the well-known result, corresponding to $\delta_1 = \delta_2 = 0$, for the interbasis expansion between parabolic and spherical bases obtained in Refs. [41-44] in the case of the hydrogen atom. Furthermore, by taking $\delta_1 = \delta_2 \neq 0$ in (52) and (54), we recover our former result [11] for the Hartmann system.

6. Prolate Spheroidal Basis

6.1. Separation in Prolate Spheroidal Coordinates

We now pass to the prolate spheroidal coordinates

$$x = \frac{R}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\cos\varphi, \quad y = \frac{R}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\sin\varphi, \quad z = \frac{R}{2}(\xi\eta+1), \tag{55}$$

$$1 \le \xi < \infty, \qquad -1 \le \eta \le 1, \qquad 0 \le \varphi < 2\pi,$$

where R is the interfocus distance. In the limits where $R \to 0$ and $R \to \infty$, the prolate spheroidal coordinates give back the spherical coordinates and the parabolic coordinates, respectively [27, 44]. In the system of prolate spheroidal coordinates, the potential V can be written as

$$V = \alpha\frac{2}{R(\xi+\eta)} + \frac{4}{R^2(\xi+\eta)}\left[c_1\frac{1}{(\xi+1)(1+\eta)} + c_2\frac{1}{(\xi-1)(1-\eta)}\right]. \tag{56}$$

The Schrödinger equation (4) for the potential (56) is separable in prolate spheroidal coordinates. As a point of fact, by looking for a solution of this equation in the form

$$\Psi(\xi,\eta,\varphi) = \psi_1(\xi)\psi_2(\eta)e^{im\varphi}, \qquad m \in \mathbf{Z}, \tag{57}$$

we obtain the two ordinary differential equations

$$\left[\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi} + \frac{(|m|+\delta_1)^2}{2(\xi+1)} - \frac{(|m|+\delta_2)^2}{2(\xi-1)} - 2\alpha R\xi + \frac{ER^2}{2}(\xi^2-1)\right]\psi_1 = +\lambda(R)\psi_1, \tag{58}$$

$$\left[\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta} - \frac{(|m|+\delta_1)^2}{2(1+\eta)} - \frac{(|m|+\delta_2)^2}{2(1-\eta)} + 2\alpha R\eta + \frac{ER^2}{2}(1-\eta^2)\right]\psi_2 = -\lambda(R)\psi_2, \tag{59}$$

where $\lambda(R)$ is a separation constant in prolate spheroidal coordinates. By eliminating the energy E from Eqs. (58) and (59), we produce the operator

$$\Lambda = \frac{1}{\xi^2-\eta^2}\left[(1-\eta^2)\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} - (\xi^2-1)\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right] + \frac{2-\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}$$
$$-\alpha R\frac{\xi\eta+1}{\xi+\eta} + 2c_1\frac{(\xi+\eta)^2+(\xi-1)(1-\eta)}{(\xi+\eta)(\xi+1)(1+\eta)} + 2c_2\frac{(\xi+\eta)^2-(\xi+1)(1+\eta)}{(\xi+\eta)(\xi-1)(1-\eta)}, \tag{60}$$

the eigenvalues of which are $\lambda(R)$ and the eigenfunctions of which are $\psi_1(\xi)\psi_2(\eta)$. The significance of the (self-adjoint) operator Λ can be found by switching to Cartesian coordinates. A long calculation gives

$$\Lambda = M + RX, \tag{61}$$

where X is the constant of motion (38) and M is the following constant of motion

$$M = L^2 + c_1\frac{1}{\cos^2\frac{\theta}{2}} + c_2\frac{1}{\sin^2\frac{\theta}{2}}, \tag{62}$$

the operator L^2 being the square of the angular momentum operator. The prolate spheroidal wavefunctions ψ_1 and ψ_2 could be obtained by solving (58) and (59). However, it is more economical to proceed in the following way that shall give us, at the same time, the global wavefunction (57), i.e., $\Psi(\xi,\eta,\varphi;R;\delta_1,\delta_2)$, and the interbasis expansion coefficients.

6.2. Interbasis Expansions for the Prolate Spheroidal Wavefunctions

From what preceds, we have three sets of commuting operators, viz., $\{H, L_z, M\}$, $\{H, L_z, X\}$, and $\{H, L_z, \Lambda\}$ corresponding to the spherical, parabolic, and prolate spheroidal coordinates, respectively. (The operators L_z and H are the z-component of the angular momentum and the Hamiltonian for the generalized Kepler-Coulomb system, respectively.) In particular, we have

$$M\Psi_{nlm}(r,\theta,\varphi;\delta_1,\delta_2) = \left(l+\frac{\delta_1+\delta_2}{2}\right)\left(l+\frac{\delta_1+\delta_2}{2}+1\right)\Psi_{nlm}(r,\theta,\varphi;\delta_1,\delta_2), \tag{63}$$

$$X\Psi_{n_1n_2m}(\mu,\nu,\varphi;\delta_1,\delta_2) = -\alpha\frac{n_1-n_2+\frac{\delta_1-\delta_2}{2}}{n+\frac{\delta_1+\delta_2}{2}}\Psi_{n_1n_2m}(\mu,\nu,\varphi;\delta_1,\delta_2), \tag{64}$$

and

$$\Lambda\Psi_{nqm}(\xi,\eta,\varphi;R;\delta_1,\delta_2) = \lambda_q(R)\Psi_{nqm}(\xi,\eta,\varphi;R;\delta_1,\delta_2) \tag{65}$$

for the spherical, parabolic, and prolate spheroidal bases, respectively. In Eq. (65), the index q labels the eigenvalues of the operator Λ and varies in the range $0 \le q \le n-|m|-1$. We are now ready to deal with the interbasis expansions

$$\Psi_{nqm}(\xi,\eta,\varphi;R;\delta_1,\delta_2) = \sum_{l=|m|}^{n-1} T_{nqm}^{l}(R;\delta_1,\delta_2)\Psi_{nlm}(r,\theta,\varphi;\delta_1,\delta_2), \tag{66}$$

$$\Psi_{nqm}(\xi,\eta,\varphi;R;\delta_1,\delta_2) = \sum_{n_1=0}^{n-|m|-1} U_{nqm}^{n_1}(R;\delta_1,\delta_2)\Psi_{n_1n_2m}(\mu,\nu,\varphi;\delta_1,\delta_2), \tag{67}$$

for the prolate spheroidal basis in terms of the spherical and parabolic bases. [Equation (66) was first considered by Coulson and Joseph [28] in the particular case $\delta_1=\delta_2=0$.]

First, we consider Eq. (66). Let the operator Λ act on both sides of (66). Then, by using Eqs. (61), (63), and (65) as well as the orthonormality property of the spherical basis, we find that

$$\left[\lambda_q(R) - \left(l+\frac{\delta_1+\delta_2}{2}\right)\left(l+\frac{\delta_1+\delta_2}{2}+1\right)\right] T_{nqm}^{l}(R;\delta_1,\delta_2) = R\sum_{l'=|m|}^{n-1} T_{nqm}^{l'}(R;\delta_1,\delta_2)(X)_{ll'}, \tag{68}$$

where

$$(X)_{ll'} = \int_0^\infty\int_0^\pi\int_0^{2\pi} \Psi_{nlm}^{*}(r,\theta,\varphi;\delta_1,\delta_2)X\Psi_{nl'm}(r,\theta,\varphi;\delta_1,\delta_2)\,r^2\sin\theta\,dr\,d\theta\,d\varphi. \tag{69}$$

The calculation of the matrix element $(X)_{ll'}$ can be done by expanding the spherical wavefunctions in (69) in terms of parabolic wavefunctions [see Eq. (53)] and by making use of the eigenvalue equation for X [see Eq. (64)]. This leads to

$$(X)_{ll'} = -\frac{\alpha}{n+\frac{\delta_1+\delta_2}{2}} \sum_{n_1=0}^{n-|m|-1} \left(2n_1 - n + |m| + \frac{\delta_1-\delta_2}{2} + 1\right) \widetilde{W}^{n_1}_{nlm}(\delta_1,\delta_2)\widetilde{W}^{n_1}_{nl'm}(\delta_1,\delta_2). \tag{70}$$

Then, by using Eq. (54) together with the recursion relation [37]

$$C^{c\gamma}_{a\alpha;b\beta} = -\left[\frac{4c^2(2c+1)(2c-1)}{(c+\gamma)(c-\gamma)(-a+b+c)(a-b+c)(a+b-c+1)(a+b+c+1)}\right]^{1/2}$$
$$\cdot\left\{\left[\frac{(c-\gamma-1)(c+\gamma-1)(-a+b+c-1)(a-b+c-1)(a+b-c+2)(a+b+c)}{4(c-1)^2(2c-3)(2c-1)}\right]^{1/2} C^{c-2,\gamma}_{a\alpha;b\beta}\right.$$
$$\left. - \frac{(\alpha-\beta)c(c-1)-\gamma a(a+1)+\gamma b(b+1)}{2c(c-1)} C^{c-1,\gamma}_{a\alpha;b\beta}\right\} \tag{71}$$

and the orthonormality condition

$$\sum_{\alpha,\beta} C^{c\gamma}_{a\alpha;b\beta} C^{c'\gamma'}_{a\alpha;b\beta} = \delta_{c'c}\delta_{\gamma'\gamma}, \tag{72}$$

we find that $(X)_{ll'}$ is given by

$$(X)_{ll'} = \frac{2\alpha}{2n+\delta_1+\delta_2}\left(A^{l+1}_{nm}\delta_{l',l+1} + A^{l}_{nm}\delta_{l',l-1}\right) - \frac{\alpha(2|m|+\delta_1+\delta_2)(\delta_1-\delta_2)}{(2l+\delta_1+\delta_2)(2l+\delta_1+\delta_2+2)}\delta_{l'l}, \tag{73}$$

where

$$A^{l}_{nm} = \frac{2}{2l+\delta_1+\delta_2}\left[\frac{(l-|m|)(l+|m|+\delta_1+\delta_2)(l+\delta_1)(l+\delta_2)(n-l)(n+l+\delta_1+\delta_2)}{(2l+\delta_1+\delta_2-1)(2l+\delta_1+\delta_2+1)}\right]^{1/2}. \tag{74}$$

Now by introducing (73) into (68), we get the following three-term recursion relation for the coefficient T^{l}_{nqm}

$$\left[\left(l+\frac{\delta_1+\delta_2}{2}\right)\left(l+\frac{\delta_1+\delta_2}{2}+1\right) + \frac{\alpha R(2|m|+\delta_1+\delta_2)(\delta_2-\delta_1)}{(2l+\delta_1+\delta_2)(2l+\delta_1+\delta_2+2)} - \lambda_q(R)\right] T^{l}_{nqm}(R;\delta_1,\delta_2)$$
$$+ \frac{\alpha R}{2n+\delta_1+\delta_2}\left[A^{l+1}_{nm}T^{l+1}_{nqm}(R;\delta_1,\delta_2) + A^{l}_{nm}T^{l-1}_{nqm}(R;\delta_1,\delta_2)\right] = 0. \tag{75}$$

The recursion relation (75) provides us with a system of $n-|m|$ linear homogeneous equations which can be solved by taking into account the normalization condition

$$\sum_{l=|m|}^{n-1} |T^{l}_{nqm}(R;\delta_1,\delta_2)|^2 = 1. \tag{76}$$

The eigenvalues $\lambda_q(R)$ of the operator Λ then follow from the vanishing of the determinant for the latter system.

Second, let us concentrate on the expansion (67) of the prolate spheroidal basis in terms of the parabolic basis. By employing a technique similar to the one used for deriving Eq. (68), we get

$$\left[\lambda_q(R) + \alpha R\frac{n_1 - n_2 + \frac{\delta_1-\delta_2}{2}}{n + \frac{\delta_1+\delta_2}{2}}\right] U^{n_1}_{nqm}(R;\delta_1,\delta_2) = \sum_{n'_1=0}^{n-|m|-1} U^{n'_1}_{nqm}(R;\delta_1,\delta_2)(M)_{n_1 n'_1}, \tag{77}$$

where

$$(M)_{n_1 n'_1} = \int_0^\infty \int_0^\infty \int_0^{2\pi} \Psi^*_{n_1 n_2 m}(\mu,\nu,\varphi;\delta_1,\delta_2) M \Psi_{n'_1 n'_2 m}(\mu,\nu,\varphi;\delta_1,\delta_2)\, \frac{\mu+\nu}{4} d\mu d\nu d\varphi. \tag{78}$$

The matrix elements $(M)_{n_1 n'_1}$ can be calculated in the same way as $(X)_{ll'}$ except that now we must use the relation [37]

$$\begin{aligned}[(b-a+c)(a-b+c+1)]^{1/2} C^{c\gamma}_{a\alpha;b\beta} &= [(a-\alpha+1)(b-\beta)]^{1/2} C^{c\gamma}_{a+1/2,\alpha-1/2;b-1/2,\beta+1/2} \\ &+ [(a+\alpha+1)(b+\beta)]^{1/2} C^{c\gamma}_{a+1/2,\alpha+1/2;b-1/2,\beta-1/2}\end{aligned} \tag{79}$$

and the orthonormality condition

$$\sum_{c,\gamma} C^{c\gamma}_{a\alpha;b\beta} C^{c\gamma}_{a\alpha';b\beta'} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}, \tag{80}$$

instead of Eqs. (71) and (72). This yields the matrix element

$$\begin{aligned}(M)_{n_1 n'_1} = &\left[(n-n_1-|m|-1)(n_1+1) + (n_1+|m|+\delta_1)(n-n_1+\delta_2) + \frac{1}{4}(\delta_1-\delta_2)(\delta_1-\delta_2-2)\right]\delta_{n'_1 n_1} \\ &-[(n-n_1-|m|-1)(n_1+1)(n_1+|m|+\delta_1+1)(n-n_1+\delta_2-1)]^{1/2}\,\delta_{n'_1,n_1+1} \\ &-[n_1(n-n_1-|m|)(n_1+|m|+\delta_1)(n-n_1+\delta_2)]^{1/2}\,\delta_{n'_1,n_1-1}.\end{aligned} \tag{81}$$

Finally, the introduction of (81) into (77) leads to the three-term recursion relation

$$\begin{aligned}&\left[(n-n_1-|m|-1)(n_1+1)(n_1+|m|+\delta_1)(n-n_1+\delta_2) + \frac{1}{4}(\delta_1-\delta_2)(\delta_1-\delta_2-2)\right. \\ &\left. -\alpha R\frac{2n_1 - n + |m| + 1 + \frac{\delta_1-\delta_2}{2}}{n+\frac{\delta_1+\delta_2}{2}} - \lambda_q(R)\right] U^{n_1}_{nqm}(R;\delta_1,\delta_2) = \\ &[(n-n_1-|m|-1)(n_1+1)(n_1+|m|+\delta_1+1)(n-n_1+\delta_2-1)]^{1/2} U^{n_1+1}_{nqm}(R;\delta_1,\delta_2) \\ &+[n_1(n-n_1-|m|)(n_1+|m|+\delta_1)(n-n_1+\delta_2)]^{1/2} U^{n_1-1}_{nqm}(R;\delta_1,\delta_2)\end{aligned} \tag{82}$$

for the expansion coefficients $U^{n_1}_{nqm}(R;\delta_1,\delta_2)$. This relation can be iterated by taking account of the normalization condition

$$\sum_{n_1=0}^{n-|m|-1} |U^{n_1}_{nqm}(R;\delta_1,\delta_2)|^2 = 1. \tag{83}$$

Here again, the eigenvalues $\lambda_q(R)$ may be obtained by solving a system of $n - |m|$ linear homogeneous equations.

In the case $\delta_1 = \delta_2 = 0$, from Eqs. (75) and (82) we obtain three-term recursion relations for the coefficients of interbasis expansions of the prolate spheroidal basis in spherical and parabolic bases for the hydrogen atom ; these coefficients were calculated in Refs. [28, 44, 45].

Finally, it should be noted that the following four limits

$$\lim_{R\to\infty} U_{nqm}^{n_1}(R;\delta_1,\delta_2) = \delta_{n_1 q}, \qquad \lim_{R\to 0} U_{nqm}^{n_1}(R;\delta_1,\delta_2) = \widetilde{W}_{nqm}^{n_1}(\delta_1,\delta_2), \tag{84}$$

$$\lim_{R\to 0} T_{nqm}^{l}(R;\delta_1,\delta_2) = \delta_{lq}, \qquad \lim_{R\to\infty} T_{nqm}^{l}(R;\delta_1,\delta_2) = W_{nqm}^{l}(\delta_1,\delta_2) \tag{85}$$

furnish a useful means for checking the calculations presented in Sections 5 and 6.

7. Concluding Remarks

One of the main results of this paper concerns the construction of the prolate spheroidal basis for the generalized Kepler-Coulomb system (corresponding to $\delta_1 \neq 0$ and $\delta_2 \neq 0$) as a superposition of either the spherical basis or the parabolic basis. In this respect, our work is a continuation of the pioneer work by Coulson and Joseph [28] on the ordinary Kepler-Coulomb system (corresponding to $\delta_1 = 0$ and $\delta_2 = 0$). We have obtained three-term recursion relations for the coefficients of the interbasis expansions of the prolate spheroidal basis in terms of the spherical basis, on one hand, and of the parabolic basis, on the other hand. These recursion relations can be easily implemented by using symbolic programming languages (like MAPLE, MATHEMATICA, etc.) especially, in the framework of perturbation theory, for small or large values of the spheroidal separation constant R.

We have also calculated the coefficients of interbasis expansions between the spherical basis and the parabolic basis. As we could expect from the limiting case $\delta_1 = \delta_2 = 0$, the latter coefficients are Clebsch-Gordan coefficients for the special unitary group SU(2) modulo an analytic continuation to real values of their arguments.

It was realized long time ago that prolate spheroidal coordinates may be useful in quantum chemistry even in situations exhibiting spherical symmetry [28, 29]. This work shows the relevance of prolate spheroidal coordinates in axial symmetry. This is indeed the kind of symmetry that is encountered in the theory of the chemical bond.

We close this paper with a remark of interest for mathematical physics (and mathematical chemistry). Most of the δ_1- and δ_2-dependent expressions (e.g., the ring-shaped functions) in this work present nice properties with respect to the arguments δ_1 and δ_2. It would be worth to study some of these expressions in connection with the theory of orthogonal polynomials.

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Appendix: An Alternative Proof for the Bi-Orthogonality of the Radial Wavefunctions

We start from two copies of Eq. (15): one for the pair ($E \equiv E_n, R \equiv R_{nl}$) and the other one for ($E \equiv E_{n'}, R \equiv R_{n'l'}$). After multiplication of the first copy (respectively second copy) by $R_{n'l'}$ (respectively R_{nl}) and integration, with the measure $r^2 dr$, on the half real line, we obtain

$$(l' - l)(l + l' + \delta_1 + \delta_2 + 1) \int_0^\infty R_{n'l'}(r; \delta_1, \delta_2) R_{nl}(r; \delta_1, \delta_2)\, dr$$

$$= 2(E_n - E_{n'}) \int_0^\infty R_{n'l'}(r; \delta_1, \delta_2) R_{nl}(r; \delta_1, \delta_2) r^2\, dr. \tag{86}$$

From the latter equation, it readily follows that

$$\int_0^\infty R_{n'l}(r; \delta_1, \delta_2) R_{nl}(r; \delta_1, \delta_2) r^2 dr = 0 \quad \text{for } n' \neq n \tag{87}$$

and

$$\int_0^\infty R_{nl'}(r; \delta_1, \delta_2) R_{nl}(r; \delta_1, \delta_2)\, dr = 0 \quad \text{for } l' \neq l. \tag{88}$$

This completes the proof of the two orthogonality relations $I_{nn'} \sim \delta_{nn'}$ and $J_{ll'} \sim \delta_{ll'}$. It should be emphasized that Eq. (87) turns out to be a direct consequence of the independence of the energy E on the quantum number l.

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