Expectation values in relativistic Coulomb problems

Sergei K Suslov

School of Mathematical and Statistical Sciences and Mathematical, Computational, and Modeling Sciences Center, Arizona State University, Tempe, AZ 85287-1804, USA
E-mail: sks@asu.edu

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Abstract
We evaluate the matrix elements $\langle O r^p \rangle$, where $O = \{1, \beta, i\alpha n\}$ are the standard Dirac matrix operators and the angular brackets denote the quantum-mechanical average for the relativistic Coulomb problem, in terms of generalized hypergeometric functions $3F_2(1)$ for all suitable powers. Their connections with the Chebyshev and Hahn polynomials of a discrete variable are emphasized. As a result, we derive two sets of Pasternack-type matrix identities for these integrals, when $p \to -p - 1$ and $p \to -p - 3$, respectively. Some applications to the theory of hydrogenlike relativistic systems are reviewed.

1. Introduction

Recent experimental progress has renewed interest in quantum electrodynamics of atomic hydrogenlike systems. Experimentalists and theorists in atomic and particle physics are discovering problems of common interest with new ideas and methods. A current account of the status of this fundamental area of quantum physics, which is more than a century old, is given in [29, 30, 38, 58]. Exciting research topics vary from experimental testing of quantum electrodynamics (QED) to fruitful training models for the bound-state quantum chromodynamics and Bose–Einstein condensation [14, 29, 30, 31, 38, 58, 63].

The highly charged ions are an ideal testing ground for the strong-field bound-state QED. They possess a strong static Coulomb field of the nucleus and a simple electronic structure which can be accurately computed from first principles. It is possible nowadays to make massive highly charged ions with a strong nuclear charge and only one electron through the periodic table up to uranium, the most highly charged ion [26, 27]. These systems are truly relativistic and require the Dirac wave equation as a starting point in a detailed investigation of their spectra [38, 55]. The binding energy of a single K -shell electron in the electric field of a uranium nucleus corresponds to roughly one third of the electron rest mass. For the simple hydrogen atom, the nonrelativistic Schrödinger approximation can be used [8].

In the last decade, the two-time Green’s function method of deriving formal expressions for the energy shift of a bound-state level of high-Z few-electron systems was developed [55], and numerical calculations of QED effects in heavy ions were performed in excellent agreement with current experimental data [26, 27] (see [52–54, 57, 58, 63] and references therein for more details). These advances motivate, among other technical things, evaluation of the expectation values $\langle O r^p \rangle$ for the standard Dirac matrix operators $O = \{1, \beta, i\alpha n\}$ between the bound-state relativistic Coulomb wavefunctions. Special cases appear in calculations of the magnetic dipole hyperfine splitting, the electric quadrupole hyperfine splitting, the anomalous Zeeman effect and the relativistic recoil corrections in hydrogenlike ions (see, for example, [1, 54, 56] and references therein). We discuss convenient closed forms of these integrals in general and derive matrix symmetry relations among them which can be useful in the theory of relativistic Coulomb systems.

This paper is organized as follows. In the following section, we review the relativistic Coulomb wavefunctions and set up the notations. The expectation values $\langle O r^p \rangle$ are evaluated in section 3 in terms of the generalized hypergeometric functions $3F_2(1)$ for all admissible powers of $r$. Their Pasternack-type matrix symmetry relations are established in section 4, and recurrence relations are given in section 5. We discuss special matrix elements and review some of their applications in section 6. An attempt to collect the available literature is made. Appendix A contains the definition of the generalized hypergeometric series and the proof of a required transformation identity. Appendix B deals with the Dirac matrices and inner product.
2. Wavefunctions for the relativistic Coulomb problem

The exact solutions of the stationary Dirac equation

\[ H\psi = (c\alpha p + mc^2\beta - Z e^2/r)\psi = E\psi \]  

(2.1)

corresponding (bispinor) Dirac wavefunctions were found by Darwin [16] and Gordon [25] at the early stage of discovery of the ‘new’ wave mechanics (see also [9] for a modern discussion of ‘Sommerfeld’s puzzle’). These classical results are nowadays included in all textbooks on relativistic quantum mechanics, quantum field theory and advanced texts on mathematical physics (see, for example, [2, 7, 8, 28, 37, 40]). The end result is

\[ \psi = \left( \varphi \chi \right) = \left( Y_{jm}^{\pm}(n)F(r) \right) \left( Y_{jm}^{\pm}(n)G(r) \right), \]

(2.2)

where the spinor spherical harmonics \( Y_{jm}^{\pm}(n) \) are given explicitly in terms of the ordinary spherical functions \( Y_{jm}(n) \), \( n = n(\theta, \varphi) = r/r \) and the special Clebsch–Gordan coefficients with the spin 1/2 as follows [2, 7, 46, 61].

\[ Y_{jm}^{\pm}(n) = \sqrt{ \frac{(j+1/2)!m!}{j! (j+1/2)! (m-1/2)!}} \left( \begin{array}{c} Y_{j+1/2, m-1/2}(\theta, \varphi) \end{array} \right) \]

(2.3)

with the total angular momentum \( j = 1/2, 3/2, 5/2, \ldots \) and its projection \( m = -j, -j+1, \ldots, j-1, j \) (see also section VI A of [60] for the properties of the spinor spherical harmonics).

The radial functions \( F(r) \) and \( G(r) \) can be presented as [40]

\[ \left( \begin{array}{c} F(r) \\ G(r) \end{array} \right) = \frac{a^2 \beta^{3/2}}{v} \sqrt{ \frac{(\varepsilon - v) (n-1)!}{\mu (v-k) (n+2v)}} e^{-\varepsilon/2} \]

\[ \times \left( \begin{array}{c} f_1 \\ f_2 \\ g_1 \\ g_2 \end{array} \right) \left( \begin{array}{c} \xi L_{\nu+1}^{2\nu+1}(\xi) \\ \xi L_{\nu-1}^{2\nu-1}(\xi) \end{array} \right), \]

(2.4)

Here, \( L_{\nu}^{2\nu}(\xi) \) are the Laguerre polynomials given by (A.2), and we use the following notations:

\[ \kappa = \pm (j + 1/2), \quad v = \sqrt{\kappa^2 - \mu^2}, \]

\[ \mu = aZ = Ze^2/hc, \quad a = \sqrt{1 - \varepsilon^2}, \]

\[ \varepsilon = E/mc^2, \quad \beta = mc/h = 1/\lambda, \]

and

\[ \xi = 2a\beta r = 2\sqrt{1 - \varepsilon^2 mc^2/\hbar r}. \]

The elements of the \((2 \times 2)\)-transition matrix in (2.4) are given by

\[ f_1 = \frac{a \mu}{\varepsilon - \kappa - v}, \quad f_2 = \kappa - v, \quad g_1 = \frac{a(\kappa - v)}{\varepsilon - \kappa - v}, \quad g_2 = \mu. \]

(2.7)

This particular form of the relativistic radial functions is due to Nikiforov and Uvarov [40]; it is very convenient for taking the nonrelativistic limit \( c \to \infty \) (see also [60]).

The relativistic discrete energy levels \( \varepsilon = \varepsilon_n = E_n/E_0 \) with the rest mass energy \( E_0 = mc^2 \) are given by the Sommerfeld–Dirac fine structure formula:

\[ E_n = \frac{mc^2}{\sqrt{1 + \mu^2/ (n + \nu)^2}}. \]

(2.8)

Here, \( n = n_r = 0, 1, 2, \ldots \) is the radial quantum number and \( \kappa = \pm (j + 1/2) = \pm 1, \pm 2, \pm 3, \ldots \). The following quantities

\[ \varepsilon \mu = a (v + n), \quad \varepsilon \mu + av = a (n + 2v), \quad \varepsilon \mu - av = an, \]

\[ \varepsilon^2 k^2 - v^2 = a^2 n (n + 2v) = \mu^2 - a^2 \kappa^2 \]

(2.9)

are useful in the calculation of the matrix elements below.

The familiar recurrence relations for the Laguerre polynomials allow us to present the radial functions (2.4) in a traditional form [2, 7, 15, 34, 60] as follows:

\[ \left( \begin{array}{c} F(r) \\ G(r) \end{array} \right) = a^2 \beta^{3/2} \sqrt{ \frac{n!}{\mu (\kappa - v) (\kappa + v) (n + 2v)}} e^{-\varepsilon/2} \]

\[ \times \left( \begin{array}{c} \alpha_1 \alpha_2 \beta_1 \beta_2 \\ \beta_1 \beta_2 \end{array} \right) \left( \begin{array}{c} L_{n+1}^{2\nu+1}(\xi) \\ L_{n-1}^{2\nu-1}(\xi) \end{array} \right), \]

(2.10)

where

\[ \alpha_1 = \sqrt{1 + \varepsilon (\kappa - v) \sqrt{1 + \varepsilon + \mu \sqrt{1 - \varepsilon}}}, \]

\[ \alpha_2 = -\sqrt{1 + \varepsilon (\kappa - v) \sqrt{1 + \varepsilon - \mu \sqrt{1 - \varepsilon}}}, \]

\[ \beta_1 = \sqrt{1 - \varepsilon (\kappa - v) \sqrt{1 + \varepsilon + \mu \sqrt{1 - \varepsilon}}}, \]

\[ \beta_2 = \sqrt{1 - \varepsilon (\kappa - v) \sqrt{1 + \varepsilon - \mu \sqrt{1 - \varepsilon}}} \]

and a convenient identity holds

\[ ((\kappa - v) \sqrt{1 + \varepsilon - \mu \sqrt{1 - \varepsilon}})^2 = 2(\kappa - v)(\kappa - ve \pm a\mu). \]

(2.13)

We give the explicit form of the radial wavefunctions (2.4) for the \( 1s_l \) state, when \( n = n_r = 0, l = 0, j = 1/2 \) and \( \kappa = -1 \):

\[ \left( \begin{array}{c} F(r) \\ G(r) \end{array} \right) = \left( \begin{array}{c} 2Z^2 \alpha_0 \\ 2\sqrt{2\nu_1 + 1} \end{array} \right) \]

\[ \times \left( \begin{array}{c} -1 \sqrt{1 - \nu_1} \varepsilon^{\nu_1-1} \varepsilon^{-\varepsilon/2} \end{array} \right). \]

(2.14)

Here, \( \nu_1 = \sqrt{1 - \mu^2} = \xi_1, \xi_2 = 2\sqrt{1 - \xi_2^2 \beta r} = 2Z (r/\alpha_0), \) and \( \alpha_0 = \hbar^2/mc^2 \) is the Bohr radius. One can see also [2, 7, 8, 16, 19, 25, 28, 34, 37, 50] and references therein for more information on the relativistic Coulomb problem.

3. Evaluation of the matrix elements

We evaluate the following integrals of the radial functions:

\[ A_p = \int_0^\infty r^{p+2} (F^2(r) + G^2(r)) \, dr, \]

(3.1)

\[ B_p = \int_0^\infty r^{p+2} (F^2(r) - G^2(r)) \, dr, \]

(3.2)
in terms of generalized hypergeometric series. (Their relations 
with the expectation values \( \langle \text{Or}^p \rangle \), where \( \text{Or} = \{ 1, \beta, \text{ion} \beta \} \), are discussed in appendix B.) The final results with the notations from the previous page can be presented in two different closed forms. Use of the traditional radial functions \( \mu(\epsilon_κ) \) takes one of the radial wavefunctions from (2.4) and another one from (2.10). We leave the details to the reader.

The averages of \( \text{Or}^p \) for the relativistic hydrogen atom were evaluated by Davis [15] in a form which is slightly different from our equations (3.4) and (3.7), see also [3] and [60] for a simple proof of the second formula including evaluation of the corresponding integral of the product of two Laguerre polynomials:

\[
\int_0^\infty e^{-x} x^{s\alpha \beta} L_n^{\beta}(x)L_m^{\alpha}(x) dx
\]

\[
= (-1)^{n-m} \frac{\Gamma(\alpha + s + 1) \Gamma(\beta + m + 1) \Gamma(s + 1)}{m! (n-m)! \Gamma(\beta + 1) \Gamma(s - n + m + 1)} \times 3F_2 \left( \begin{array}{c} -m, s + 1, \beta - \alpha - s \\ \beta + 1, \ n - m + 1 \end{array} \right), \quad n \geq m.
\]

(The limit \( c \to \infty \) of the integral \( A_p \) is discussed in [60].) Equations (3.5)–(3.6) and (3.8)–(3.9), which we have not been able to find in the available literature, can be derived in a similar fashion. It does not appear to have been noticed that the corresponding \( 3F_2 \) functions can be expressed in terms of Hahn polynomials:

\[
h_n^{(c, \beta)}(x, N) = (-1)^n \frac{\Gamma(N) \Gamma(\beta + 1)_n}{n! \Gamma(N - n)} \times 3F_2 \left( \begin{array}{c} -n, \alpha + \beta + n + 1, -x \\ \beta + 1, \ n - N \end{array} \right).
\]

The ease of handling of these matrix elements for the discrete levels is greatly increased if use is made of the known properties of these polynomials [20, 39, 40].

For example, the difference-differentiation formulae (4.34)–(4.35) of [60] (see also (A.5)) take the following convenient form:

\[
\frac{p(p + 1)}{n + 2v} \times 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2v + 1, 2 \end{array} \right)
\]

\[
= \frac{p(p + 1)}{2v + 1} \times 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 2 \\ 2v + 1, 2 \end{array} \right) = 3F_2 \left( \begin{array}{c} -n, -p, p + 1 \\ 2v + 1, 1 \end{array} \right) - 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2v + 1, 1 \end{array} \right),
\]

\[
(3.12)
\]

in terms of generalized hypergeometric series. (Their relations 
with the expectation values \( \langle \text{Or}^p \rangle \), where \( \text{Or} = \{ 1, \beta, \text{ion} \beta \} \), are discussed in appendix B.) The final results with the notations from the previous page can be presented in two different closed forms. Use of the traditional radial functions \( \mu(\epsilon_κ) \) takes one of the radial wavefunctions from (2.4) and another one from (2.10). We leave the details to the reader.

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\[
\int_0^\infty e^{-x} x^{s\alpha \beta} L_n^{\beta}(x)L_m^{\alpha}(x) dx
\]

\[
= (-1)^{n-m} \frac{\Gamma(\alpha + s + 1) \Gamma(\beta + m + 1) \Gamma(s + 1)}{m! (n-m)! \Gamma(\beta + 1) \Gamma(s - n + m + 1)} \times 3F_2 \left( \begin{array}{c} -m, s + 1, \beta - \alpha - s \\ \beta + 1, \ n - m + 1 \end{array} \right), \quad n \geq m.
\]

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\[
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\]

\[
= \frac{p(p + 1)}{2v + 1} \times 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 2 \\ 2v + 1, 2 \end{array} \right) = 3F_2 \left( \begin{array}{c} -n, -p, p + 1 \\ 2v + 1, 1 \end{array} \right) - 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2v + 1, 1 \end{array} \right),
\]

\[
(3.12)
\]
in terms of the generalized hypergeometric functions. (Another proof of these identities is given in appendix A.)

As a result, the linear relation holds [1, 51]

\[ 2\kappa (A_p - \varepsilon B_p) - (p + 1)(B_p - \varepsilon A_p) = 4\mu C_p, \]  

(3.13)

and we can rewrite (3.4)–(3.5) in the following matrix form:

\[ 2(p + 1)\alpha \mu (2\alpha \beta)^p \frac{\Gamma (2v + p + 1)}{\Gamma (2v + p + 1)} \begin{pmatrix} A_p \\ B_p \end{pmatrix} = \begin{pmatrix} \gamma_1 & \gamma_2 \\ \delta_1 & \delta_2 \end{pmatrix} \begin{pmatrix} 1 - n, -p, p + 1 \\ 2v + 1, 1 \end{pmatrix} (p \neq -1), \]

\[ \frac{\delta_2}{3} \begin{pmatrix} 1 - n, -p, p + 1 \\ 2v + 1, 1 \end{pmatrix} \]

(3.14)

where

\[ \gamma_1 = (\mu + a\kappa)(a(2\kappa + p + 1) - 2\varepsilon \mu), \]

(3.15)

\[ \gamma_2 = (\mu - a\kappa)(a(2\kappa + p + 1) + 2\varepsilon \mu), \]

\[ \delta_1 = (\mu - a\kappa)(a(2\kappa + \varepsilon(p + 1)) - 2\mu), \]

(3.16)

\[ \delta_2 = (\mu - a\kappa)(a(2\kappa + \varepsilon(p + 1)) + 2\mu). \]

This representation of integrals \( A_p \) and \( B_p \) involves the Chebyshev polynomials of a discrete variable \( h_p^{(0,0)}(x, -2v) \) at \( x = n, n - 1 \) only; see also equation (3.6) for \( C_p \). The corresponding dual Hahn polynomials [39] may be considered as difference analogues of the Laguerre polynomials in equation (2.10) for the relativistic radial functions.

4. Inversion formulae

Due to the symmetry of the hypergeometric functions in (3.4)–(3.6) under the transformation \( p \rightarrow -p - 1 \), one obtains

\[ A_{-p-1} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p)}{\Gamma(2v + p + 1)} \frac{(1 + \varepsilon^2)p + \varepsilon^2) A_p - (2p + 1)\varepsilon B_p}{(1 - \varepsilon^2)p}, \]

(4.1)

\[ B_{-p-1} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p)}{\Gamma(2v + p + 1)} \frac{(2p + 1)\varepsilon A_p - ((1 + \varepsilon^2)p + 1)B_p}{(1 - \varepsilon^2)p}, \]

(4.2)

\[ C_{-p-1} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p)}{\Gamma(2v + p + 1)} C_p. \]

(4.3)

(These relations allow us to evaluate all the convergent integrals with \( p \leq -2 \).) Indeed,

\[ A_{-p-1} - \varepsilon B_{-p-1} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p)}{\Gamma(2v + p + 1)} (A_p - \varepsilon B_p), \]

(4.4)

\[ B_{-p-1} - \varepsilon A_{-p-1} = \frac{p + 1}{p} (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p)}{\Gamma(2v + p + 1)} (B_p - \varepsilon A_p), \]

(4.5)

which gives the first two equations, if \( B_p \neq \varepsilon A_p \) and \( p \neq 0, -1 \). The last one follows from (3.6). Special cases \( p = 0, -1 \) of (4.4)–(4.5) are simply identity (6.16) and Fock’s virial theorem (6.13), respectively. In view of our formulæ (3.4)–(3.5), equation \( B_p = \varepsilon A_p \) occurs only when \( p = 0 \) or \( n = 0 \).

The symmetry of the hypergeometric functions in (3.7)–(3.9) under another reflection \( p \rightarrow -p - 3 \) gives

\[ A_{-p-3} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p - 2)}{\Gamma(2v + p + 3)} \times \left( 4\mu^2(2p + 3) + (p + 2)(4\varepsilon^2 + (p + 1)(p + 2)) \frac{A_p}{p + 2} \right. \]

\[ - 2\kappa(2p + 3)B_p - 8\kappa \mu \frac{2p + 3}{p + 2} C_p \right), \]

(4.6)

\[ B_{-p-3} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p - 2)}{\Gamma(2v + p + 3)} \times \left( -2\kappa(2p + 3)A_p + (4\varepsilon^2 + (p + 1)(p + 2))B_p + 4\mu(2p + 3)C_p \right), \]

(4.7)

\[ C_{-p-3} = (2\alpha \beta)^{2p+1} \frac{\Gamma(2v - p - 2)}{\Gamma(2v + p + 3)} \times \left( 2\mu \frac{2p + 3}{p + 2} C_p - \mu(2p + 3)B_p \right. \]

\[ - 4\mu^2(2p + 3) + (p + 1)(4\varepsilon^2 - (p + 2)^2) \frac{C_p}{p + 2} \right), \]

(4.8)

as a result of elementary matrix multiplications. These relations can be used for all the convergent integrals with \( p \leq -3 \). Further details are left to the reader.

The corresponding single two-term nonrelativistic relation was found by Pasternack [41, 42] (see also [51] and references therein). We have been unable to find the relativistic matrix identities (4.1)–(4.3) and (4.6)–(4.8) in the available literature (see equation (18) of [3] as the closest analogue).

5. Recurrence relations

A set of useful recurrence relations between the relativistic matrix elements was derived by Shabatov [51] (see also [1, 18, 56, 62]) on the basis of a hypervirial theorem:

\[ 2\kappa A_p - (p + 1)B_p = 4\mu C_p + 4\beta \varepsilon C_{p+1}, \]

(5.1)

\[ 2\kappa B_p - (p + 1)A_p = 4\beta C_{p+1}, \]

(5.2)

\[ \mu B_p - (p + 1)C_p = \beta(A_{p+1} - \varepsilon B_{p+1}), \]

(5.3)

Linear relation (3.13) and convenient recurrence formulæ

\[ A_{p+1} = -(p + 1) \times \frac{4\varepsilon^2 p + 2\kappa(p + 2) + \varepsilon(p + 1)(2\kappa\varepsilon + p + 2)}{4(1 - \varepsilon^2)(p + 2)\beta \mu} A_p \]

\[ + \frac{4\mu^2(p + 2) + (p + 1)(2\kappa\varepsilon + p + 1)(2\kappa\varepsilon + p + 2)}{4(1 - \varepsilon^2)(p + 2)\beta \mu} B_p, \]

(5.4)
\[ B_{p+1} = -\left(p + 1\right) \frac{4\nu^2 + 2k \varepsilon^2 (p + 3) + \varepsilon^2 (p + 1)(p + 2)}{4(1 - \varepsilon^2)(p + 2)\beta\mu} A_p + 4\mu^2 \varepsilon(p + 2)(p + 1)(2k \varepsilon + 2p + 1) (2k \varepsilon + \varepsilon(p + 2)) B_{p'}, \]

\[ C_{p+1} = \frac{1}{4\mu} (2k + \varepsilon(p + 2)) A_{p+1} - \frac{1}{4\mu} (2k \varepsilon + p + 2) B_{p+1}, \]

are obtained from these equations (see [1, 51, 56] for more details). Their connections with the theory of generalized hypergeometric functions will be discussed elsewhere.

### 6. Special expectation values and their applications

The Sommerfeld–Dirac formula (2.8) is derived for a point charge atomic nucleus with infinite mass and no internal structure (an electron moving in the static Coulomb field). In reality, the electron’s mass is not negligibly small compared with the nuclear mass, and one has to consider the effect of nuclear motion on the energy levels. Actual nuclei have a finite size and possess some internal structure, such as an internal angular momentum or spin, a magnetic dipole moment and a small electric quadrupole moment associated with the spin, which also affect the energy levels. Radiative corrections are introduced by the quantization of the electromagnetic radiation field. (See [8, 11, 22–55, 63, 58] and references therein for more details.) Calculations of the real energy levels of the high-Z one-electron systems with the help of the perturbation theory require special relativistic matrix elements.

From the explicit expressions (3.4)–(3.9), one can derive the following special matrix elements:

\[ A_2 = \left(\frac{r}{r}\right) = \frac{5n(n + 2\nu) + 4\nu^2 + 1 - \varepsilon\kappa(2k \varepsilon + 3)}{2(\alpha\beta)^2}, \]

\[ A_1 = \left(\frac{\partial E}{\partial \lambda}\right) = \frac{3\varepsilon^2 \mu^2 - \kappa(1 - \varepsilon^2)(1 + \varepsilon\kappa)}{2\beta\mu(1 - \varepsilon^2)}, \]

\[ A_0 = \left(1\right) = 1, \]

\[ A_{-1} = \left(\frac{1}{r}\right) = \frac{\beta \varepsilon^2 (1 - \varepsilon^2)(\varepsilon\nu + \mu\sqrt{1 - \varepsilon^2})}{m^2 e^4 - E^2}, \]

\[ A_{-2} = \left(\frac{1}{r^2}\right) = \frac{2\alpha^2 \beta^2 \varepsilon^2 (2k \varepsilon - 1)}{\mu \nu (4\nu^2 - 1)}, \]

\[ A_{-3} = \left(\frac{1}{r^3}\right) = \frac{2(\alpha^2 \beta^2 - 3k \varepsilon^2 - \varepsilon^2 + 1)}{v(v^2 - 1)(4v^2 - 1)}. \]

(Note that \(A_{-3}\) exists only if \(|\kappa| \geq 2\) [51].) The average distance between the electron and the nucleus \(\langle r \rangle\) is given by \(A_1\). The mean square deviation of the nucleus–electron separation is \(\langle r^2 \rangle = A_2 - (A_1)^2\). The energy eigenvalue \(\langle E \rangle\), mean radius \(\langle r \rangle\) and mean square radius \(\langle r^2 \rangle\) are frequently used when making comparisons of wavefunctions computed by different approximation methods. The integrals \(A_1\) and \(A_2\) have been evaluated in [13, 23, 44, 60] (see also [3] for closed-form expressions for \(|A_p|\) to \(\infty\)). Matrix element \(A_3\) appears in the calculation of the electric quadrupole hyperfine splitting [43, 52, 56]. Integrals \(A_p\) are also part of the expression for the effective electrostatic potential for the relativistic hydrogenlike atom [60]:

\[ B_2 = (\beta r^2) = \frac{2\alpha^2 \beta^2}{m^2 e^4} \left[5n(n + 2\nu) + 2\nu^2 + 1 - 3\varepsilon\kappa\right] \]

\[ = \frac{3\varepsilon^2 \mu^2 + (5\mu^2 + 3\varepsilon^2 - 1)\varepsilon^3 - 3\varepsilon^2 - 3\varepsilon^2 + 1}{2\beta^2(1 - \varepsilon^2)^2}, \]

\[ B_1 = (\beta r) = \frac{3\varepsilon^2 \mu^2 - (1 - \varepsilon^2)(\varepsilon\kappa + \varepsilon^2)}{2\beta \mu(1 - \varepsilon^2)}, \]

\[ B_0 = (\beta) = \varepsilon = \frac{E}{m c^2}. \]

The integrals \(B_0\) appears in the virial theorem for the Dirac equation in a Coulomb field,

\[ E = m c^2 \langle \beta \rangle, \]

established by Fock [22] and then developed by many authors (see [11, 12, 17, 18, 21, 24, 32, 36, 45, 47–49, 51, 56], and references therein). Relation (6.13) can also be obtained with the help of the Hellmann–Feynman theorem,

\[ \frac{\partial E}{\partial \lambda} = \langle \frac{\partial H}{\partial \mu} \rangle, \]

\[ \frac{\partial E}{\partial Z} = -\varepsilon^2 \left(\frac{1}{r}\right) = -\varepsilon^2 A_{-1}, \]

\[ \frac{\partial E}{\partial \kappa} = 2\hbar c A_{-1}. \]

The following identities hold

\[ A_{-1} - \varepsilon B_{-1} = \frac{\alpha^2 \beta}{\varepsilon} = \frac{1}{\beta} \left(\mu B_{-2} + C_{-2}\right), \]

by (5.3). The integral \(B_{-1}\) is evaluated in [11] and \(A_{-1}, A_{-2}, B_{-2}, C_{-2}\) and \(A_{-3}\) are given in [51] (see also [56]).

The relativistic recoil corrections to the energy levels, when nuclear motion is taken into consideration, require matrix elements \(A_{-2}, B_{-1}\) and \(C_{-2}\) (see [1, 11, 53, 54] and references therein):

\[ C_2 = \frac{\kappa a^2}{4\mu (\alpha^2 \beta^2)} \]

\[ = \frac{\kappa (1 - \varepsilon^2)(1 - \varepsilon^2) + 3\varepsilon^2 \mu^2 (\varepsilon \kappa - 1)}{4\mu \beta^2(1 - \varepsilon^2)}. \]
Table 1. Expectation values for the 1s1/2 state.

|   | $A_p$ | $B_p$ | $C_p$ |
|---|---|---|---|
| 2 | $\frac{1}{2} \left( \frac{1}{2} \right)^2 (v_1 + 1) (2v_1 + 1)$ | $\frac{1}{2} \left( \frac{1}{2} \right)^2 v_1 (v_1 + 1) (2v_1 + 1) - \frac{\hbar}{2} \left( v_1 + 1 \right) (2v_1 + 1)$ | $\frac{1}{2} (2v_1 + 1)$ |
| 1 | $\frac{3}{2} \left( \frac{1}{2} \right)^2$ | $\frac{3}{2} \hbar v_1$ | $\frac{3}{2} \hbar v_1$ |
| 0 | 1 | $v_1$ | $v_1$ |
| -1 | $\frac{1}{2} \left( \frac{1}{2} \right)^2$ | $\frac{1}{2} \left( \frac{1}{2} \right)^2 v_1$ | $\frac{1}{2} \left( \frac{1}{2} \right)^2 v_1$ |
| -2 | $\left( \frac{3}{2} \right)^2 \left( \frac{1}{2} \right)^2 (v_1 + 1)$ | $\left( \frac{3}{2} \right)^2 \left( \frac{1}{2} \right)^2 (v_1 + 1)$ | $\left( \frac{3}{2} \right)^2 \left( \frac{1}{2} \right)^2 (v_1 + 1)$ |
| -3 | $\frac{3}{2} \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} \right)^2$ | $\frac{3}{2} \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} \right)^2$ | $\frac{3}{2} \left( \frac{1}{2} \right)^2 \left( \frac{1}{2} \right)^2$ |

(6.18) (for all the suitable integers $p > -2v_1 - 1 > -3$) follow directly from (3.4), (3.5) and (3.7), (3.9). (The formal expressions for $A_{-3}$, $B_{-3}$ and $C_{-3}$, when the integrals diverge, are included into the table for ‘completeness’; see [1] for more details.) The reflection relation (4.3) holds for all the convergent integrals $A_p, B_p$ and $C_p$.

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Appendix A. Generalized hypergeometric series

The generalized hypergeometric series is defined as follows [4, 20],

$$p F_q (a_1, a_2, \ldots, a_p; b_1, b_2, \ldots, b_q; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \cdots (a_p)_n z^n}{(b_1)_n (b_2)_n \cdots (b_q)_n n!},$$

(A.1)

where $(a)_n = a (a + 1) \cdots (a + n - 1) = \Gamma (a + n) / \Gamma (a)$. In this paper, we always have $p = 3, q = 2, z = 1$, and $a_1$ is a negative integer when the series terminates. The Laguerre polynomials are given by [20, 39, 40]:

$$L_n^\alpha (x) = \frac{\Gamma (\alpha + n + 1)}{n! \Gamma (\alpha + 1)} \frac{\hbar}{\lambda} F_1 \left( \frac{-n}{\alpha + 1}; x \right).$$

(A.2)

The required identity (3.12) can be derived from the theory of classical polynomials in the following fashion. Let us start from the difference equation for the Hahn polynomials $y_m = h^{(a, b)}_m (x, N)$ [39]:

$$(\sigma (x) \nabla + \lambda (x)) \Delta y_m + \lambda_m y_m = 0,$$

(A.3)

where $\Delta f (x) = \nabla f (x + 1) - f (x)$ and

$$\sigma (x) = x (a + N - x),$$

(A.4)

$$\lambda_m = m (a + \beta + m + 1),$$

where $\Delta f (x) = \nabla f (x + 1) - f (x)$ and

$$\sigma (x) = x (a + N - x),$$

(A.4)

$$\lambda_m = m (a + \beta + m + 1).$$

(A.4)
and use the familiar difference-differentiation formula:
\[ \Delta h_{m}^{(\alpha,\beta)}(x, N) = (\alpha + \beta + m + 1)h_{m-1}^{(\alpha+1,\beta+1)}(x, N - 1). \]  
(A.5)
As a result,
\[ (\sigma(x)\nabla + \tau(x))h_{m}^{(\alpha,\beta)}(x, N - 1) + m h_{m}^{(\alpha,\beta)}(x, N) = 0. \]  
(A.6)
Letting \( \alpha = \beta \) and \( \beta \to -1 \), one gets
\[ x(N-x-1)\nabla h_{m}^{(0,0)}(x, N - 1) = -m \lim_{\beta \to -1} h_{m}^{(\alpha,\beta)}(x, N) \]
\[ = (-1)^{m}m(m-1) \frac{\Gamma(N-1)}{\Gamma(N-m-1)} \frac{1}{r_{2}} \left( \frac{1 - m, m, 1 - x}{2}, \frac{2}{2}, \frac{2 - N}{2} \right) \]
(A.7)
by (3.11). The last identity takes the form (3.12), if the Chebyshev polynomials of a discrete variable \( h_{m}^{(0,0)}(x, N - 1) \) are replaced by the corresponding generalized hypergeometric functions. (Use of (A.5) in (A.7) gives the special \( \text{F}_{2} \) transformation.)

**Appendix B. Dirac matrices and inner product**

We use the standard representations of the Dirac and Pauli matrices:
\[ \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]
(B.1)
\[ \sigma_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]
(B.2)
with
\[ 0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \]
(B.3)
The inner product of two Dirac (bispinor) wavefunctions
\[ \langle \psi, \phi \rangle = \int \psi^{\dagger} \phi \, dv = \int \psi_{1}^{\dagger} \phi_{1} \, dv \]
\[ = \int \psi_{2}^{\dagger} \phi_{2} \]  
(B.4)
and the corresponding expectation values of a matrix operator \( A \) are given by
\[ \langle A \rangle = \langle \psi, A \psi \rangle. \]
(B.6)
From this definition one gets
\[ \langle \beta^{p} \rangle = B_{p}, \quad \langle \alpha \beta^{p} \rangle = -2C_{p}, \]
(B.7)
where the integrals \( A_{p}, B_{p}, \) and \( C_{p} \) are given by (3.1)–(3.3), respectively.

Indeed, the first relation is derived, for example, in [60] and the second one can be obtained by integrating the identity
\[ r^{p} \psi^{\dagger} \beta \psi = r^{p} (\varphi^{\dagger}, \chi^{\dagger}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \varphi \\ -\chi \end{pmatrix} = r^{p} (\varphi^{\dagger}, \chi^{\dagger}) (F^{2} - G^{2}) \]
(B.8)
(we leave details to the reader) in a similar fashion.

In the last case, we start from the matrix identity
\[ (\alpha \beta \psi) = \begin{pmatrix} 0 & \sigma \nu \\ \sigma \nu & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ -\chi \end{pmatrix} = \begin{pmatrix} (\sigma \nu) \chi \\ (\sigma \nu) \varphi \end{pmatrix} \]
(B.9)
and use the Ansatz [60]
\[ \varphi = \varphi(r) = \gamma^{(n)}(r), \]
\[ \chi = \chi(r) = -i (\sigma \nu)(n) \gamma^{(n)}(r), \]
where \( n = r/r \) and \( \gamma^{(n)}(n) \) are the spinor spherical harmonics given by (2.3). As a result,
\[ ir^{p} \psi^{\dagger} ((\alpha \beta \psi) = ir^{p} (\varphi^{\dagger}, \chi^{\dagger}) (\sigma \nu) \chi) \]
\[ = ir^{p} (F \gamma^{(n)}(n), i G \gamma^{(n)}(n)) (\gamma^{(n)}(n)) \]
\[ = -r^{p} (\gamma^{(n)}(n)) F G - r^{p} (\gamma^{(n)}(n)) G F \]
\[ = -2r^{p} (\gamma^{(n)}(n)) F G \]
(B.11)
with the help of the familiar identity \( (\sigma \nu)^{2} = n^{2} = 1 \).

Integration over \( \mathbb{R}^{3} \) in the spherical coordinates completes the proof.

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