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Exact atomic wavefunctions: a generalised power series expansion using hyperspherical coordinates

H Klar†

Fakultät für Physik der Universität Freiburg, Hermann-Herder-Strasse 3, D-7800 Freiburg, West Germany

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Abstract. The Schrödinger equation for an atom having N electrons ($N = 1, 2, 3, \dots$) has been solved exactly within the framework of generalised power series. The members of this series can easily be calculated from a two-term recursion. The present formulation is suitable both for computational as well as for analytical work.

1. Introduction

Exact atomic wavefunctions were first considered by Fock (1958) in the case of helium in the 1S symmetry. Fock introduced hyperspherical coordinates to describe the position vectors of the two electrons r_i ($i = 1, 2$) putting

$$\begin{aligned} r &= (r_1^2 + r_2^2)^{1/2} \\ \tan \alpha &= r_1 / r_2 \\ \cos \vartheta &= \hat{r}_1 \cdot \hat{r}_2 \end{aligned} \tag{1}$$

and showed that exact eigenfunctions possess in the neighbourhood of the point $r = 0$ an expansion of the structure

$$\psi(r, \alpha, \vartheta) = \sum_{n=0}^{\infty} r^n \sum_{m=0}^{[n/2]} (\ln r)^m \psi_{nm}(\alpha, \vartheta). \tag{2}$$

Substituting this ansatz into the wave equation for helium he derived a coupled system of equations for the angular functions $\psi_{nm}(\alpha, \vartheta)$. The actual calculation of the angular functions however turns out to be extremely difficult. We remark also that the Fock expansion, equation (2), represents one particular solution that is finite at the origin ($r = 0$). Fock did not derive expansions for other linearly independent solutions in order to construct a fundamental system of solutions. Application of physical boundary conditions needs such a complete system of solutions.

Fock expansions in terms of hyperspherical partial waves have been investigated by Knirk (1974a, b) for many-electron atoms of any symmetry. Knirk derived a coupled system of hyperradial equations, and following Nyswander (1929) he obtained an expansion of radial functions into power of r and into powers of $\ln r$. The calculation of the expansion coefficients requires either multiple derivatives with respect to some parameter (Knirk 1974a) or the treatment of two-dimensional algebraic recurrence

† Present address: Fachbereich Physik, Universität Kaiserslautern, D6750 Kaiserslautern, West Germany.

relations (Knirk 1974b). Both methods are very difficult to handle, and inconvenient for numerical computation.

Knirk's approach was recently reconsidered by Haftel and Mandelzweig (1983) for three-body Coulomb systems. These authors solve the system of hyperradial equations following a method described by Gantmacher (1959). Gantmacher derives generalised power series solutions for first-order systems of ordinary differential equations with one weak singularity. This power series contains matrix powers of the independent variable (r in our case). Logarithmic terms are thus generated by upper or lower triangular matrices as an exponent of r . Haftel and Mandelzweig (1983) apply Gantmacher's method to second-order systems. Their system of recurrence relations for a truncated set of differential equations has a triangular structure, i.e. the n th order matrix coefficient as the solution of the recurrence formula requires knowledge of *all* matrices of lower order. Nevertheless, this procedure does not require matrix inversions, and is suitable for numerical computation. The procedure also allows the construction of regular and irregular fundamental systems. The convergence of this generalised power series was shown by Gantmacher (1959).

The method described in this article to solve hyperradial equations for N -electron atoms ($N \geq 1$) is based on a more modern treatment of first-order linear systems with one weak singularity (Harris *et al* 1969, Walter 1976). We show explicitly that our second-order system of equations to be solved is equivalent to a first-order system that belongs to that class of first-order systems treated by Walter (1976). In our particular case of Coulomb systems, however, we have got the impression that it is easier to attack directly the second-order equations. In contrast to earlier work of other authors we derive a two-term recursion formula which can immediately be solved in any order. Our method may be regarded as formal generalisation of the standard treatment for the hydrogen atom. The method allows us to construct regular and irregular fundamental systems.

The paper is organised as follows. Section 2 derives the system of equations to be solved. Section 3 develops generalised power series solutions, and § 4 constructs a regular fundamental system of solutions. A rigorous proof for the convergence of the generalised power series presented here will be given elsewhere (Klar 1984).

2. Preliminaries

We start from the Hamiltonian (in atomic units) of an atom with N electrons

$$H = \sum_{i=1}^N \left(\frac{1}{2} \mathbf{p}_i^2 - \frac{z}{r_i} \right) + \sum_{i < j} \frac{1}{r_{ij}} \quad (3)$$

and look for stationary solutions ψ ,

$$H\psi = E\psi. \quad (4)$$

In configuration space representation equation (4) is a partial differential equation depending on $3N$ variables. This form is rather inconvenient for a mathematical investigation. Below we will convert equation (4) into a linear system of ordinary differential equations, since the theory for such systems is better established than for partial differential equations.

To this end we introduce hyperspherical coordinates (r, ω) parametrising the electron position vectors

$$\mathbf{r}_i = r f_i(\omega) \quad (5)$$

with

$$\sum_{i=1}^N f_i(\omega)^2 = 1 \quad (6)$$

i.e.

$$r = \left(\sum_{i=1}^N r_i^2 \right)^{1/2}. \quad (7)$$

The quantity r is called the hyperradius and the symbol ω stands for a set of $3N-1$ angles. The choice of the parametrisation $f_i(\omega)$ is not important here. A particular parametrisation was given for instance by Knirk (1974a). For two-electron systems (helium-like atoms) two alternative parametrisations are frequently used (see Fano 1983). For helium S-states Fock (1958) used the parametrisation given in equation (1). The Hamiltonian equation (3) reads in hyperspherical coordinates

$$H = -\frac{1}{2} r^{1-3N} \frac{\partial}{\partial r} r^{3N-1} \frac{\partial}{\partial r} + \frac{\Lambda^2}{2r^2} + \frac{C(\omega)}{r}. \quad (8)$$

Here Λ^2 is the sum of the squared generators for rotations in $3N$ dimensions. This operator is independent of r and acts only in the angles ω . The function $C(\omega)$, also independent of r , is equal to the total potential energy multiplied by r :

$$C(\omega) = r \left(-Z \sum_{i=1}^N \frac{1}{r_i} + \sum_{i<j} \frac{1}{r_{ij}} \right). \quad (9)$$

Next we introduce antisymmetry-adapted hyperspherical harmonics (Knirk 1974a). These are harmonics on the sphere

$$S_{3N-1} = \{(\mathbf{r}_1, \dots, \mathbf{r}_N) | r = 1\} \quad (10)$$

and eigenfunctions of the total spin. A complete description of how to construct these antisymmetry-adapted harmonics was given by Knirk (1974a) and we refer the reader to that work. Here we need only that these harmonics are eigenfunctions of the operator Λ^2 :

$$\Lambda^2 Y_{\lambda g}(\omega) = \lambda(\lambda + 3N - 2) Y_{\lambda g}(\omega) \quad (11)$$

with $\lambda = 0, 1, 2, \dots$. Each eigenvalue $\lambda \neq 0$ is, in general, degenerate; degenerate states within a λ multiplet are labelled by the index $g = g(\lambda)$.

Since the antisymmetry-adapted harmonics form a complete set of orthonormal functions on $S_{3N-1} \times \Sigma$, Σ being the spin space, we may expand the wavefunction according to

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{\lambda g} \psi_{\lambda g}(r) Y_{\lambda g}(\omega) \quad (12)$$

where the spin variables are not explicitly written down. It is expected that this series converges in the mean (Erdélyi *et al* 1953, p241f), i.e.

$$\lim_{\lambda' \rightarrow \infty} \int d\omega \left| \psi(\mathbf{r}_1, \dots, \mathbf{r}_N) - \sum_{\lambda=\lambda_{\min}}^{\lambda'} \sum_g \psi_{\lambda g}(r) Y_{\lambda g}(\omega) \right|^2 = 0. \quad (13)$$

Substitution of equation (12) into equation (4) leads to a system of second-order ordinary differential equations:

$$\left(-\frac{1}{2} r^{1-3N} \frac{\partial}{\partial r} r^{3N-1} \frac{\partial}{\partial r} + \frac{\lambda(\lambda+3N-2)}{2r^2} \right) \psi_{\lambda g}(r) + \frac{1}{r} \sum_{\lambda' g'} C_{\lambda g \lambda' g'} \psi_{\lambda' g'}(r) = E \psi_{\lambda g}(r) \quad (14)$$

with the constant Hermitian matrix

$$C_{\lambda g \lambda' g'} = \int d\omega Y_{\lambda g}(\omega)^\dagger C(\omega) Y_{\lambda' g'}(\omega). \quad (15)$$

For two-electron systems, for instance, this matrix can be calculated analytically (Klar and Klar 1980, Pelikan and Klar 1983).

In the following we use matrix notation and rewrite equation (14) in the form

$$\left(-\frac{1}{2} r^{1-3N} \frac{\partial}{\partial r} r^{3N-1} \frac{\partial}{\partial r} + \frac{1}{2r^2} \Lambda(\Lambda+3N-2) + \frac{1}{r} C - E \right) \psi(r) = 0. \quad (16)$$

Here $\psi(r)$ is the column vector with components $\psi_{\lambda g}(r)$, Λ is the diagonal matrix with components

$$\Lambda_{\lambda g \lambda' g'} = \lambda \delta_{\lambda \lambda'} \delta_{g g'} \quad (17)$$

and the elements of the matrix C are given in equation (15). Below the threshold for N free electrons ($E < 0$) we put

$$\kappa^2 = -2E. \quad (18)$$

Further it is convenient to use the variable

$$z = \kappa r \quad (19)$$

and to introduce the vector $\phi(z)$ by

$$\psi(r) = \exp(-z) \phi(z). \quad (20)$$

Equation (16) then reads

$$\left[\frac{d^2}{dz^2} + \left(\frac{3N-1}{z} - 2 \right) \frac{d}{dz} - \frac{1}{z^2} \Lambda(\Lambda+3N-2) - \frac{1}{z} \left(\frac{2}{\kappa} C + 3N-1 \right) \right] \phi(z) = 0. \quad (21)$$

Let us briefly look at the behaviour of solutions of equation (21) at the origin $z=0$. Disregarding terms with $1/z$ we find constant vectors

$$\phi_0 = \lim_{z \rightarrow 0} z^{-\alpha} \phi(z) \quad (22)$$

with

$$\alpha = \begin{cases} \lambda_0 & \text{for regular solutions} \\ -\lambda_0 - 3N + 2 & \text{for irregular solutions.} \end{cases} \quad (23)$$

In the special case of a diagonal matrix C solutions of equation (21) are confluent hypergeometric functions describing a hydrogen atom in $d=3N$ dimensions. For a non-diagonal matrix C equation (20) has no trivial 'matrix generalisation' of a Kummer

series as a solution because the eigenvalues λ are integers. This last circumstance leads to logarithmic terms in power series expansions.

3. Generalised power series solutions

Equation (21) is equivalent to a first-order system with one weak singularity at $z = 0$,

$$W(z)' = z^{-1}(A_0 + zA_1)W(z), \tag{24}$$

For such systems generalised power series solutions are known (Nyswander 1929, Gantmacher 1959, Walter 1976). Before we apply this technique to the second-order equation (21) we show the equivalence between equations (21) and (24). To this end we introduce the auxiliary vector

$$u(z) = \phi(z)' - \frac{1}{z} \Lambda \phi(z)$$

and put

$$W(z) = \begin{pmatrix} \phi(z) \\ u(z) \end{pmatrix}.$$

With help of the identity

$$\left(\frac{d}{dz} + \frac{\lambda + 3N - 1}{z}\right)\left(\frac{d}{dz} - \frac{\lambda}{z}\right) = \frac{d}{dz^2} + \frac{3N - 1}{z} \frac{d}{dz} + \frac{\lambda(\lambda + 3N - 2)}{z^2}$$

we obtain an equation having the structure of equation (24) where the constant matrices A_0 and A_1 are given by

$$A_0 = \begin{bmatrix} \Lambda & \mathbf{0} \\ 2\Lambda + (2/\kappa)C + (3N - 1)\mathbb{1} & -\Lambda - (3N - 1)\mathbb{1} \end{bmatrix}$$

$$A_1 = \begin{bmatrix} \mathbf{0} & \mathbb{1} \\ \mathbf{0} & 2\mathbb{1} \end{bmatrix}.$$

In our example however it is more advantageous to solve directly the second-order equation for two reasons:

(a) One circumvents the calculation of the unnecessary auxiliary vectors $u(z)$.

(b) Recursion formulae for the members of a power series are easier to solve for second-order equations than for first-order equations.

We start therefore solving equation (21) employing the ansatz

$$\phi(z) \equiv \varphi(s) = \sum_{k=0}^{\infty} \exp[(\alpha + k)s]\varphi_k(s) \tag{25}$$

with $z = e^s$ and α given by equation (23).

From the behaviour at $z = 0$ (see equation (23)), we conclude that the vector $\phi_0(s)$ in equation (25) must be constant (independent of s) and equal to

$$\varphi_0 = \lim_{z \rightarrow 0} z^{-\alpha} \phi(z) = \phi_0. \tag{26}$$

Now we put the expansion (25) into equation (21) and thus obtain the following set of equations for the vectors $\phi_k(s)$:

for $k = 0$:

$$(\lambda_0 \mathbb{1} - \Lambda)\varphi_0 = 0 \tag{27}$$

for $k \geq 1$:

$$\begin{aligned} \varphi_k(s)'' + (2\alpha + 2k + 3N - 2)\varphi_k(s)' + [(\alpha + k)(\alpha + k + 3N - 2) - \Lambda(\Lambda + 3N - 2)]\varphi_k(s) \\ = 2\varphi_{k-1}(s)' + \left(\frac{2}{\kappa} C + 2k + 3\alpha + 3N - 3\right)\varphi_{k-1}(s). \end{aligned} \tag{28}$$

In order to solve equation (28) it is convenient to rewrite this equation in factorised form

$$\begin{aligned} (D + \alpha + k + 3N - 2 + \Lambda)(D + \alpha + k - \Lambda)\varphi_k(s) \\ = \left(2D + \frac{2}{\kappa} C + 2\alpha + 2k + 3N - 3\right)\varphi_{k-1}(s) \end{aligned} \tag{28'}$$

with

$$D = \frac{d}{ds}. \tag{29}$$

Assume now that the RHS of equation (28') is a polynomial vector of degree $m \geq 0$. Then there exists a unique solution $\phi_k(s)$ provided the two diagonal matrices

$$M_1 = (\alpha + k + 3N - 2)\mathbb{1} + \Lambda \tag{30a}$$

and

$$M_2 = (\alpha + k)\mathbb{1} - \Lambda \tag{30b}$$

are regular. It is easily seen that this solution is a polynomial vector of the same degree m . If however at least one of the matrices M_i ($i = 1, 2$) is singular equation (28') has more than one polynomial solution $\phi_k(s)$ of degree $m + 1$. This has the following consequences. For *regular solutions* ($\alpha = \lambda_0 \geq 0$) the matrix M_1 is regular because all diagonal elements are positive ($k \geq 1, N \geq 1$). The matrix M_2 is singular in the block $\lambda = \lambda' = \lambda_0 + k$. Since parity conservation connects in the matrix C only even (odd) values with even (odd) values of λ the matrix M_2 becomes singular only for even values of $k \geq 2$. Therefore regular solutions consist of vector polynomials $\phi_k(s)$ whose degree is

$$\text{deg } \varphi_k(s) = [k/2]. \tag{31}$$

For *irregular solutions* ($\alpha = -\lambda_0 - 3N + 2$) the situation is less obvious because both matrices M_i ($i = 1, 2$) may become singular. M_1 becomes singular in the block $\lambda = \lambda' = \lambda_0 - k$; this is possible for $k = 2, 4, \dots, (\lambda_0 - \lambda_{\min})$ where λ_{\min} , depending on spin and parity, is the smallest value of λ appearing in the expansion (12). The matrix M_2 becomes singular in the block $\lambda = \lambda' = -\lambda_0 - 3N + 2 + k$; this is possible for $k \geq \lambda_0 + \lambda_{\min} + 3N - 2$ which may be even or odd. The degree of irregular vector polynomials is therefore

$$\text{deg } \varphi_k(s) = \begin{cases} \frac{1}{2}(\lambda_0 - \lambda_{\min}) & \text{for } k < \lambda_0 + \lambda_{\min} + 3N - 2 \\ [(k - 3N + 4)/2] - \lambda_{\min} & \text{for } k \geq \lambda_0 + \lambda_{\min} + 3N - 2. \end{cases} \tag{32}$$

Note that $\lambda_0 - \lambda_{\min}$ is even and not negative.

Let us briefly consider the hydrogen atom in $d = 3N$ dimensions. All λ states are then decoupled because the matrix C is diagonal in this case. For regular solutions both matrices M_i ($i = 1, 2$) are then regular, i.e. regular Coulomb wavefunctions contain no logarithmic terms. For irregular solutions the matrix M_2 becomes singular at one k value only, given by $k_0 = 2\lambda_0 + 3N - 2$. The expansion (25) for irregular Coulomb wavefunctions therefore contains linear terms in $s = \ln z$

$$\phi(z) = A(z) \ln z + B(z)$$

where $A(z)$ and $B(z)$ have power series expansions with leading terms z^{λ_0} and $z^{-(\lambda_0 + 3N - 2)}$, respectively. This is in agreement with Abramowitz and Stegun (1964) for $N = 3$.

4. Regular solutions

We now focus attention on regular solutions putting $\alpha = \lambda_0$ in equation (28'). We define a sequence of operators

$$O_k = (D + \lambda_0 - \mathbf{A} + k)^{-1} (D + \lambda_0 + 3N - 2 + \mathbf{A} + k)^{-1} \left(D + \frac{1}{\kappa} C + \lambda_0 + \frac{3}{2} N - \frac{3}{2} + k \right) \quad (33)$$

$k \geq 1$. The inverse of an operator $D + a$, $a \in \mathbb{R}$, which appears in equation (33) has to be defined such that

$$y(s) = (D + a)^{-1} q(s) \quad (34)$$

is a polynomial solution of the equation

$$y'(s) + ay(s) = q(s)$$

provided $q(s)$ is a polynomial. We obtain

$$(D + a)^{-1} = \begin{cases} \sum_{n=0}^{\infty} (-1)^n a^{-(n+1)} D^n & \text{for } a \neq 0 \\ D^{-1} & \text{for } a = 0 \end{cases} \quad (35)$$

where D^{-1} means integration:

$$D^{-1} q(s) = y_0 + \int_{s_0}^s ds' q(s'). \quad (36)$$

In terms of the operator O_k equation (28') may be written in the form

$$\phi_k(s) = 2O_k \phi_{k-1}(s). \quad (37)$$

Without loss of generality we standardise the solution vectors $\phi_k(s)$ putting

$$D^{-1} q(s) = \int_0^s ds' q(s') \quad (36)$$

instead of equation (36). This special choice is obviously permitted. Assume we solve a truncated system of dimension N_0 . This system has N_0 regular, linearly independent solution vectors $\phi^{(n)}(z)$, $n = 1, \dots, N_0$ which may generated, for instance, from linear

combinations of standardised vectors $\phi_{st}^{(n)}(z)$:

$$\phi^{(n)}(z) = \sum_{m=1}^{N_0} \phi_{st}^{(m)}(z) c_{mn} \tag{38}$$

provided the standardised vectors are linearly independent. Our standardisation (36') corresponds therefore to a transformation given by (38). The standardised vector solutions are linearly independent for all values of z if they are linearly independent at one value of z . It is therefore sufficient to start with linearly independent solutions ϕ_0 of equation (27).

With the above notations the polynomial vectors $\varphi(s)$ are given by

$$\varphi_k(s) = 2^k \prod_{l=0}^k O_l \varphi_0 \tag{39}$$

where the product is ordered according to

$$\prod_{l=0}^k O_l = O_k O_{k-1} \dots O_1 O_0 \tag{40}$$

with $O_0 = \mathbb{1}$.

Substitution of equation (39) into equation (24) yields a solution in closed form. This may be regarded as an operator-generalisation of a hypergeometrical function

$${}_2F_2(a, b; c, d; z) = 1 + \frac{z}{1!} \frac{ba}{dc} + \frac{z^2}{2!} \frac{(b+1)b(a+1)a}{(d+1)d(c+1)c} + \dots \tag{41}$$

(see Slater 1966). We consider here non-singular operators represented by quadratic matrices $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ and construct a sequences of operators:

$$p_k = \begin{cases} \mathbb{1} & \text{for } k = 0 \\ (\mathbf{d} + k\mathbb{1})^{-1} (\mathbf{c} + k\mathbb{1})^{-1} (\mathbf{b} + k\mathbb{1}) (\mathbf{a} + k\mathbb{1}) & \text{for } k \geq 1. \end{cases} \tag{42}$$

The definition

$${}_2\mathcal{F}_2(\mathbf{a}, \mathbf{b}; \mathbf{c}, \mathbf{d}; z) = \mathbb{1} + \frac{z}{1!} p_1 + \frac{z^2}{2!} p_2 p_1 + \frac{z^3}{3!} p_3 p_2 p_1 + \dots = \sum_{k=0}^{\infty} \frac{z^k}{k!} \prod_{l=0}^k p_l \tag{43}$$

generalises equation (41) to operator-valued parameters.

In terms of this definition the regular solutions are thus obtained in the form

$$\phi(z) = z^{\lambda_0} {}_2\mathcal{F}_2(\mathbf{a}, \mathbf{b}; \mathbf{c}, \mathbf{d}; 2z) \varphi_0 \tag{44}$$

with

$$\begin{aligned} \mathbf{a} &= \mathbb{1}D + \frac{1}{\kappa} C + (\lambda_0 + \frac{3}{2}N - \frac{1}{2})\mathbb{1} \\ \mathbf{b} &= \mathbb{1} \\ \mathbf{c} &= \mathbb{1}D + (\lambda_0 + 1)\mathbb{1} - \mathbf{A} \\ \mathbf{d} &= \mathbb{1}D + (\lambda_0 + 3N - 1)\mathbb{1} + \mathbf{A}. \end{aligned} \tag{45}$$

We note that the derivative

$$D = \frac{d}{ds} = \frac{d}{d(\ln z)}$$

does *not* act on the argument $2z$ of the function ${}_2F_2$, see equation (43).

Let us again consider the special case of hydrogen for the purpose of illustration. The matrix C is then equal to

$$C = -Z_0 \mathbb{1}$$

Z_0 being the nuclear charge. Since all λ states decouple, equations (45) reduce to

$$a \rightarrow -\frac{Z_0}{\kappa} + \lambda_0 + \frac{3}{2}N - \frac{1}{2}$$

$$b \rightarrow 1$$

$$c \rightarrow 1$$

$$d \rightarrow 2\lambda_0 + 3N - 1$$

and the hypergeometric function equation (43) reduces to a confluent hypergeometric function. The regular solutions read therefore

$$\phi(z) = z^{\lambda_0} {}_1F_1(-\nu; 2\lambda_0 + 3N - 1; 2z) \varphi_0 \tag{46}$$

with

$$\nu = \frac{Z_0}{\kappa} - \lambda_0 - \frac{3}{2}N + \frac{1}{2}. \tag{47}$$

Normalisability for bound states requires ν to be an integer. This yields the discrete eigenvalues in $d = 3N$ dimensions

$$E = -\frac{\kappa^2}{2} = -\frac{Z_0^2}{2(\lambda_0 + \nu + \frac{3}{2}N - \frac{1}{2})^2} \tag{48}$$

Finally we compare our result with Fock's (1958) in the case of helium 1S . Fock's angular functions $\psi_{nm}(\alpha, \vartheta)$ are related to our vectors $\phi_k(s)$ by

$$e^{-z} \sum_{k=0}^{\infty} z^k \sum_{\lambda g} Y_{\lambda g}(\alpha, \vartheta) \varphi_{k, \lambda g}(s) = \sum_{k=0}^{\infty} z^k \sum_{m=0}^{[k/2]} (\ln z)^m \psi_{km}(\alpha, \vartheta) \tag{49}$$

see equations (2), (20) and (25). The index g stands in this example for the orbital angular momentum $l_1 = l_2 = l$ of each electron. We expand now the exponential in equation (49) and compare the coefficient functions. The first few Fock functions are then given by

$$\psi_{00}(\alpha, \vartheta) = \sum_{\lambda l} Y_{\lambda l}(\alpha, \vartheta) \varphi_{0, \lambda l} \tag{50a}$$

$$\psi_{10}(\alpha, \vartheta) = \sum_{\lambda l} Y_{\lambda l}(\alpha, \vartheta) \varphi_{1, \lambda l} - \psi_{00}(\alpha, \vartheta) \tag{50b}$$

$$\psi_{21}(\alpha, \vartheta) = \frac{\partial}{\partial s} \sum_{\lambda l} Y_{\lambda l}(\alpha, \vartheta) \varphi_{2, \lambda l} \Big|_{s=0}. \tag{50c}$$

Since Fock (1958) considers only wavefunctions being finite at $r = 0$ we put in equations

(50) $\lambda_0 = 0$. The normalised vector ϕ_0 , see equation (27), therefore has the components

$$\varphi_{0,\lambda l} = \delta_{\lambda 0} \delta_{l 0}.$$

It is now straightforward to employ the technique presented in this section. We find:

$$\psi_{00}(\alpha, \vartheta) = Y_{00} = \text{constant} \quad (51a)$$

$$\psi_{10}(\alpha, \vartheta) = 2 \sum_{\lambda l} Y_{\lambda l}(\alpha, \vartheta) (O_1)_{\lambda l, 00} Y_{00} - \psi_{00}$$

which is equal to

$$\psi_{10}(\alpha, \vartheta) = \frac{2}{\kappa} (5 - \Lambda^2) \left(-\frac{Z_0}{r_1} - \frac{Z_0}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right) \quad (51b)$$

$$\psi_{20}(\alpha, \vartheta) = \sum_{l=0,1} \frac{1}{4} Y_{2l}(\alpha, \vartheta) \int d\omega' Y_{2l}(\alpha', \vartheta') \left(\frac{7}{2} + \frac{1}{\kappa} C(\alpha', \vartheta') \right) Y_{00}. \quad (51c)$$

Using the identities

$$(5 - \Lambda^2)^{-1} (r_i)^{-1} = \frac{1}{2} r_i \quad (i = 1, 2)$$

$$(5 - \Lambda^2)^{-1} |\mathbf{r}_1 - \mathbf{r}_2|^{-1} = \frac{1}{4} |\mathbf{r}_1 - \mathbf{r}_2|$$

we rediscover in equations (50b, c) Fock's result up to a different normalisation, equation (53a).

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