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Spheroidal analysis of the hydrogen atom

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Abstract. A hydrogen atom is analysed in spheroidal coordinates. Limiting transformations $R \to 0$ and $R \to \infty$, R being a dimensional parameter characterising the spheroidal coordinates, are considered in trinomial recurrence relations and spheroidal wavefunctions. Expansions are found for normalised spheroidal wavefunctions of the hydrogen atom over spherical and parabolic bases, and relevant limiting transformations are studied.

1. Introduction

Quantum systems with hidden symmetry possess a remarkable property: variables in the Schrödinger equation for such systems separate in several systems of coordinates, and the corresponding solutions for a given energy are complete bases with respect to other quantum numbers. This property is a manifestation of the accidental degeneracy. A basis is chosen by reason of convenience, and often it is necessary to go from one basis to another. An example of such an interconverting transformation is the expansion of a plane wave over spherical waves in scattering theory. At present the problem of interconverting transformations constitutes an independent trend of the theory of systems with hidden symmetry; many of its aspects are described by Miller (1977), Malkin and Man'ko (1979) and Komarov *et al* (1976). Some interconverting transformations are applied in the three-body problem (Faifman *et al* 1976), in low-energy nuclear physics (Smirnov and Shitikova 1977) and in calculating overlap integrals in quantum molecular theory (Bell 1970, Doktorov *et al* 1976). The discovery of hidden symmetry in the hydrogen atom (Fock 1935) and the success of symmetry schemes in elementary particle physics have stimulated the development of a group-theoretical approach to problems with a Coulomb field (Bander and Itzykson 1966). The theory of interconverting transformations was pioneered by Eisenhart (1948) where the problem of separation of variables in the Schrödinger equation in different coordinate systems was solved. In the literature the first interconverting transformation in the Coulomb field was apparently the result found by Stone (1956). Stone derived, in momentum representation, an expansion of the hydrogen parabolic basis over the spherical one. Later, based on work by Fock (1935) and Bargmann (1936), Park (1960) found an expansion of the coordinate parabolic basis of the hydrogen atom over the spherical one. Then Tarter (1970) repeated the result of Park by a pure analytic approach, i.e. without group-theoretical methods. Perelomov and Popov

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(1968) obtained an expansion of the Rutherford wavefunction over the spherical basis and Majumdar and Basu (1974) found an expansion of the general, not necessarily scattering, parabolic basis over the spherical one. Pogosyan and Ter-Antonyan (1980) derived an expansion of the spherical over the parabolic basis for the continuous spectrum. Coulson and Robinson (1958) investigated the hydrogen atom in spheroidal coordinates, while Coulson and Joseph (1967) obtained trinomial recurrence relations for the matrix of transformation from the spheroidal to the spherical basis.

Spheroidal coordinates represent a natural means of investigating many problems in mathematical physics (Komarov *et al* 1976). These include the diffraction of scalar and electromagnetic waves on prolate and oblate spheroids (Bowman *et al* 1969), the induced electromagnetic radiation from a spheroidal antenna (Page 1944), normal modes of an open resonator (Boyd and Gordon 1961), the behaviour of a particle in a spheroidal potential well (Rainwater 1950), the propagation of neutrons (Cupta 1968) and others. In quantum mechanics the spheroidal coordinates turned out to be useful in describing the behaviour of a charged particle in the field of two Coulomb centres. The distance between centres R is taken as a dimensional parameter characterising spheroidal coordinates and has a dynamic meaning, i.e., it enters into the energy-spectrum expression. We have studied most thoroughly the system H_2^+, knowledge of whose properties is required to solve various problems in astrophysics, plasma physics, the theory of the chemical bond, atomic physics, etc. Many studies are devoted to the energy spectrum of a hydrogen molecular ion; the corresponding references are given by Bates and Reid (1968). If the charge of one centre is put as zero, one arrives at a one-centre problem, and the parameter R becomes purely kinematic; this simplifies the problem considerably. At the same time the mathematical structure of the spheroidal coordinates remains the same, because the energy enters into both the radial and angular equations. Consequently, the spheroidal analysis of a hydrogen atom becomes the first step in the investigation of the two-centre Coulomb problem. Wavefunctions of the two-centre problem provide the basis for expansions of solutions of more complicated problems (for instance, wavefunctions of a three-body problem with a Coulomb interaction).

As $R \to 0$ and $R \to \infty$ spheroidal coordinates become spherical and parabolic ones if the position of the Coulomb centre and charged particle is fixed when taking the limits. This signifies the 'correspondence principle' by which all formulae in spheroidal coordinates should change, in the above limits, into the corresponding spherical and parabolic analogues. Despite this natural principle, taking the limit is not a trivial task, because spheroidal Coulomb functions are expressed in terms of quantities obeying trinomial recurrence formulae, while spherical and parabolic Coulomb functions are constructed on the basis of binomial recurrence relations. Hence, to obtain the limiting transformation for wavefunctions, matrix elements and so forth, one should ascertain how the trinomial recurrence relations convert to the binomial ones in the above limits.

In this paper the limiting process is considered in more detail than by Coulson and Joseph (1967) and Coulson and Robinson (1958). There are several reasons for this. First, as we have already mentioned, such limits are not trivial to obtain and these require a more careful analysis. Second, formulae of the spheroidal analysis of a hydrogen atom are generally rather complicated and therefore the 'correspondence principle' provides a further argument in favour of the validity of certain results.

The paper is organised as follows. Upon recalling some information concerning the hydrogen atom in spheroidal coordinates, we investigate limiting processes $R \to 0$

and $R \to \infty$ in trinomial recurrence relations. Then the limiting transformations are obtained for the wavefunctions and it is proved that these obey the 'correspondence principle' provided the expansion for a solution of the Schrödinger equation is chosen in an appropriate way. The next step of our study is the expansion of the spheroidal over the spherical basis. Such an expansion was considered by Coulson and Joseph (1967) who found recurrence relations for coefficients generating the above expansion. We made further progress along these lines and obtained a formula which explicitly expresses these transformation coefficients in terms of coefficients defining the shape of a spheroidal wavefunction. Then we carried out a detailed analysis of limiting transformations $R \to 0$ and $R \to \infty$ in the expression obtained and established that it agrees with the 'correspondence principle'. Expansion of the spheroidal over the parabolic basis, which, as far as we know, has not yet been considered, represents an independent interest. This expansion is analysed in the latter part of the paper, where a closed expression is found for coefficients relating the spheroidal to the spherical basis and their agreement with the 'correspondence principle' is shown. In the conclusion we present some specific results.

2. Basic formulation

We now present the information necessary for further discussions. The spheroidal coordinates ξ, η and φ are determined in the following way:

$$x = \tfrac{1}{2}R[(\xi^2-1)(1-\eta^2)]^{1/2}\cos\varphi$$
$$y = \tfrac{1}{2}R[(\xi^2-1)(1-\eta^2)]^{1/2}\sin\varphi$$
$$z = \tfrac{1}{2}R(\xi\eta+1)$$

where $1 \leq \xi < \infty$, $-1 \leq \eta \leq 1$, $0 \leq \varphi \leq 2\pi$. As $R \to 0$

$$\xi \to 2r/R \qquad \eta \to \cos\theta \tag{2.1a}$$

and as $R \to \infty$

$$\xi \to 1+\mu/R \qquad \eta \to -1+\nu/R \tag{2.1b}$$

where r and θ are spherical coordinates, ν and μ are parabolic coordinates: $\nu = r+z$, $\mu = r-z$. In both the limits the point (x, y, z) and the coordinates of the Coulomb centre are considered to be fixed.

The spheroidal wavefunction of a hydrogen atom is

$$\psi_{nqm}(\xi, \eta, \varphi; R) = C_{nqm}(R)\Pi_{nqm}(\xi, R)\Xi_{nqm}(\eta, R)\frac{\exp(im\varphi)}{(2\pi)^{1/2}}. \tag{2.2}$$

Here $C_{nmq}(R)$ is the normalisation factor; the meaning of n, q and m will be explained further. It is known that

$$\Pi_{nqm}(\xi, R) = \exp(-R\xi/2n)(\xi^2-1)^{|m|/2}f(\xi, R) \tag{2.3a}$$

$$\Xi_{nqm}(\eta, R) = \exp(-R\eta/2n)(1-\eta^2)^{|m|/2}g(\eta, R) \tag{2.3b}$$

where $f(\xi, R)$ and $g(\eta, R)$ are polynomials of degree $(n-|m|-1)$ in ξ and η. The functions $\Pi_{nqm}(\xi, R)$ and $\Xi_{nqm}(\eta, R)$, usually known as radial and angular functions in the Coulomb system of units, satisfy the equations

$$\frac{d}{d\xi}\left((\xi^2-1)\frac{d\Pi}{d\xi}\right)+\left(R\xi+\frac{ER^2}{2}\xi^2-\frac{m^2}{\xi^2-1}+A\right)\Pi=0 \tag{2.4a}$$

$$\frac{d}{d\eta}\left((1-\eta^2)\frac{d\Xi}{d\eta}\right)+\left(-R\eta-\frac{ER^2}{2}\eta^2-\frac{m^2}{1-\eta^2}-A\right)\Xi=0. \tag{2.4b}$$

A is a separation constant in spheroidal coordinates; it depends on R and the quantum numbers n, q and m, where n is the principal quantum number ($E=-1/2n^2$), m is the azimuthal quantum number, and q varies in the limits $1\leqslant q\leqslant n-|m|$ and denotes $n-|m|$ possible values of the separation constant A at fixed n and $|m|$.

The orthogonality conditions in index q are

$$\int_1^\infty \Pi^*_{nq'm}(\xi, R)\Pi_{nqm}(\xi, R)\,d\xi=0 \tag{2.5a}$$

$$\int_{-1}^1 \Xi^*_{nq'm}(\eta, R)\Xi_{nqm}(\eta, R)\,d\eta=0. \tag{2.5b}$$

Being eigenfunctions of the Hamiltonian and z projection of the angular momentum, the wavefunctions (2.2) are also orthogonal in the other two indices, n and m.

3. Wavefunctions

In the literature various types of expansions are used for the functions $f(\xi, R)$ and $g(\eta, R)$ in powers $(\xi-1)$ and $(\eta-1)$, over the Laguerre polynomials of appropriate combinations of the variables ξ and η, etc. Further we shall keep to the expansions

$$f(\xi, R)=\sum_{s=0}^{n-|m|-1} a_s(\xi-1)^s \tag{3.1a}$$

$$g(\eta, R)=\sum_{s=0}^{n-|m|-1} b_s(1+\eta)^s. \tag{3.1b}$$

In § 5 it will be shown that it is just these expansions that satisfy the 'correspondence principle'. Formulae (2.3), (2.4) and (3.1) result in the trinomial recurrence relations

$$\alpha_s a_{s+1}+\beta_s a_s+R\gamma_s a_{s-1}=0 \tag{3.2a}$$

$$-\alpha_s b_{s+1}+\tilde{\beta}_s b_s+R\gamma_s b_{s-1}=0 \tag{3.2b}$$

where

$$\alpha_s=2(s+1)(s+|m|+1) \tag{3.3a}$$

$$\beta_s=(s+|m|)(s+|m|+1)+(R/n)(n-|m|-1-2s)-(R^2/4n^2)+A \tag{3.3b}$$

$$\tilde{\beta}_s=(s+|m|)(s+|m|+1)-(R/n)(n-|m|-1-2s)-(R^2/4n^2)+A \tag{3.3c}$$

$$\gamma_s=(n-|m|-s)/n. \tag{3.3d}$$

The 'cut-off conditions'

$$a_0 = 1 \qquad a_{-1} = a_{n-|m|} = 0$$

$$b_0 = 1 \qquad b_{-1} = b_{n-|m|} = 0$$

hold as well.

Let the wavefunction obey the normalisation condition

$$\int_1^\infty \int_{-1}^1 \int_0^{2\pi} |\psi_{nqm}(\xi, \eta, \varphi; R)|^2 \tfrac{1}{8} R^3 (\xi^2 - \eta^2)\, d\xi\, d\eta\, d\varphi = 1.$$

Hence, as will be shown further, it follows that

$$C_{nqm}(R) \xrightarrow{R\to 0} \exp(i\phi_0) \frac{\sqrt{2}}{n^2} \left(\frac{R}{n}\right)^l \left(\frac{[(l+|m|)!]^3 (n+l)!}{(l-|m|)!(n-l-1)!(2l+1)}\right)^{1/2} \frac{2^{l-2|m|} l!}{[(2l)!]^2 (|m|!)^2} \tag{3.4a}$$

$$C_{nqm}(R) \xrightarrow{R\to\infty} \exp(i\phi_\infty) \frac{\sqrt{2}}{n^2} \left(\frac{R}{2n}\right)^{|m|} \left(\frac{(n_1+|m|)!(n_2+|m|)!}{n_1! n_2!}\right)^{1/2} \frac{1}{(|m|!)^2} \tag{3.4b}$$

where l, n_1 and n_2 are known spherical and parabolic quantum numbers, and the phases ϕ_0 and ϕ_∞ are as yet arbitrary.

4. Limiting transformations in recurrence relations

The recurrence relation (3.2a) is a set of linear homogeneous equations for a_s, and thus the corresponding determinant should vanish. In the limit $R \to \infty$, one may neglect coefficients α_s in this determinant compared with infinite coefficients β_s and $R\gamma_s$ and represent the determinant by a product of all β_s. In order that the determinant vanish one of the multipliers β_s must vanish as well. Replacing the s in β_s by n_2 we have

$$A(R) \xrightarrow{R\to\infty} -(R/n)(n-|m|-1-2n_2) + (R^2/4n^2). \tag{4.1a}$$

Analogously, for (3.2b) we can show that there should exist some n_1, for which $\tilde{\beta}_{n_1} = 0$ and consequently

$$A(R) \xrightarrow{R\to\infty} (R/n)(n-|m|-1-2n_1) + (R^2/4n^2). \tag{4.1b}$$

Formulae (4.1a) and (4.1b) are compatible if $n = n_1 + n_2 + |m| + 1$, i.e. if n_1 and n_2 are parabolic quantum numbers. From (4.1), (3.3b) and (3.3c) it follows that at $s \neq n_1$, $s \neq n_2$,

$$\beta_s \xrightarrow{R\to\infty} R\beta_s^{(1)} \tag{4.2a}$$

$$\tilde{\beta}_s \xrightarrow{R\to\infty} R\beta_s^{(2)} \tag{4.2b}$$

where the quantities $\beta_s^{(1)}$ and $\beta_s^{(2)}$ are independent of R and have the form

$$\beta_s^{(1)} = 2(n_2 - s)/n \qquad \beta_s^{(2)} = -2(n_1 - s)/n. \tag{4.2c}$$

These formulae and the cut-off conditions $a_{-1}=0$ and $b_{-1}=0$ show that trinomial recurrence relations (3.2) in the limit $R\to\infty$ become the binomial relations

$$\alpha_s a_{s+1}+R\beta_s^{(1)}a_s=0 \tag{4.3a}$$

$$-\alpha_s b_{s+1}+R\beta_s^{(2)}b_s=0 \tag{4.3b}$$

if $0\leqslant s\leqslant n_1-1$ and $0\leqslant s\leqslant n_2-1$. Using formulae (4.2) and the cut-off conditions $a_{n-|m|}=0$ and $b_{n-|m|}=0$, we see that in the limit $R\to\infty$ (3.2) becomes

$$\beta_s^{(1)}a_s+\gamma_s a_{s-1}=0 \tag{4.4a}$$

$$\beta_s^{(2)}b_s+\gamma_s b_{s-1}=0 \tag{4.4b}$$

if $n_1+1\leqslant s\leqslant n-|m|-1$ or $n_2+1\leqslant s\leqslant n-|m|-1$.

Consider now the cases when $s=n_1$ and $s=n_2$. As $R\to\infty$ the constant A can be expanded in powers of $1/R$ and according to (4.1a) and (4.1b) this expansion can contain only terms with powers of $1/R$ not higher than -2.

Thus, it follows that

$$A(R)\xrightarrow{R\to\infty}A_0-(R/n)(n-|m|-1-2n_2)+(R^2/4n^2) \tag{4.5a}$$

$$A(R)\xrightarrow{R\to\infty}A_0+(R/n)(n-|m|-1-2n_1)+(R^2/4n^2) \tag{4.5b}$$

as there the condition $n=n_1+n_2+|m|+1$ must hold. Substituting these formulae into (3.3b) and (3.3c) we obtain

$$\beta_{n_2}=(n_2+|m|)(n_2+|m|+1)+A_0$$

$$\tilde{\beta}_{n_1}=(n_1+|m|)(n_1+|m|+1)+A_0.$$

The constant A_0 can be determined from the recurrence relation (3.2a) at $s=n_2$:

$$\alpha_{n_2}a_{n_2+1}+\beta_{n_2}a_{n_2}+R\gamma_{n_2}a_{n_2-1}=0$$

if we use the expressions

$$a_{n_2-1}=-\frac{1}{R}\frac{\alpha_{n_2-1}}{\beta^{(1)}_{n_2-1}}a_{n_2}\qquad a_{n_2+1}=-\frac{\gamma_{n_2+1}}{\beta^{(1)}_{n_2+1}}a_{n_2}$$

resulting from the binomial recurrence relations (4.3a) and (4.4a). Then we have

$$A_0=2n_2^2-2n_1(n-|m|-1)-(|m|+1)(n-1).$$

Note that this formula has been obtained by Coulson and Robinson (1958) from the analysis of recurrence relations arising in the case when the functions $f(\xi,R)$ and $g(\eta,R)$ are represented by expansions over the Laguerre polynomials.

The limit $R\to 0$ may be investigated analogously. In this case equations (3.2) become the binomial recurrence relations

$$\alpha_s a_{s+1}+\bar{\beta}_s a_s=0 \tag{4.6a}$$

$$-\alpha_s b_{s+1}+\bar{\beta}_s b_s=0 \tag{4.6b}$$

if $0\leqslant s\leqslant l-|m|-1$ and

$$\bar{\beta}_s a_s+R\gamma_s a_{s-1}=0 \tag{4.7a}$$

$$\bar{\beta}_s b_s+R\gamma_s b_{s-1}=0 \tag{4.7b}$$

if $l-|m|+1 \leqslant s \leqslant n-|m|-1$. In these relations

$$\bar{\beta}_s = (s+|m|)(s+|m|+1)+A(0). \tag{4.7c}$$

Consider the case when $s = l-|m|$. At small R

$$A(R) \xrightarrow{R\to 0} A(0) + R(\mathrm{d}A/\mathrm{d}R)_{R=0} + \mathrm{O}(R^2).$$

Coulson and Robinson (1958) showed that $A(0) = -l(l+1)$. With this and (3.3b) and (3.3c) taken into account we obtain

$$\beta_{l-|m|} \xrightarrow{R\to 0} \varepsilon_{l-|m|}R + \mathrm{O}(R^2) \tag{4.8a}$$

$$\bar{\beta}_{l-|m|} \xrightarrow{R\to 0} \bar{\varepsilon}_{l-|m|}R + \mathrm{O}(R^2) \tag{4.8b}$$

where

$$\varepsilon_{l-|m|} = \left(\frac{\mathrm{d}A}{\mathrm{d}R}\right)_{R=0} + \frac{n+|m|-1-2l}{n}$$

$$\bar{\varepsilon}_{l-|m|} = \left(\frac{\mathrm{d}A}{\mathrm{d}R}\right)_{R=0} - \frac{n+|m|-1-2l}{n}.$$

It follows from these formulae that the recurrence relations (3.2) at $s = l-|m|$ take the form

$$\alpha_{l-|m|}a_{l-|m|+1} + \varepsilon_{l-|m|}Ra_{l-|m|} + R\gamma_{l-|m|}a_{l-|m|-1} = 0 \tag{4.9a}$$

$$-\alpha_{l-|m|}b_{l-|m|+1} + \bar{\varepsilon}_{l-|m|}Rb_{l-|m|} + R\gamma_{l-|m|}b_{l-|m|-1} = 0. \tag{4.9b}$$

According to (4.6) and (4.7) the quantities $a_{l-|m|+1}$, $a_{l-|m|-1}$, $b_{l-|m|+1}$ and $b_{l-|m|-1}$ are expressed via $a_{l-|m|}$ and $b_{l-|m|}$. Therefore equations (4.9) should lead to constraints under which the cut-off conditions at $s=-1$ and $s = n-|m|$ are consistent. Using equations (4.8) we can easily show that the condition $(\mathrm{d}A/\mathrm{d}R)_{R=0} = 0$ is just such a restriction.

5. Limiting transformations for the wavefunction

The functions $f(\xi, R)$ and $g(\eta, R)$ as $R\to\infty$ according to (2.1b) are

$$f(\xi,R) \xrightarrow{R\to\infty} \sum_{s=0}^{n_1+n_2} \frac{a_s}{R^s}\mu^s \qquad g(\eta,R) \xrightarrow{R\to\infty} \sum_{s=0}^{n_1+n_2} \frac{b_s}{R^s}\nu^s.$$

From the binomial recurrence relations (4.3) and (4.4) it follows that

$$a_s \xrightarrow{R\to\infty} (-1)^s \frac{\beta_0^{(1)}\ldots\beta_{s-1}^{(1)}}{\alpha_0\ldots\alpha_{s-1}}R^s \qquad 1\leqslant s\leqslant n_2 \tag{5.1a}$$

$$b_s \xrightarrow{R\to\infty} \frac{\beta_0^{(2)}\ldots\beta_{s-1}^{(2)}}{\alpha_0\ldots\alpha_{s-1}}R^s \qquad 1\leqslant s\leqslant n_1 \tag{5.1b}$$

$$a_s \xrightarrow{R\to\infty} (-1)^{s-n_2} \frac{\gamma_{n_2+1}\ldots\gamma_s}{\beta_{n_2+1}^{(1)}\ldots\beta_s^{(1)}}a_{n_2} \qquad n_2+1\leqslant s\leqslant n_1+n_2 \tag{5.1c}$$

$$b_s \xrightarrow{R\to\infty} (-1)^{s-n_1} \frac{\gamma_{n_1+1} \ldots \gamma_s}{\beta^{(2)}_{n_1+1} \ldots \beta^{(2)}_s} b_{n_1} \qquad n_1+1 \leqslant s \leqslant n_1+n_2 \tag{5.1d}$$

so the functions $f(\xi, R)$ and $g(\eta, R)$ become polynomials of powers n_2 and n_1, respectively. According to (5.1*a*), (5.1*b*), (3.3*a*) and (4.2*c*)

$$a_s \xrightarrow{R\to\infty} \frac{(-1)^s}{n^s} \frac{n_2!}{(n_2-s)!} \frac{|m|!}{(s+|m|)!} \frac{R^s}{s!} \qquad 1 \leqslant s \leqslant n_2 \tag{5.2a}$$

$$b_s \xrightarrow{R\to\infty} \frac{(-1)^s}{n^s} \frac{n_1!}{(n_1-s)!} \frac{|m|!}{(s+|m|)!} \frac{R^s}{s!} \qquad 1 \leqslant s \leqslant n_1 \tag{5.2b}$$

and, consequently,

$$f(\xi, R) \xrightarrow{R\to\infty} F(-n_2; |m|+1; \mu/n)$$

$$g(\eta, R) \xrightarrow{R\to\infty} F(-n_1; |m|+1; \nu/n).$$

Now by using (3.4*b*) it is easy to show that as $R \to \infty$ (2.2) becomes the normalised wavefunction in parabolic coordinates:

$$\begin{aligned}\psi_{n_1 n_2 m}(\nu, \mu, \varphi) = {} & \frac{\sqrt{2}}{n^2} \frac{1}{(|m|!)^2} \left(\frac{(n_1+|m|)!(n_2+|m|)!}{n_1! n_2!} \right)^{1/2} \left(\frac{\nu}{n}\right)^{|m|/2} \left(\frac{\mu}{n}\right)^{|m|/2} \\ & \times \exp[-(\nu+\mu)/2n] F(-n_1; |m|+1; \nu/n) \\ & \times F(-n_2; |m|+1; \mu/n) \exp(im\varphi)/\sqrt{2\pi}\end{aligned} \tag{5.3}$$

if $\phi_\infty = 0$.

In the limit $R \to 0$ according to (2.1*a*)

$$\Pi(\xi, R) \xrightarrow{R\to 0} \exp(-r/n) \left(\frac{2r}{R}\right)^{|m|} \sum_{s=0}^{n-|m|-1} \frac{a_s}{R^s} (2r)^s \tag{5.4a}$$

$$\Xi(\eta, R) \xrightarrow{R\to 0} (\sin\theta)^{|m|} \sum_{s=0}^{n-|m|-1} b_s (1+\cos\theta)^s. \tag{5.4b}$$

From the binomial recurrence relations (4.6) and (4.7) it follows that

$$a_s \xrightarrow{R\to 0} (-1)^s \frac{\bar\beta_0 \ldots \bar\beta_{s-1}}{\alpha_0 \ldots \alpha_{s-1}} \tag{5.5a}$$

$$b_s \xrightarrow{R\to 0} \frac{\bar\beta_0 \ldots \bar\beta_{s-1}}{\alpha_0 \ldots \alpha_{s-1}} \tag{5.5b}$$

if $1 \leqslant s \leqslant l-|m|$ and

$$a_s \xrightarrow{R\to 0} (-1)^{s-l+|m|} \frac{\gamma_{l-|m|+1} \ldots \gamma_s}{\bar\beta_{l-|m|+1} \ldots \bar\beta_s} R^{s-l+|m|} a_{l-|m|} \tag{5.5c}$$

$$b_s \xrightarrow{R\to 0} (-1)^{s-l+|m|} \frac{\gamma_{l-|m|+1} \ldots \gamma_s}{\bar\beta_{l-|m|+1} \ldots \bar\beta_s} R^{s-l+|m|} b_{l-|m|} \tag{5.5d}$$

if $l-|m|+1 \leqslant s \leqslant n-|m|-1$. Substituting γ, α and $\bar\beta$ from (3.3*d*), (3.3*a*) and (4.7*c*) into (5.5*c*) and (5.5*b*) we obtain

$$a_{s+l-|m|} \xrightarrow{R\to 0} (-1)^s \frac{(n-l-1)!}{(n-l-s-1)!} \frac{(2l+1)!}{(2l+s+1)!} \frac{R^s}{n^s s!} a_{l-|m|} \tag{5.6a}$$

$$b_s \xrightarrow{R\to 0} (-1)^s \frac{(l-|m|)!}{(l-|m|-s)!} \frac{(l+|m|+s)!\,|m|!}{(l+|m|)!\,(|m|+s)!} \frac{1}{2^s s!}. \tag{5.6b}$$

In the first case $1 \leqslant s \leqslant n-l-1$, while in the second $1 \leqslant s \leqslant l-|m|$. It follows from these formulae that

$$\Pi(\xi, R) \xrightarrow{R\to 0} a_{l-|m|} \exp(-r/n) \left(\frac{2r}{R}\right)^l F(-n+l+1; 2l+2; 2r/n) \tag{5.7a}$$

$$\Xi(\eta, R) \xrightarrow{R\to 0} (\sin\theta)^{|m|} F(-l+|m|, l+|m|+1; |m|+1; \tfrac{1}{2}(1+\cos\theta)). \tag{5.7b}$$

With (3.4*a*) it is easy to show that the wavefunction (2.2) becomes the normalised wavefunction in spherical coordinates

$$\psi_{nlm}(r,\theta,\varphi) = \frac{2}{n^2}\left(\frac{(n+l)!}{(n-l-1)!}\right)^{1/2} \left(\frac{2r}{n}\right)^l \frac{\exp(-r/n)}{(2l+1)!} F(-n+l+1; 2l+2; 2r/n) Y_{lm}(\theta,\varphi) \tag{5.8}$$

if $\phi_0 = \pi[l + \frac{1}{2}(m-|m|)]$. It is necessary here to use the formula (Varshalovich *et al* 1975)

$$Y_{lm}(\theta,\varphi) = (-1)^{[l+\frac{1}{2}(m-|m|)]} \frac{\exp(im\varphi)}{\sqrt{2\pi}} \left(\frac{2l+1}{2} \frac{(l+|m|)!}{(l-|m|)!}\right)^{1/2} \frac{(\sin\theta)^{|m|}}{2^{|m|}|m|!}$$
$$\times F(-l+|m|; l+|m|+1; |m|+1, \tfrac{1}{2}(1+\cos\theta)).$$

So, it is proved that the wavefunction (2.2) does satisfy the 'correspondence principle'.

6. Spherical-basis expansion

Let us write the expansion we are interested in as

$$\psi_{nqm}(\xi,\eta,\varphi; R) = \sum_{l=|m|}^{n-1} W_{nq}^{lm} \psi_{nlm}(r,\theta,\varphi) \tag{6.1}$$

and perform the following operations. First, we change ψ_{nlm} from spherical coordinates to spheroidal ones

$$r = \tfrac{1}{2}R(\xi+\eta) \qquad \cos\theta = (1+\xi\eta)/(\xi+\eta)$$

and then let ξ tend to infinity on both sides of (6.1). As a result

$$r \xrightarrow{\xi\to\infty} \tfrac{1}{2}R\xi \qquad \cos\theta \xrightarrow{\xi\to\infty} \eta$$

and the dependence on the variable ξ in (6.1) is removed. Using this fact we multiply both sides of (6.1) by $P_l^{|m|}(\eta)$ and integrate over η. Then owing to the orthogonality condition of the associated Legendre polynomials we get the equality

$$W_{nq}^{lm}(R) = D_n^{lm} \frac{C_{nqm}(R)}{R^{n-1}} a_{n-|m|-1} E_{nq}^{lm}(R)$$

where

$$D_n^{lm}=(-1)^{n-l-1+\frac{1}{2}(m+|m|)}\frac{n^{n+1}}{2}\left(\frac{2l+1}{2}\frac{(l-|m|)!}{(l+|m|)!}(n+l)!\,(n-l-1)!\right)^{1/2}$$

$$E_{nq}^{lm}(R)=\int_{-1}^{1}(1-\eta^2)^{|m|/2}P_l^{|m|}(\eta)g_{nqm}(\eta,R)\,\mathrm{d}\eta.$$

With the use of (3.1b) the latter integral can be expressed via the coefficients b_s:

$$E_{nq}^{lm}(R)=\sum_{s=0}^{n-|m|-1}b_s(R)\int_{-1}^{1}(1-\eta^2)^{|m|/2}(1+\eta)^sP_l^{|m|}(\eta)\,\mathrm{d}\eta.$$

By integration by parts we find that the integral in the sum is not zero only at $l-|m|\leqslant s\leqslant n-|m|-1$, and consequently, by changing the sum index we obtain

$$E_{nq}^{lm}(R)=\frac{1}{2^l l!}\frac{(l+|m|)!}{(l-|m|)!}\sum_{s=0}^{n-l-1}b_{s+l-|m|}\frac{(s+l-|m|)!}{s!}J^{ls}$$

where

$$J^{ls}=\int_{-1}^{1}(1-\eta^2)^l(1+\eta)^s\,\mathrm{d}\eta=2^{2l+s+1}\frac{l!\,(s+l)!}{(2l+s+1)!}.$$

As a result

$$W_{nq}^{lm}(R)=(-1)^{n-l-1+\frac{1}{2}(m+|m|)}\frac{n^{n+1}}{R^{n-1}}C_{nqm}(R)a_{n-|m|-1}2^l$$
$$\times\left(\frac{2l+1}{2}\frac{(l+|m|)!}{(l-|m|)!}(n+l)!\,(n-l-1)!\right)^{1/2}B_{nlm}(R)\tag{6.2}$$

where

$$B_{nlm}(R)=\sum_{s=0}^{n-l-1}b_{s+l-|m|}\frac{2^s(s+l)!\,(s+l-|m|)!}{s!\,(s+2l+1)!}.\tag{6.3}$$

Now we turn to the limiting transformations. As $R\to0$ the separation constant $A(R)\to-l'(l'+1)$ so, according to (3.3b),

$$\beta_s\xrightarrow{R\to0}\bar{\beta}_s\equiv(s+|m|-l')(s+|m|+l'+1).$$

Then, from (5.5d) we obtain

$$b_{s+l-|m|}\overset{R\to0}{\sim}\frac{R^{s+l-l'}}{\Gamma(l-l'+1)}.$$

It follows that at $l>l'$, $b_{s+l-|m|}\to0$ for $s\geqslant0$, and at $l<l'$, $b_{s+l-|m|}=0$ due to a gamma function in the denominator. At $l=l'$ in the sum (6.3) as $R\to0$ only the term with $s=0$ differs from zero, so taking (3.4a) and (5.6b) into account we conclude that at $l=l'$ $W_{nq}^{lm}(R)\to1$ and therefore

$$W_{nq}^{lm}(R)\xrightarrow{R\to0}\delta_{ll'}.$$

Consider now the limit $R \to \infty$. From (3.4b), (5.1a) and (5.1c) it follows that

$$\frac{C_{nqm}(R)}{R^{n-1}} a_{n-|m|-1} \overset{R\to\infty}{\sim} \frac{1}{R^{n_1}}.$$

That means that in (6.3) we can restrict ourselves to the summation, starting from $s = n_1$ i.e.

$$B_{nlm}(R) \xrightarrow{R\to\infty} \sum_{s=0}^{n_2} b_{s+n_1} \frac{2^{s+n_1-l+|m|}(s+n_1+|m|)!\,(s+n_1)!}{(s+n_1-l+|m|)!\,(s+n_1+|m|+l+1)!}.$$

From (4.2c) and (5.1d) it follows that

$$b_{s+n_1} \xrightarrow{R\to\infty} (-1)^s \frac{n_2!\, b_{n_1}}{2^s s!\,(n_2-s)!}.$$

Thus, B_{nlm} can be written in the form

$$B_{nlm}(R) \xrightarrow{R\to\infty} 2^{n_1-l+|m|} \frac{n_1!\,(n_1+|m|)!\, b_{n_1}}{(n_1-l+|m|)!\,(n_1+l+|m|+1)!}\, {}_3F_2\left\{ \begin{matrix} -n_2,\, n-n_2,\, n-n_2-|m| \\ n-n_2+l+1,\, n-n_2-l \end{matrix} \middle| 1 \right\}.$$

Now we use the two formulae

$${}_3F_2\left\{ \begin{matrix} c,\, b,\, e-a \\ e,\, 1+b+c-f \end{matrix} \middle| 1 \right\} = \frac{\Gamma(1-f+a)\Gamma(1+b+c-f)}{\Gamma(1+e-f)\Gamma(1-e-f+a+b+c)}\, {}_3F_2\left\{ \begin{matrix} e-a,\, e-b,\, e-c \\ e,\, 1+e-f \end{matrix} \middle| 1 \right\} \tag{6.4}$$

$${}_3F_2\left\{ \begin{matrix} s,\, s',\, -N \\ t',\, 1-N-t \end{matrix} \middle| 1 \right\} = \frac{\Gamma(t+s+N)\Gamma(t)}{\Gamma(t+s)\Gamma(t+N)}\, {}_3F_2\left\{ \begin{matrix} s,\, t'-s',\, -N \\ t',\, t+s \end{matrix} \middle| 1 \right\}. \tag{6.5}$$

The first is taken from Smorodinsky and Shepelev (1971), the second from Bailey (1935). Successively applying them we obtain

$$B_{nlm}(R) \xrightarrow{R\to\infty} 2^{n_1-l+|m|} \frac{(n_1+|m|)!\,(n_2+|m|)!}{(|m|)!\,(n+l)!} \frac{(n-|m|-1)!}{(n-l-1)!} b_{n_1}$$
$$\times\, {}_3F_2\left\{ \begin{matrix} -n_2,\, -l+|m|,\, l+|m|+1 \\ |m|+1,\, |m|+1-n \end{matrix} \middle| 1 \right\}.$$

Further, according to (5.1c), (5.2a) and (5.2b)

$$a_{n-|m|-1} = \frac{(-1)^{n_2}}{n^{n_2}} \frac{|m|!}{(n_2+|m|)!} \frac{R^{n_2}}{2^{n_1}}$$

$$b_{n_1} = \frac{(-1)^{n_1}}{n^{n_1}} \frac{|m|!}{(n_1+|m|)!} R^{n_1},$$

so with (3.4b) taken into account at $\phi_\infty = 0$ we have

$$W_{nq}^{lm} \xrightarrow{R\to\infty} (-1)^{l+\frac{1}{2}(m-|m|)} \frac{(n-|m|-1)!}{|m|!} \left(\frac{(2l+1)(n_1+|m|)!\,(n_2+|m|)!\,(l+|m|)!}{n_1!\,n_2!\,(n+l)!\,(n-l-1)!\,(l-|m|)!} \right)^{1/2}$$
$$\times\, {}_3F_2\left\{ \begin{matrix} -l+|m|,\, l+|m|+1,\, -n_2 \\ |m|+1,\, -n+|m|+1 \end{matrix} \middle| 1 \right\}. \tag{6.6}$$

The limiting expression obtained coincides with the result of a paper by Tarter (1970). Thus, in both the limits required formulae have been established.

7. Parabolic-basis expansion

We write an expansion we are looking for in the form

$$\psi_{nqm}(\xi,\eta,\varphi;R)=\sum_{n_1+n_2=n-|m|-1} U_{qm}^{n_1n_2}(R)\psi_{n_1n_2m}(\nu,\mu,\varphi). \tag{7.1}$$

According to (5.3) the parabolic wavefunction is expressed via the Laguerre polynomials of the variables

$$\mu=\tfrac{1}{2}R(\xi-1)(1-\eta)$$

and

$$\nu=\tfrac{1}{2}R(\xi+1)(1+\eta).$$

Let $\eta=-1$ in (7.1). Taking the new variable $t=\xi-1$ and using the property of orthogonality

$$\int_0^\infty \exp\left(-\frac{Rt}{n}\right)\left(\frac{Rt}{n}\right)^{|m|} F\left(-n_2;|m|+1;\frac{Rt}{n}\right)F\left(-n_2';|m|+1;\frac{Rt}{n}\right)\mathrm{d}t$$
$$=\frac{n}{R}\frac{(|m|!)^2 n_2!}{(n_2+|m|)!}\delta_{n_2n_2'}$$

we obtain

$$U_{qm}^{n_1n_2}(R)=C_{nqm}(R)\frac{Rn}{\sqrt{2}}2^{|m|}\left(\frac{(n_2+|m|)!}{(n_1+|m|)!}\frac{n_1!}{n_2!}\right)^{1/2}$$
$$\times\sum_{s=0}^{n-|m|-1} a_s\int_0^\infty t^{|m|+s}\exp\left(-\frac{Rt}{n}\right)F\left(-n_2;|m|+1;\frac{Rt}{n}\right)\mathrm{d}t.$$

Further, as

$$\int_0^\infty t^{s+|m|}\exp\left(-\frac{Rt}{n}\right)F\left(-n_2;|m|+1;\frac{Rt}{n}\right)\mathrm{d}t$$
$$=\left(\frac{n}{R}\right)^{s+|m|+1}(-1)^{n_2}\frac{|m|!s!(|m|+s)!}{(n_2+|m|)!\Gamma(s+1-n_2)}$$

then

$$U_{qm}^{n_1n_2}(R)=(-1)^{n_2}C_{nqm}(R)\frac{n^2}{\sqrt{2}}|m|!\left(\frac{|n_1|!|n_2|!}{(n_1+|m|)!(n_2+|m|)!n_2!}\right)^{1/2}$$
$$\times\left(\frac{2n}{R}\right)^{|m|}\sum_{s=0}^{n_1+n_2}\frac{a_s}{R^s}n^s\frac{(|m|+s)!s!}{\Gamma(s+1-n_2)}.$$

Now we investigate the limiting cases. As $R\to\infty$, as mentioned before, there exists such a value $s=n_2'$, for which $\beta_{n_2'}=0$. According to (5.1a) and (5.1c) the ratio a_s/R^s in this limit is different from zero when $0\leqslant s\leqslant n_2'$ so the maximum value of s in the sum (7.2) can be changed to n_2'. Thus, using (5.1a) and (3.4b) we see that at $n_2'<n_2$ the sum in (7.2) becomes zero, and at $n_2'\geqslant n_2$

$$U_{qm}^{n_1n_2}(R)\xrightarrow{R\to\infty}\left(\frac{n_1!n_2!(n_1'+|m|)!(n_2'+|m|)!}{n_1'!n_2'!(n_1+|m|)!(n_2+|m|)!}\right)^{1/2}\sum_{s=0}^{n_2'-n_2}\frac{(-1)^s}{s!\Gamma(n_2'-n_2-s+1)}.$$

It is easy to show that the latter can take only two values: zero and unity. This depends on either $n_2' > n_2$ or $n_2' = n_2$. Therefore,

$$U_{qm}^{n_1 n_2}(R) \xrightarrow{R\to\infty} \delta_{n_2' n_2}.$$

Consider now the limit $R \to 0$. From (5.5*a*), (5.6*a*) and (3.4*b*) it follows that in this limit

$$U_{qm}^{n_1 n_2}(R) \xrightarrow{R\to 0} (-1)^{n_2+l+\frac{1}{2}(m-|m|)}\left(\frac{(2l+1)(l+|m|)!\,(l-|m|)!\,(n+l)!\,n_1!}{(n_1+|m|)!\,(n_2+|m|)!\,(n-l-1)!\,n_2!}\right)^{1/2}$$

$$\times \frac{l!}{(2l+1)!\,(l-|m|-n_2)!}\,{}_3F_2\left\{\begin{matrix}-n+l+1,\, l+1,\, l-|m|+1\\ l-|m|-n_2+1,\, 2l+2\end{matrix}\,\Big|\, 1\right\}.$$

Using formulae (6.4) and (6.5) we obtain

$$U_{qm}^{n_1 n_2}(R) \xrightarrow{R\to 0} (-1)^{l+\frac{1}{2}(m-|m|)}\frac{(n-|m|-1)!}{|m|!}\left(\frac{(2l+1)(l+|m|)!\,(n_1+|m|)!\,(n_2+|m|)!}{n_1!\,n_2!\,(l-|m|)!\,(n-l-1)!}\right)^{1/2}$$

$$\times {}_3F_2\left\{\begin{matrix}-l+|m|,\, l+|m|+1,\, -n_2\\ |m|+1,\, -n+|m|+1\end{matrix}\,\Big|\, 1\right\},$$

i.e. the result of Tarter (1970).

Formulae (3.4*a*) and (3.4*b*) have been used essentially in the investigation of the limiting transformations for the wavefunction (2.2) and transformation coefficients. The result is the following. Substituting expansions (3.1*a*) and (3.1*b*) into the normalisation condition of the wavefunction (2.2), we obtain

$$2^{4m+1}R^3|C_{nqm}(R)|^2 \sum_{s,s',t,t'} 2^{s+s'+t+t'} a_s a_{s'} b_t b_{t'} (I_{ss'}^{|m|} J_{tt'}^{|m|+1} + I_{ss'}^{|m|+1} J_{tt'}^{|m|}) = 1$$

where the summation runs over all the indices in the limits $(0, n-|m|-1)$, and $I_{ss'}^{m}$, $J_{tt'}^{|m|}$ are expressed via confluent hypergeometric functions (Bateman and Erdelyi 1953):

$$I_{ss'}^{m} = (|m|+s+s')!\,\psi(|m|+s+s'+1;\, 2|m|+s+s'+2;\, 2R/n)$$

$$J_{tt'}^{|m|} = \frac{|m|!\,(|m|+t+t')!}{(2|m|+t+t'+1)!}F(|m|+t+t'+1;\, 2|m|+t+t'+2;\, -2R/n).$$

Using asymptotes of these functions as $R \to 0$ and $R \to \infty$ and formulae (5.1) and (5.5), we arrive at just the results (3.4*a*) and (3.4*b*).

8. Particular cases and tables

Let us introduce the notation

$$\tilde{W}_{nq}^{lm}(R) = W_{nq}^{lm}(R)/C_{nqm}(R).$$

As the transformation coefficients $W_{nq}^{lm}(R)$ satisfy the condition

$$\sum_{l=|m|}^{n-1} (W_{nq}^{lm})^2 = 1$$

we obtain the formula convenient for the calculation of the normalisation constant

$$C_{nqm}(R) = \left(\sum_{l=|m|}^{n-1} (\tilde{W}_{nq}^{lm})^2\right)^{-1/2}.$$

Let us present here some particular results:

$$C_{1q0}=\sqrt{2} \qquad C_{3q2}=\frac{\sqrt{2}}{648}R^2$$

$$C_{2q1}=\frac{\sqrt{2}}{16}R \qquad C_{3q1}=\frac{R}{27}\left(\frac{A'+6}{A'+4}\right)^{1/2}$$

$$C_{2q0}=\frac{1}{2\sqrt{2}}\left(\frac{A'+2}{A'+1}\right)^{1/2} \qquad C_{3q0}=\left(\frac{2}{27}\right)^{1/2}\left(1+\frac{27}{8}\frac{(A')^2}{R^2}+\frac{1}{2}\frac{A'^2}{(A'+6)^2}\right)^{-1/2}$$

where $A'=A-R^2/4n^2$. Possible values of A and the normalised spheroidal wavefunctions have the form

$$\psi_{1q0}=(1/\sqrt{\pi})\exp[-\tfrac{1}{2}R(\xi+\eta)] \qquad A'=0$$

$$\psi_{2q1}=\tfrac{1}{16}R\exp[-\tfrac{1}{4}(\xi+\eta)][(\xi^2-1)(1-\eta^2)]^{1/2}\exp(\mathrm{i}\varphi)/\sqrt{2\pi} \qquad A'+2=0$$

$$\psi_{2q0}=\frac{1}{4\sqrt{\pi}}\left(\frac{A'+2}{A'+1}\right)^{1/2}[1+\tfrac{1}{2}A'(1+\xi\eta)-\tfrac{1}{4}R(\xi+\eta)]\exp[-\tfrac{1}{4}R(\xi+\eta)]$$

$$A'(A'+2)=\tfrac{1}{4}R^2$$

$$\psi_{3q2}=\frac{R^2}{648}\exp[-\tfrac{1}{6}R(\xi+\eta)](\xi^2-1)(1-\eta^2)\frac{\exp(2\mathrm{i}\varphi)}{\sqrt{\pi}} \qquad A'+6=0$$

$$\psi_{3q1}=\frac{R}{27}\left(\frac{A'+6}{A'+4}\right)^{1/2}\exp[-\tfrac{1}{6}R(\xi+\eta)][(\xi^2-1)(1-\eta^2)]^{1/2}$$

$$\times[1+\tfrac{1}{4}(A'+2)(1+\xi\eta)-\tfrac{1}{12}R(\xi+\eta)]\frac{\exp(\mathrm{i}\varphi)}{\sqrt{2\pi}}$$

$$(A'+2)(A'+6)=\tfrac{1}{9}R^2$$

$$\psi_{3q0}=\frac{\exp[-\tfrac{1}{6}R(\xi+\eta)]}{\sqrt{27\pi}}\left[1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{1}{2}\left(\frac{A'}{A'+6}\right)^2\right]^{-1/2}$$

$$\times\left[1-\frac{R}{3}(\xi+\eta)+\frac{A'^2}{2}(1+\xi\eta)-\frac{A'R}{24}(1+\xi\eta)(\xi+\eta)\right.$$

$$\left.+\frac{R^2}{27}\left(\frac{A'+8}{A'+6}\right)(\xi+\eta)^2+\frac{A'R^2}{72(A'+6)}(1+\xi\eta)^2\right]$$

$$A'(A'+2)(A'+6)=\tfrac{4}{9}R^2(A'+4).$$

It is easy to show that these formulae coincide to within normalisation constants with analogous formulae given by Coulson and Robinson (1958).

We recall that the index q denotes the eigenvalues of the separation constant A and takes the values $1\leqslant q\leqslant n-|m|$. These eigenvalues are determined from the equations together with the wavefunctions. For illustration we write down the transformation coefficients W_{nq}^{lm} and $U_{qm}^{n_1 n_2}$ in the same particular cases (see tables 1 and 2).

The transformation coefficients were first tabulated by Coulson and Joseph (1967) for several values of the quantum numbers. We have enlarged this table slightly and, as can be verified, have obtained agreement with their results. Substituting the values

Table 1. The transformation coefficients W_{nq}^{lm}.

n	m	l	$W_{nq}^{lm}(R)$	A'
1	0	0	1	$A'=0$
2	0	0	$\frac{1}{\sqrt{2}}\left(\frac{A'+2}{A'+1}\right)^{1/2}$	$A'(A'+2)=\frac{1}{4}R^2$
2	0	1	$\frac{A'\sqrt{2}}{R}\left(\frac{A'+2}{A'+1}\right)^{1/2}$	$A'(A'+2)=\frac{1}{4}R^2$
2	1	1	-1	$A'+2=0$
3	0	0	$\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	0	1	$\frac{A'}{R}\left(\frac{27}{8}\right)^{1/2}\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	0	2	$\frac{A'}{\sqrt{2}(A'+6)}\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	1	1	$-\frac{1}{\sqrt{2}}\left(\frac{A'+6}{A'+4}\right)^{1/2}$	$(A'+2)(A'+6)=\frac{1}{9}R^2$
3	1	2	$-\frac{3}{\sqrt{2}}\frac{(A'+2)}{R}\left(\frac{A'+6}{A'+4}\right)^{1/2}$	$(A'+2)(A'+6)=\frac{1}{9}R^2$
3	2	2	1	$A'+6=0$

Table 2. The transformation coefficients $U_{qm}^{n_1n_2}$.

n	m	n_2	$U_{qm}^{n_1n_2}$	A'
1	0	0	1	$A'=0$
2	0	0	$-\left(\frac{A'}{R}-\frac{1}{2}\right)\left(\frac{A'+2}{A'+1}\right)^{1/2}$	$A'(A'+2)=\frac{1}{4}R^2$
2	0	1	$\left(\frac{A'}{R}+\frac{1}{2}\right)\left(\frac{A'+2}{A'+1}\right)^{1/2}$	$A'(A'+2)=\frac{1}{4}R^2$
2	1	0	1	$A'+2=0$
3	0	0	$\frac{\sqrt{3}}{2}\left(\frac{A'+4}{A'+6}-\frac{3A'}{2R}\right)\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	0	1	$\frac{2\sqrt{3}}{A'+6}\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	0	2	$\frac{\sqrt{3}}{2}\left(\frac{A'+4}{A'+6}+\frac{3A'}{2R}\right)\left(1+\frac{27}{8}\frac{A'^2}{R^2}+\frac{A'^2}{2(A'+6)^2}\right)^{-1/2}$	$A'(A'+2)(A'+6)=\frac{4}{9}R^2(A'+4)$
3	1	0	$-\frac{3}{2R}\left(A'+2-\frac{R}{3}\right)\left(\frac{A'+6}{A'+4}\right)^{1/2}$	$(A'+2)(A'+6)=\frac{1}{9}R^2$
3	1	1	$\frac{3}{2R}\left(A'+2+\frac{R}{3}\right)\left(\frac{A'+6}{A'+4}\right)^{1/2}$	$(A'+2)(A'+6)=\frac{1}{9}R^2$
3	2	0	1	$A'+6=0$

of coefficients W_{nq}^{lm} and $U_{qm}^{n_1n_2}$ into relations (6.1) and (7.1) one can easily find strong connections. In the following, spheroidal, spherical and parabolic wavefunctions are denoted by $|nqm\rangle$, $\|nlm\rangle$ and $|||n_1n_2m\rangle$, respectively.

$$|110\rangle = \|100\rangle \qquad A' = 0$$

$$|210\rangle = \left(\frac{(1+\frac{1}{4}R^2)+(1+\frac{1}{4}R^2)^{1/2}}{2(1+\frac{1}{4}R^2)}\right)^{1/2} \|200\rangle + \frac{R}{2}\{2[(1+\tfrac{1}{4}R^2)+(1+\tfrac{1}{4}R^2)^{1/2}]\}^{-1/2}\|210\rangle$$

$$(A')_1 = -1+(1+\tfrac{1}{4}R^2)^{1/2}$$

$$|220\rangle = \left(\frac{(1+\frac{1}{4}R^2)-(1+\frac{1}{4}R^2)^{1/2}}{2(1+\frac{1}{4}R^2)}\right)^{1/2} \|200\rangle - \frac{R}{2}\{2[(1+\tfrac{1}{4}R^2)-(1+\tfrac{1}{4}R^2)^{1/2}]\}^{-1/2}\|210\rangle$$

$$(A')_2 = 1-(1+\tfrac{1}{4}R^2)^{1/2}$$

$$|211\rangle = -\|211\rangle \qquad A' = -2$$

$$|311\rangle = -\left(\frac{(1+\frac{1}{36}R^2)+(1+\frac{1}{36}R^2)^{1/2}}{2(1+\frac{1}{36}R^2)}\right)^{1/2} \|311\rangle$$

$$-\frac{R}{6}\{2[(1+\tfrac{1}{36}R^2)+(1+\tfrac{1}{36}R^2)^{1/2}]\}^{-1/2}\|321\rangle$$

$$(A')_1 = -4+2(1+\tfrac{1}{36}R^2)^{1/2}$$

$$|321\rangle = -\left(\frac{(1+\frac{1}{36}R^2)-(1+\frac{1}{36}R^2)^{1/2}}{2(1+\frac{1}{36}R^2)}\right)^{1/2} \|311\rangle$$

$$+\frac{R}{6}\{2[(1+\tfrac{1}{36}R^2)-(1+\tfrac{1}{36}R^2)^{1/2}]\}^{-1/2}\|321\rangle$$

$$(A')_2 = -4-2(1+\tfrac{1}{36}R^2)^{1/2}$$

$$|312\rangle = \|322\rangle \qquad A' = -6$$

$$|110\rangle = |||000\rangle \qquad A' = 0$$

$$|210\rangle = \left[\frac{1}{2}+\frac{1}{R}-(1+\tfrac{1}{4}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{4}R^2)+(1+\frac{1}{4}R^2)^{1/2}}{(1+\frac{1}{4}R^2)}\right)^{1/2} |||100\rangle$$

$$+\left[\frac{1}{2}-\frac{1}{R}+(1+\tfrac{1}{4}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{4}R^2)+(1+\frac{1}{4}R^2)^{1/2}}{(1+\frac{1}{4}R^2)}\right)^{1/2} |||010\rangle$$

$$(A')_1 = -1+(1+\tfrac{1}{4}R^2)^{1/2}$$

$$|220\rangle = \left[\frac{1}{2}+\frac{1}{R}+(1+\tfrac{1}{4}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{4}R^2)-(1+\frac{1}{4}R^2)^{1/2}}{(1+\frac{1}{4}R^2)}\right)^{1/2} |||100\rangle$$

$$+\left[\frac{1}{2}-\frac{1}{R}-(1+\tfrac{1}{4}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{4}R^2)-(1+\frac{1}{4}R^2)^{1/2}}{(1+\frac{1}{4}R^2)}\right)^{1/2} |||010\rangle$$

$$(A')_2 = -1-(1+\tfrac{1}{4}R^2)^{1/2}$$

$$|211\rangle = |||001\rangle \qquad A' = -2$$

$$|311\rangle = \frac{3}{R}\left[\frac{R}{6}+3-(1+\tfrac{1}{36}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{36}R^2)+(1+\frac{1}{36}R^2)^{1/2}}{(1+\frac{1}{36}R^2)}\right)^{1/2} |||101\rangle$$

$$+\frac{3}{R}\left[\frac{R}{6}-1+(1+\tfrac{1}{36}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{36}R^2)+(1+\frac{1}{36}R^2)^{1/2}}{(1+\frac{1}{36}R^2)}\right)^{1/2} |||011\rangle$$

$$(A')_1 = -4+2(1+\tfrac{1}{36}R^2)^{1/2}$$

$$|321\rangle = \frac{3}{R}\left[\frac{R}{6}+3+(1+\tfrac{1}{36}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{36}R^2)-(1+\frac{1}{36}R^2)^{1/2}}{(1+\frac{1}{36}R^2)}\right)^{1/2} |||101\rangle$$

$$+\frac{3}{R}\left[\frac{R}{6}-1-(1+\tfrac{1}{36}R^2)^{1/2}\right]\left(\frac{(1+\frac{1}{36}R^2)-(1+\frac{1}{36}R^2)^{1/2}}{(1+\frac{1}{36}R^2)}\right)^{1/2} |||011\rangle$$

$$(A')_2 = -4-2(1+\tfrac{1}{36}R^2)^{1/2}$$

$$|312\rangle = |||002\rangle \qquad A' = -6.$$

9. Conclusion

In this paper we have developed a spheroidal analysis of the hydrogen atom in which conditions following from the 'correspondence principle' are fulfilled at all steps: equations, recurrence relations, wavefunctions, transformation coefficients, etc. The formula suitable for calculating the normalisation constant and expansions of the spheroidal wavefunction over the spherical basis and parabolic basis are found.

Systematic spheroidal analysis of the Coulomb problem comprises a lot of related problems. The present paper is the first step to the solution of this problem. The next step concerns the continuous spectrum.

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