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The N -dimensional Coulomb problem: Stark effect in hyperparabolic and hyperspherical coordinates

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Abstract

We calculate the first-order energy shifts for the N -dimensional hydrogen atom exposed to a static electric field. The results are compared with numerical diagonalization of the Hamiltonian in a finite basis. Using simple scaling relations, we show how corrections to arbitrarily high order may be obtained from known results for the three-dimensional Coulomb problem.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The generalization of three-dimensional quantum problems to higher dimensions is of fundamental interest. In addition, such generalizations are useful in certain aspects of mathematical modelling. For example, the problem of two interacting particles in three dimensions may be described by basis functions corresponding to a six-dimensional extension of three-dimensional noninteracting problems. This is, for example, the essence of the application of six-dimensional hyperspherical coordinates [1] to describe the excitation spectrum of He [2, 3]. Another area of application is in dimensional scaling: energies in three-dimensional space may in some situations be obtained from interpolation or extrapolations from higher dimensions where the particular system may be analytically solvable [4, 5].

The N -dimensional analogy of the hydrogen atom has been studied extensively over the years [1, 6–13] generalizing many of the known properties of three-dimensional hydrogen. In this paper, we add to this theory by investigating the N -dimensional hydrogen atom in the presence of a static electric field. Matrix elements for the linear Stark effect are obtained using a basis of hyperparabolic eigenfunctions for the unperturbed system and results are compared with a numerical diagonalization of the applied electric field in the hyperspherical basis. Moreover, we generalize the scaling approach of Tanaka *et al* [14] to obtain energy corrections to second order in N dimensions. This technique relies on results from the three-dimensional case and may be extended to deal with any order in the perturbation.

For completeness and readability we offer a brief account of the solutions to the N -dimensional Coulomb problem in both hyperspherical and hyperparabolic coordinates. These details as well as the definitions of the coordinates are given in appendix A and appendix B. Atomic units ($\hbar = m_e = e = a_0 = 1$) are used throughout.

2. Stark effect: first- and second-order treatments and numerical diagonalization

The external linear electric field is given as

$$Fx_N = Fr \cos(\phi_{N-1}) = F \frac{1}{2}(\xi - \eta), \quad (1)$$

with F the field strength, and with x_N defined in equations (A.1) and (B.1) in hyperspherical and hyperparabolic coordinates, respectively.

In the following we first pursue the diagonalization of this Hamiltonian to first order in the hyperparabolic set of coordinates. To this end, we note that the hyperparabolic eigenfunctions for the N -dimensional Coulomb problem obtained in appendix B, the so-called Stark states, are also eigenstates of the combined Coulomb potential and linear electric field along the x_N direction within a single shell with principal quantum number n . This is a well-known result from three dimensions and also applies in the general N -dimensional case.

To first order in the perturbation, we have

$$E_n \approx E_n^{(0)} + E_n^{(1)}, \quad (2)$$

where $E_n^{(0)} = 1/[2(n + (N - 3)/2)^2]$ is the field-free energy of level n (see appendix A, (A.8)) and where the first-order correction to the energy $E_n^{(1)} = \langle n | Fx_N | n \rangle$ is evaluated using the eigenstates derived in appendix B and given in (B.6), i.e., $|n\rangle = \mathcal{U} = \mathcal{U}_{n_1, n_2, l_{N-2}, \dots, l_1}(\xi, \eta, \Omega_{N-2}) = f(\xi)g(\eta)\mathcal{Y}(\Omega_{N-2})$ where $\{l_{N-2}, \dots, l_1\}$ are angular momentum quantum numbers and n_1, n_2 are the parabolic quantum numbers. The perturbation does not depend on any of the angles $\phi_1, \dots, \phi_{N-2}$, and therefore no coupling exists between states of different angular quantum numbers $\{l_{N-2}, \dots, l_1\}$. Likewise there is no coupling of states with different n_1 and n_2 [15]. This verifies that the perturbation is diagonal in the Stark basis. Thus the required integration is

$$\int |\mathcal{U}_{n_1, n_2, l_{N-2}, \dots, l_1}|^2 \frac{1}{2} F(\xi - \eta) d^N r. \quad (3)$$

The volume element is given in equation (B.7). All angles integrate to unity, leaving the two-dimensional integral

$$\langle Fx_N \rangle = \frac{1}{8} F \int_0^\infty \int_0^\infty f(\xi)^2 g(\eta)^2 (\xi^2 - \eta^2) (\xi\eta)^{\frac{N-3}{2}} d\xi d\eta, \quad (4)$$

where the integrations over ξ and η are separable and solvable [17]. The result is

$$E_n^{(1)} = \frac{3}{2} F \left(n + \frac{N-3}{2} \right) k, \quad (5)$$

with the Stark quantum number $k = n_1 - n_2$ and the total energy to first order in the perturbation is given by

$$E_n = -\frac{1}{2} \frac{1}{\left(n + \frac{N-3}{2} \right)^2} + \frac{3}{2} F \left(n + \frac{N-3}{2} \right) k. \quad (6)$$

It is easily shown that each principal level splits into $2n - 1$ energy levels. Within a given principal shell, k remains a ‘good’ quantum number and the Stark states remain eigenfunctions. The maximum splitting is related to the degeneracy of the quantum numbers $\{l_{N-1}, l_{N-2}\}$

or $\{(n_1, n_2), l_{N-2}\}$ for given n , giving $n(n + 1)/2$ energy levels. The degeneracy of the hyperspherical harmonics is discussed in [18].

Calculating higher order corrections is tedious. With a simple substitution, however, it is possible to generalize all well-known matrix elements from the three-dimensional Stark effect to higher dimensions. In all matrix elements the integration over ξ and η reduces to integrals which are familiar from the three-dimensional case when substituting $m \rightarrow m - \frac{N-3}{2}, n_1 \rightarrow n_1 - \frac{N-3}{2}, n_2 \rightarrow n_2 - \frac{N-3}{2}$ and $n \rightarrow n - \frac{N-3}{2}$. This is readily verified using the volume element of equation (B.7). Similar substitutions also reduce matrix elements of the radial functions in (A.6) to familiar three-dimensional integrals. The radial part of the volume element is in this case r^{N-1} . This technique was used to calculate second-order energy corrections to the Stark effect in two-dimensional hydrogen [14]. For instance we have the second-order energy corrections in three dimensions [19]

$$E_{3D}^{(2)} = -\frac{F^2}{16}n^4(17n^2 - 3k^2 - 9m^2 + 19), \tag{7}$$

and using the substitutions introduced above, we obtain for general N ,

$$E_{ND}^{(2)} = -\frac{F^2}{16}\left(n + \frac{N-3}{2}\right)^4 \left[17\left(n + \frac{N-3}{2}\right)^2 - 3k^2 - 9\left(m + \frac{N-3}{2}\right)^2 + 19 \right]. \tag{8}$$

Higher order corrections may be obtained as described in [20].

The two-dimensional case is special since both substitutions $m \rightarrow \frac{1}{2}$ and $m \rightarrow -\frac{1}{2}$ transform the matrix elements into the corresponding three-dimensional integrals [14]. Of course one also obtains the linear corrections of (5) with the present scaling approach.

We now compare the first- and second-order results with diagonalization of the Hamiltonian in a restricted basis, $n \leq 6$. In this approach, we take into account the inter-shell mixing that occurs at non-perturbative field strengths and we work in hyperspherical coordinates, cf appendix A. In the numerical calculation the Hamiltonian matrix for the N -dimensional problem is set up with nondiagonal matrix elements of the type $\langle n\mathcal{L}|r \cos(\phi_{N-1})|n'\mathcal{L}'\rangle$, where $|n'\mathcal{L}'\rangle$ are the eigenfunctions of the N -dimensional Coulomb problem, equations (A.6), (A.14). All hyperangles except ϕ_{N-1} integrate to unity, leaving only the evaluation of the matrix elements $\langle n l_{N-1}|r \cos(\phi_{N-1})|n' l'_{N-1}\rangle$. These matrix elements involve the calculation of the angular integral

$$I_{l,l'}^m(N) = \int_{-1}^1 dx (1-x^2)^{m+\frac{N-3}{2}} x C_{l-m}^{(\frac{N-3}{2})}(x) C_{l'-m}^{(\frac{N-3}{2})}(x). \tag{9}$$

Using the three-term recursion relation for Gegenbauer polynomials [15] we obtain two standard integrals. Each of these contribute with non-vanishing matrix elements, provided $\Delta l = \pm 1$. The results are

$$I_{l,l+1}^m(N) = \sqrt{\frac{(l-m)(l+m+N-3)}{(2l+N-4)(2l+N-2)}} \tag{10}$$

and

$$I_{l,l-1}^m(N) = \sqrt{\frac{(l+1)(l+N-2) - m(m+N-3)}{(2l+N)(2l+N-2)}}. \tag{11}$$

The radial integrals may be obtained generalizing the 3D treatment [19].

Figure 1 shows the numerically computed corrections, together with first- and second-order corrections for the selected level with principal quantum number $n = 3$, and for dimensions $N = 3, 4, 6$ and 9 . As expected from (6), we observe an increase in the splitting

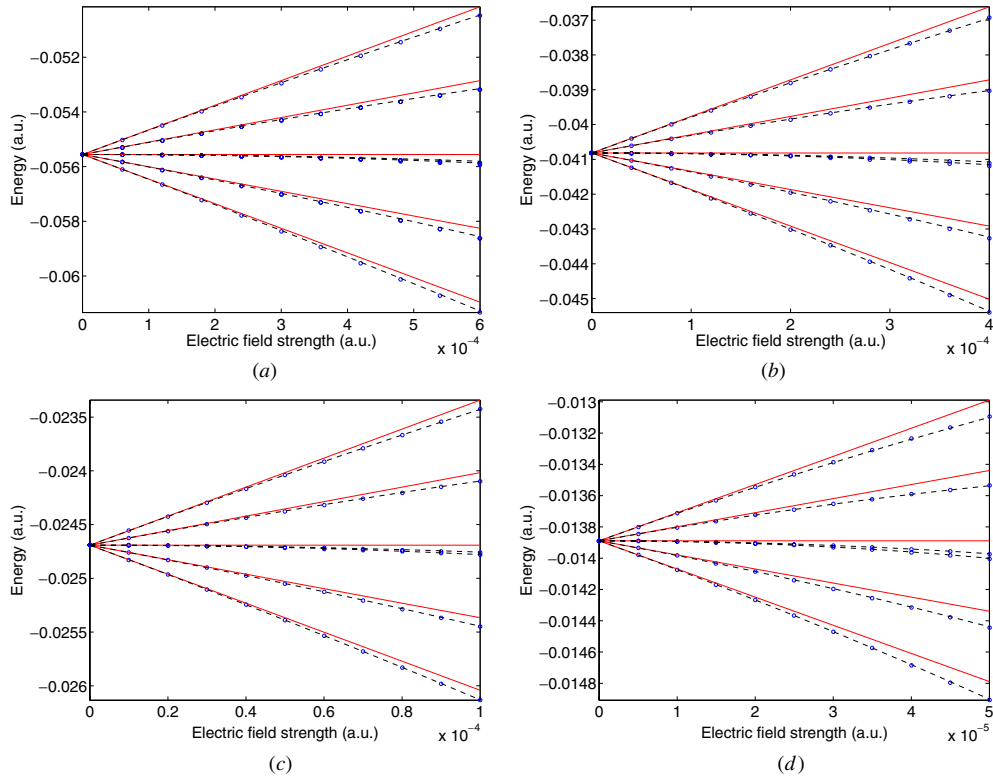


Figure 1. Stark effect in (a): $N = 3$, (b): $N = 4$, (c): $N = 6$ and (d): $N = 9$ dimensional hydrogen for principal shell $n = 3$. The curves show the diverging prediction of results obtained in first-order perturbation theory (solid curve), second-order perturbation theory (dashed curve), and numerical results (circles) obtained by diagonalization of the Hamiltonian matrix in a basis with $n \leq 6$.

with N . This follows from an accompanying increase in the polarizability of the system. From the figure, we see an excellent agreement between the two first-order scaling relations for weak fields. As expected, both the numerical and second-order energy levels diverge from those predicted with linear theory, due to interactions between principal shells for higher field strengths. Note a splitting in five energy levels for the solid lines contrary to a splitting in six levels for the exact diagonalization and second-order corrections. Even for arbitrarily small field strengths, there is a coupling to the continuum under the Stark perturbation; although for low n and weak fields this can often be neglected. The diagonalization above uses a limited basis of bound state functions (L2) and does not include the continuum, while the second-order results incorporates continuum corrections. Due to the excellent agreement between these results, we conclude that continuum contributions are negligible in the considered regime.

3. Summary and conclusion

In this paper we investigated the Stark effect in N -dimensional hydrogen. We calculated the first- and second-order corrections and compared these energies with results obtained by numerical matrix diagonalization. The comparison showed that the first-order theory performs excellent in the weak-field limit for any dimension N . For higher field strengths, we found good agreement between the numerical result obtained in a finite basis and the second-order result.

Apart from the fundamental results presented here, the present theory adds to the basis for applications of hyperspherical or hyperparabolic basis functions in the theoretical/computational description of few or many particle problems in atomic physics such as, e.g., dynamics of electrons in parabolic quantum dots or many-electron atoms exposed to intense light sources.

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Appendix A. The N -dimensional Coulomb problem: separation in hyperspherical coordinates

The hyperspherical coordinates are

$$\begin{aligned} x_1 &= r \sin(\phi_{N-1}) \sin(\phi_{N-2}) \dots \sin(\phi_1), \\ x_2 &= r \sin(\phi_{N-1}) \sin(\phi_{N-2}) \dots \cos(\phi_1), \\ &\vdots \\ x_{N-1} &= r \sin(\phi_{N-1}) \cos(\phi_{N-2}), \\ x_N &= r \cos(\phi_{N-1}), \end{aligned} \quad (\text{A.1})$$

with $r = (\sum_{i=1}^N x_i^2)^{1/2}$ the hyperradius. The hyperangles $\{\phi_2 \dots \phi_{N-1}\}$ range from 0 to π and ϕ_1 range from 0 to 2π [10].

In the Schrödinger equation $\{-\frac{1}{2}\nabla^2 + V(\vec{r})\}\Psi(r, \Omega) = E\Psi(r, \Omega)$, the Laplace operator is given by [21],

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r} \frac{\partial}{\partial r} - \frac{1}{r^2} \hat{\Lambda}^2(N), \quad (\text{A.2})$$

where the grand angular momentum operator, $\hat{\Lambda}^2(N)$, may be written recursively

$$-\hat{\Lambda}^2(N) = \frac{\partial^2}{\partial \phi_{N-1}^2} + (N-2) \cot(\phi_{N-1}) \frac{\partial}{\partial \phi_{N-1}} - \frac{\hat{\Lambda}^2(N-1)}{\sin^2(\phi_{N-1})} \quad \text{for } N \geq 2, \quad (\text{A.3})$$

defining $\hat{\Lambda}^2(1) = 0$. For a central symmetric potential, $V(r)$, the Schrödinger equation is separable in a radial and an angular part, $\Psi(r, \Omega) = R(r)\mathcal{Y}(\Omega_N)$. The corresponding equations read

$$\hat{\Lambda}^2(N)\mathcal{Y}(\Omega_N) = l_{N-1}(l_{N-1} + N - 2)\mathcal{Y}(\Omega_N) \quad (N > 1), \quad (\text{A.4})$$

$$\left[-\frac{1}{2} \left(\frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} - \frac{l_{N-1}(l_{N-1} + N - 2)}{r^2} \right) + V(r) \right] R(r) = ER(r). \quad (\text{A.5})$$

A.1. Radial solutions for the $-1/r$ potential

For the N -dimensional hydrogen atom we use the generalized Coulomb potential $-1/r$. The radial solutions are analogous to the three-dimensional solutions [22],

$$R_{nl}(\rho) = \mathcal{N}_{nl} e^{-\rho/2} \rho^l h(\rho), \quad (\text{A.6})$$

with the scaled coordinate $\rho = 2\epsilon r$, where ϵ defines the energy $E = -\frac{1}{2}\epsilon^2$. The function $h(\rho)$ is a generalized Laguerre polynomial, $L_{\frac{1}{\epsilon}+1/2-N/2-l_{N-1}}^{(2l_{N-1}+N-2)}(\rho)$ [15]. Details on the N -dimensional generalization can be found elsewhere [16]. With the principal quantum number

$$n = \frac{1}{\epsilon} - \frac{N-3}{2}, \tag{A.7}$$

we have $n = 1, 2, 3, \dots$ and $l_{N-1} \leq n - 1$, together with the energy

$$E_n = -\frac{1}{2\left(n + \frac{N-3}{2}\right)^2}, \quad n = 1, 2, 3, \dots \tag{A.8}$$

The normalization constant is calculated using the properties of Laguerre polynomials [15] and an integral given in [17],

$$\mathcal{N}_{nl} = \frac{2^{N/2}}{\left(n + \frac{N-3}{2}\right)^{N/2}} \times \left(\frac{\Gamma(n-l)}{2\left(n + \frac{N-3}{2}\right)\Gamma(n+l+N-2)} \right)^{1/2}. \tag{A.9}$$

A.2. Angular solutions

The recursiveness of the grand angular momentum operator (A.3) suggests that the angular solutions may be separated

$$\mathcal{Y}(\Omega_N) = \Theta(\phi_{N-1})\mathcal{Y}(\Omega_{N-1}), \tag{A.10}$$

where $\mathcal{Y}(\Omega_{N-1}) = \mathcal{Y}(\phi_{N-2}, \dots, \phi_1)$ is an eigenfunction of $\hat{\Lambda}^2(N-1)$. This separations is seen for instance in [1, 6, 9]. Given the solution in $N-1$ dimensions, all we need to solve is

$$\left[\frac{\partial^2}{\partial\phi_{N-1}^2} + (N-2)\cot(\phi_{N-1})\frac{\partial}{\partial\phi_{N-1}} + l_{N-1}(l_{N-1} + N - 2) - \frac{l_{N-2}(l_{N-2} + N - 3)}{\sin^2(\phi_{N-1})} \right] \Theta(\phi_{N-1}) = 0. \tag{A.11}$$

The angular solutions to equation (A.4) are thus obtained recursively from the solutions in lower dimensions. For the case $N = 2$ equation (A.11) becomes $\left[\frac{\partial^2}{\partial\phi_1^2} + l_1^2 \right] \Theta(\phi_1) = 0$, and we obtain the exponential function $e^{il_1\phi_1}$, for $|l_1| = 0, 1, 2, \dots$. The total angular functions for general N are named *hyperspherical harmonics* giving the familiar spherical harmonics for $N = 3$.

We now proceed to solve (A.11): for simplicity we substitute $l_{N-2} = m$ and $l_{N-1} = l$ in the following. Introducing also $x = \cos(\phi_{N-1})$ yields

$$\left[(1-x^2)\frac{\partial^2}{\partial x^2} - (N-1)x\frac{\partial}{\partial x} + l(l+N-2) - \frac{m(m+N-3)}{1-x^2} \right] \Theta(x) = 0. \tag{A.12}$$

Given that $\Theta_l^{(N)}(x)$ solves (A.12) for $m = 0$, it can be shown by induction that $\Theta_{lm}^{(N)}(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} \Theta_l^{(N)}(x)$ solves (A.12) for general m . For $N = 3$ we recognize the Legendre and associated Legendre polynomials. Equation (A.12) with $m = 0$ is a known differential equation whose solutions are the Gegenbauer polynomials [23], $\mathcal{C}_n^\alpha(x)$. Accordingly, the final solutions to equation (A.12) may be expressed as

$$\Theta_{lm}^{(N)}(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} \mathcal{C}_l^{\left(\frac{N-2}{2}\right)}(x) \sim (1-x^2)^{\frac{m}{2}} \mathcal{C}_{l-m}^{\left(\frac{N-2}{2}+m\right)}(x). \tag{A.13}$$

The hyperspherical harmonics are products of these solutions (recall we had $x = \cos \phi_{i-1}$, $i = 2, \dots, N$)

$$\mathcal{Y}_{\mathcal{L}}(\Omega_N) = \mathcal{N}_{\mathcal{L}} \Theta_{l_{N-1}, l_{N-2}}^{(N)}(\phi_{N-1}) \Theta_{l_{N-2}, l_{N-3}}^{(N-1)}(\phi_{N-2}) \dots \Theta_{l_2, l_1}^{(3)}(\phi_2) \Theta_{l_1}^{(2)}(\phi_1). \tag{A.14}$$

Here \mathcal{L} denotes the set of angular quantum numbers $\{l_{N-1}, l_{N-2}, \dots, l_1\}$. Note that all but $\Theta_{l_1}^{(2)} = e^{i l_1 \phi_1}$ are on the form of equation (A.13). The orthogonality of the hyperspherical harmonics follows directly from the hermiticity of the grand angular momentum operator. The volume element is given by,

$$|d\Omega_N| = [\sin^{N-3}(\phi_{N-1})d(\cos(\phi_{N-1}))] \cdots [\sin(\phi_3)d(\cos(\phi_3))][d(\cos(\phi_2))] d\phi_1. \quad (\text{A.15})$$

This yields for the normalization constant $\mathcal{N}_{\mathcal{L}}$, cf. [15],

$$\mathcal{N}_{\mathcal{L}} = \frac{1}{\sqrt{2\pi}} \prod_{i=3}^N 2^{l_{i-2} + \frac{1}{2}i - 2} \Gamma\left(\frac{i-2}{2} + l_{i-2}\right) \left[\frac{(l_{i-1} - l_{i-2})!(2l_{i-1} + i - 2)}{\pi \Gamma(l_{i-1} + l_{i-2} + i - 2)} \right]^{1/2}. \quad (\text{A.16})$$

The angular quantum numbers obey,

$$l_1 = 0, \pm 1, \dots, \pm l_2; \quad l_2 = 0, 1, \dots, l_3; \quad \dots; \quad l_{N-1} = 0, 1, \dots, n - 1. \quad (\text{A.17})$$

Appendix B. The N -dimensional Coulomb problem: separation in hyperparabolic coordinates. Stark states

The hyperparabolic coordinates are

$$\begin{aligned} x_1 &= \sqrt{\xi\eta} \sin(\phi_{N-2}) \dots \sin(\phi_1), \\ x_2 &= \sqrt{\xi\eta} \sin(\phi_{N-2}) \dots \cos(\phi_1), \\ &\vdots \\ x_{N-1} &= \sqrt{\xi\eta} \cos(\phi_{N-2}), \\ x_N &= \frac{1}{2}(\xi - \eta), \end{aligned} \quad (\text{B.1})$$

were the parabolic coordinates ξ and η , range from 0 to $+\infty$. The Schrödinger equation reads [9],

$$\left\{ \frac{4}{\xi + \eta} \left[\Delta(\xi) + \Delta(\eta) - \frac{\xi + \eta}{4\xi\eta} \hat{\Lambda}^2(\Omega_{N-1}) \right] + 2E + \frac{4}{\xi + \eta} \right\} \mathcal{U}_{n_1, n_2, l_{N-2}, \dots, l_1} = 0, \quad (\text{B.2})$$

with $\hat{\Lambda}^2$ defined in (A.3) and with the Laplacian $\Delta(\xi)$

$$\Delta(\xi) = \xi^{-\frac{N-3}{2}} \frac{\partial}{\partial \xi} \xi^{\frac{N-1}{2}} \frac{\partial}{\partial \xi}, \quad (\text{B.3})$$

and similarly for $\Delta(\eta)$. Thus the angular part can again be separated out. The solutions are the hyperspherical harmonics, $\mathcal{Y}_{l_{N-2}, \dots, l_1}(\phi_{N-2}, \dots, \phi_1)$ whose eigenvalues are $l_{N-2}(l_{N-2} + N - 3)$. The equation can further be separated in the two parabolic coordinates, $\mathcal{U}_{n_1, n_2, l_{N-2}, \dots, l_1}(\xi, \eta, \Omega_{N-2}) = f(\xi)g(\eta)\mathcal{Y}(\Omega_{N-2})$ yielding for $f(\xi)$,

$$\left\{ \xi \frac{\partial^2}{\partial \xi^2} + \frac{N-1}{2} \frac{\partial}{\partial \xi} + \left(\frac{E\xi}{2} - \frac{1}{4\xi} m(m + N - 3) + v_1 \right) \right\} f(\xi) = 0, \quad (\text{B.4})$$

with $m = l_{N-2}$, and similarly for $g(\eta)$, only with the separation constant v_1 replaced with v_2 . Furthermore $v_1 + v_2 = 1$. As with the radial equation in hyperspherical coordinates the solutions are on the product form $f(\xi) = e^{-\frac{1}{2}\epsilon\xi} \xi^{\frac{m}{2}} u(\xi)$, where $u(\xi)$ is a Laguerre polynomial [15],

$$u(x) = L_{n_1}^{m + \frac{N-3}{2}}(x), \quad n_1 = \frac{v_1}{\epsilon} - \frac{1}{2} \left(m + \frac{N-1}{2} \right). \quad (\text{B.5})$$

Again $E = -\frac{1}{2}\epsilon^2$ and $x = \xi\epsilon$. Similar results are obtained for $g(\eta)$ giving the complete solution to the original Schrödinger equation,

$$\mathcal{U}_{n_1, n_2, l_{N-2}, \dots, l_1} = \mathcal{N}_{n_1, n_2} e^{-\frac{1}{2}\epsilon(\xi+\eta)} \xi^{\frac{m}{2}} \eta^{\frac{m}{2}} L_{n_1}^{m+\frac{N-3}{2}}(\epsilon\xi) L_{n_2}^{m+\frac{N-3}{2}}(\epsilon\eta) \mathcal{Y}(\Omega_{N-2}). \quad (\text{B.6})$$

We shall refer to these solutions as the Stark states. The volume element is

$$d^N r = \frac{1}{4}(\xi + \eta)(\xi\eta)^{\frac{N-3}{2}} d\xi d\eta d\Omega_{N-2}. \quad (\text{B.7})$$

With the normalization of the hyperspherical harmonics, see (A.16), we obtain for the normalization constant [15],

$$\mathcal{N}_{n_1, n_2} = \frac{\sqrt{2}}{\left(n + \frac{N-3}{2}\right)^{m+(N+1)/2}} \left(\frac{n_1! n_2!}{\Gamma(n_1 + m + \frac{1}{2}(N-1)) \Gamma(n_2 + m + \frac{1}{2}(N-1))} \right)^{1/2}. \quad (\text{B.8})$$

We obtain the energy $E = -\frac{1}{2(n_1+n_2+m+\frac{N-1}{2})^2}$ giving the relation between the quantum numbers n_1, n_2 and m , and the principal quantum number n ,

$$n = n_1 + n_2 + m + 1. \quad (\text{B.9})$$

For the case $N = 3$, m corresponds to the magnetic quantum number and the absolute value should be used.

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