MATHEMATICAL STRUCTURE OF RELATIVISTIC COULOMB INTEGRALS

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ABSTRACT. We show that the diagonal matrix elements $\langle O r^p \rangle$, where $O = \{1, \beta, \alpha n \beta\}$ are the standard Dirac matrix operators and the angular brackets denote the quantum-mechanical average for the relativistic Coulomb problem, may be considered as difference analogs of the radial wave functions. Such structure provides an independent way of obtaining closed forms of these matrix elements by elementary methods of the theory of difference equations without explicit evaluation of the integrals. Three-term recurrence relations for each of these expectation values are derived as a by-product. Transformation formulas for the corresponding generalized hypergeometric series are discussed.

1. Introduction

Recent experimental and theoretical progress has renewed interest in quantum electrodynamics of atomic hydrogenlike systems (see, for example, [8], [9], [12], [13], [15], [22], and [24] and references therein). 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 [22] and numerical calculations of QED effects in heavy ions were performed with excellent agreement to current experimental data [8], [9], [24]. These advances motivate detailed study of the expectation values of the Dirac matrix operators between the bound-state relativistic Coulomb wave functions. 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], [21], [23], [25] and references therein). These expectation values can be used in calculations with hydrogenlike wave functions when a high precision is required.

In the previous paper [25], we have evaluated the relativistic Coulomb integrals of the radial functions,

$$A_p = \int_0^\infty r^{p+2} \left( F^2(r) + G^2(r) \right) dr, \quad (1.1)$$

$$B_p = \int_0^\infty r^{p+2} \left( F^2(r) - G^2(r) \right) dr, \quad (1.2)$$

$$C_p = \int_0^\infty r^{p+2} F(r) G(r) \, dr, \quad (1.3)$$

for all admissible powers $p$, in terms of three special generalized hypergeometric $3F_2$ series related to the Chebyshev polynomials of a discrete variable [16] (we concentrate on the radial integrals since,
for problems involving spherical symmetry, one can reduce all expectation values to radial integrals by use of the properties of angular momentum). These integrals are linearly dependent:

$$(2\kappa + \varepsilon (p + 1)) A_p - (2\varepsilon \kappa + p + 1) B_p = 4\mu C_p$$  \hspace{1cm} (1.4)$$

(see, for example, [1], [19], [20], and [25] for more details). Thus, eliminating, say $C_p$, one can deal with $A_p$ and $B_p$ only. The corresponding representations in terms of only two linearly independent generalized hypergeometric series are given in this paper (see (3.1)–(3.3) and (3.4)–(3.6)).

The integrals (1.1)–(1.3) satisfy numerous recurrence relations in $p$, which provide an effective way of their evaluation for small $p$ (see [1], [19], [20], [25] and references therein). The two-term recurrence relations were derived by Shabaev [19], [20] on the basis of a hypervirial theorem and by a different method using relativistic versions of the Kramers–Pasternack three-term recurrence relations in [26]. In our notations,

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

$$B_{p+1} = -(p + 1) \frac{4\mu^2 (p + 2) + (p + 1) (2\kappa \varepsilon + p + 1) (2\kappa \varepsilon + p + 2)}{4 (1 - \varepsilon^2) (p + 2) \beta \mu} B_p,$$

and

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

$$B_{p-1} = \beta \frac{4\mu^2 (p + 1) + p (2\kappa \varepsilon + p) (2\kappa \varepsilon + p + 1)}{\mu (4\nu^2 - p^2) p} B_p,$$

respectively. Here,

$$\kappa = \pm \left( j + 1/2 \right), \quad \nu = \sqrt{\kappa^2 - \mu^2},$$

$$\mu = \alpha Z = Ze^2/\hbar c, \quad a = \sqrt{1 - \varepsilon^2},$$

$$\varepsilon = E/mc^2, \quad \beta = mc/\hbar$$

with the total angular momentum $j = 1/2, 3/2, 5/2, \ldots$ (see [25] and [27] for more details).

These recurrence relations are complemented by the symmetries of the integrals $A_p$, $B_p$, and $C_p$ under reflections $p \rightarrow -p - 1$ and $p \rightarrow -p - 3$ found in [25] (see also [2]). For example,

$$A_{-p-3} = (2a\beta)^{2p+3} \frac{\Gamma (2\nu - p - 2)}{\Gamma (2\nu + p + 3)} \hspace{1cm} (1.10)$$
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\[
\times \left( -(p + 1) \frac{4\nu^2 + 2\varepsilon \kappa (2p + 3) - (p + 2)^2}{p + 2} A_p \\
+ 2\kappa (2\varepsilon \kappa - 1) \frac{2p + 3}{p + 2} B_p \right),
\]

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

for independent convergent integrals \(A_p\) and \(B_p\).

In this paper, we would like to draw reader’s attention to an interesting analogy between the explicit solutions of the first order system of difference equations (1.5)–(1.6) and the standard method of dealing with the system of differential equations for the radial relativistic Coulomb wave functions \(F\) and \(G\) (see, for example, [4], [5], [10], [17], [18], and [27] regarding solution of the Dirac equation in Coulomb field). En route, we derive the three-term recurrence relations for each of the single integrals (1.1)–(1.3) that seem to be new and convenient for their evaluation. Our observation provides an independent method of obtaining closed forms of these matrix elements, but this time, from the theory of difference equations and without explicit evaluation of the integrals. Some transformation formulas for the corresponding generalized hypergeometric series are derived.

2. THREE-TERM RECURRENCE RELATIONS

Several relativistic Kramers–Pasternack three-term vector recurrence relations for the integrals \(A_p, B_p, C_p\) have been obtained in [26]. A more general setting is as follows. Let us rewrite (1.5)–(1.6) and (1.7)–(1.8) in the matrix form

\[
\begin{bmatrix} A_p \\ B_p \end{bmatrix} = S_p \begin{bmatrix} A_{p-1} \\ B_{p-1} \end{bmatrix}, \quad \begin{bmatrix} A_{p-1} \\ B_{p-1} \end{bmatrix} = S_{p-1}^{-1} \begin{bmatrix} A_p \\ B_p \end{bmatrix}
\]

and denote

\[
S_p = \begin{bmatrix} a_p & b_p \\ c_p & d_p \end{bmatrix}, \quad S_{p-1}^{-1} = \frac{1}{\Delta_p} \begin{bmatrix} d_p & -b_p \\ -c_p & a_p \end{bmatrix}
\]

with

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

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

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

\[
d_p = \frac{4\mu^2 \varepsilon (p + 1) + p (2\kappa \varepsilon + p) (2\kappa + \varepsilon (p + 1))}{4 (1 - \varepsilon^2) (p + 1) \beta \mu}.
\]
and
\[ \Delta_p = \det S_p = \frac{(4\nu^2 - p^2) p}{(2a\beta)^2(p + 1)}. \] (2.7)

Eliminating \( A_p \) and \( B_p \), respectively, from the system (2.1), we arrive at the following three-term recurrence equations for the independent integrals
\[ A_{p+1} = \left( a_{p+1} + \frac{b_{p+1}}{b_p} d_p \right) A_p - \frac{b_{p+1}}{b_p} \Delta_p A_{p-1}, \] (2.8)
\[ B_{p+1} = \left( d_{p+1} + \frac{c_{p+1}}{c_p} a_p \right) B_p - \frac{c_{p+1}}{c_p} \Delta_p B_{p-1}, \] (2.9)

which seem are missing in the available literature.

In general, one can easily verify that the following vector three-term recurrence relation holds:
\[ \left( \begin{array}{c} A_{p+1} \\ B_{p+1} \end{array} \right) = M_p \left( \begin{array}{c} A_p \\ B_p \end{array} \right) + N_p \left( \begin{array}{c} A_{p-1} \\ B_{p-1} \end{array} \right) \] (2.10)
for two matrices \( M_p \) and \( N_p \) provided that
\[ S_{p+1} = M_p + N_p S_p^{-1}. \] (2.11)

Our equations (2.8)–(2.9) provide a diagonal matrix solution. According to (2.1), (2.10) and (2.11), a simple identity
\[ \left( \begin{array}{c} A_{p+1} \\ B_{p+1} \end{array} \right) = (S_{p+1} - N_p S_p^{-1}) \left( \begin{array}{c} A_p \\ B_p \end{array} \right) + N_p \left( \begin{array}{c} A_{p-1} \\ B_{p-1} \end{array} \right) \] (2.12)
holds for any matrix \( N_p \). The known three-term recurrence relations for the relativistic Coulomb integrals can be obtained by choosing different forms of the matrix \( N_p \). The case \( N_p = 0 \) goes back to the two-term recurrence relation (2.1) and two more explicit solutions have been found in [26]. Here we analyze another possibility and take
\[ N_p = \begin{pmatrix} \lambda_p & 0 \\ 0 & \mu_p \end{pmatrix} \quad \text{and} \quad N_p = \begin{pmatrix} 0 & \lambda_p \\ \mu_p & 0 \end{pmatrix} \]
for suitable parameters \( \lambda_p \) and \( \mu_p \). A new convenient relations are as follows
\[ \left( \begin{array}{c} A_{p+1} \\ B_{p+1} \end{array} \right) = \left( \begin{array}{cc} a_{p+1} + b_{p+1} d_p/b_p & 0 \\ 0 & d_{p+1} + c_{p+1} a_p/c_p \end{array} \right) \left( \begin{array}{c} A_p \\ B_p \end{array} \right) - \Delta_p \left( \begin{array}{cc} b_{p+1}/b_p & 0 \\ 0 & c_{p+1}/c_p \end{array} \right) \left( \begin{array}{c} A_{p-1} \\ B_{p-1} \end{array} \right), \] (2.13)
Explicit diagonal form, when the equations are separated, is given by

\[
\begin{align*}
\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} &= \begin{pmatrix} 0 & b_{p+1}/a_p \\ c_{p+1}/d_p & 0 \end{pmatrix} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} + \Delta_p \left( \begin{array}{cc} 0 & b_{p+1}/a_p \\ c_{p+1}/d_p & 0 \end{array} \right) \begin{pmatrix} A_p \\ B_p \end{pmatrix} \\
&= \begin{pmatrix} a_{p+1}/d_p & 0 \\ 0 & d_{p+1}/a_p \end{pmatrix} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} + \Delta_p \begin{pmatrix} 0 & b_{p+1}/a_p \\ c_{p+1}/d_p & 0 \end{pmatrix} \begin{pmatrix} A_p \\ B_p \end{pmatrix} \\
&\quad - \Delta_p \begin{pmatrix} 0 & a_{p+1}/c_p \\ d_{p+1}/b_p & 0 \end{pmatrix} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}.
\end{align*}
\]

(2.14) (2.15) (2.16)

Explicit diagonal form, when the equations are separated, is given by

\[
\begin{align*}
A_{p+1} &= \frac{\mu P (p)}{a^2 \beta (4 \mu^2 (p + 1) + p (2 \kappa \varepsilon + p) (2 \kappa \varepsilon + p + 1)) (p + 2)} A_p \\
&\quad - \frac{(4 \nu^2 - p^2) (4 \mu^2 (p + 2) + (p + 1) (2 \kappa \varepsilon + p + 1) (2 \kappa \varepsilon + p + 1)) p}{(2 a \beta)^2 (4 \mu^2 (p + 1) + p (2 \kappa \varepsilon + p) (2 \kappa \varepsilon + p + 1)) (p + 2)} A_{p-1},
\end{align*}
\]

(2.17) \quad \begin{align*}
B_{p+1} &= \frac{\varepsilon \mu Q (p)}{a^2 \beta (4 \nu^2 + 2 \kappa \varepsilon (2 p + 1) + \varepsilon^2 p (p + 1)) (p + 2)} B_p \\
&\quad - \frac{(4 \nu^2 - p^2) (4 \nu^2 + 2 \kappa \varepsilon (2 p + 3) + \varepsilon^2 (p + 1) (p + 2)) (p + 1)}{(2 a \beta)^2 (4 \nu^2 + 2 \kappa \varepsilon (2 p + 1) + \varepsilon^2 p (p + 1)) (p + 2)} B_{p-1},
\end{align*}

(2.18)

where

\[
\begin{align*}
P (p) &= 2 \varepsilon p^4 + (8 \kappa \varepsilon^2 + 5 \varepsilon) p^3 \\
&\quad + (8 \kappa^2 \varepsilon^3 + 8 \kappa^2 \varepsilon + 20 \kappa \varepsilon^2 - 4 \kappa - 8 \nu^2 \varepsilon + 3 \varepsilon) p^2 \\
&\quad + (12 \kappa^2 \varepsilon^3 + 20 \kappa^2 \varepsilon^2 + 16 \kappa \varepsilon^2 - 10 \kappa - 20 \nu^2 \varepsilon) p \\
&\quad + 4 \kappa^2 \varepsilon^3 + 8 \kappa^2 \varepsilon + 4 \kappa \varepsilon^2 - 4 \kappa - 12 \nu^2 \varepsilon, \\
Q (p) &= 2 \varepsilon^2 p^3 + (7 \varepsilon^2 + 8 \kappa \varepsilon - 2) p^2 \\
&\quad + (8 \nu^2 + 7 \varepsilon^2 + 16 \kappa \varepsilon - 4) p \\
&\quad + 12 \nu^2 + 2 \varepsilon^2 + 6 \kappa \varepsilon - 2.
\end{align*}
\]

(2.19) (2.20)

In comparison with other papers (see [1], [2], [19], [20], [25], [26], and references therein), our consideration provides an alternative way of the recursive evaluation of the special values \(A_p\) and \(B_p\), when one deals separately with one of these integrals only. The corresponding initial data can be found in [25]. It is important emphasizing, for the purpose of this paper, that this argument resembles the reduction of the first order system of differential equations for relativistic radial
Coulomb wave functions $F$ and $G$ to the second order differential equations (see, for example, [17] and [27]).

If one wants to solve equations (2.17)–(2.18) analytically for all admissible powers, then the major obstacle is that they are not difference equations of hypergeometric type on a quadratic lattice, solutions of which are available in the literature [16]. The following consideration helps. A linear transformation
\[
\begin{pmatrix}
X_p \\
Y_p
\end{pmatrix} = T_p \begin{pmatrix}
A_p \\
B_p
\end{pmatrix},
\]
where
\[
T_p = \begin{pmatrix}
\alpha_p & \beta_p \\
\gamma_p & \delta_p
\end{pmatrix}, \quad \det T_p = \alpha_p\delta_p - \beta_p\gamma_p \neq 0,
\]
results in a new system of the first order difference equations
\[
\begin{pmatrix}
X_p \\
Y_p
\end{pmatrix} = \tilde{S}_p \begin{pmatrix}
X_{p-1} \\
Y_{p-1}
\end{pmatrix},
\]
where the corresponding similar matrix is given by
\[
\tilde{S}_p = T_p S_p T_{p-1}^{-1} = \begin{pmatrix}
\tilde{a}_p & \tilde{b}_p \\
\tilde{c}_p & \tilde{d}_p
\end{pmatrix}
\]
with
\[
\begin{align*}
\det T_{p-1} \tilde{a}_p &= \alpha_p\delta_{p-1}a_p - \alpha_p\gamma_{p-1}b_p + \beta_p\delta_{p-1}c_p - \beta_p\gamma_{p-1}d_p, \\
\det T_{p-1} \tilde{b}_p &= -\alpha_p\beta_{p-1}a_p + \alpha_p\alpha_{p-1}b_p - \beta_p\beta_{p-1}c_p + \beta_p\alpha_{p-1}d_p, \\
\det T_{p-1} \tilde{c}_p &= \gamma_p\delta_{p-1}a_p - \gamma_p\gamma_{p-1}b_p + \delta_p\delta_{p-1}c_p - \delta_p\gamma_{p-1}d_p, \\
\det T_{p-1} \tilde{d}_p &= -\gamma_p\beta_{p-1}a_p + \gamma_p\alpha_{p-1}b_p - \delta_p\beta_{p-1}c_p + \delta_p\alpha_{p-1}d_p,
\end{align*}
\]
and
\[
\tilde{\Delta}_p = \det \tilde{S}_p = \det S_p \frac{\det T_p}{\det T_{p-1}} \neq 0.
\]
The new separated three-term recurrence equations take the similar forms
\[
\begin{align*}
X_{p+1} &= \left( \tilde{a}_{p+1} + \frac{\tilde{b}_{p+1}}{\tilde{b}_p} \tilde{d}_p \right) X_p - \frac{\tilde{b}_{p+1}}{\tilde{b}_p} \tilde{\Delta}_p X_{p-1}, \\
Y_{p+1} &= \left( \tilde{d}_{p+1} + \frac{\tilde{c}_{p+1}}{\tilde{c}_p} \tilde{a}_p \right) Y_p - \frac{\tilde{c}_{p+1}}{\tilde{c}_p} \tilde{\Delta}_p Y_{p-1}.
\end{align*}
\]
As in the case of the radial wave functions [17] and [27], there are several possibilities to choose the matrix $T_p$ in order to simplify the original equations (2.17)–(2.18). Examples of such transformations, when the resulting equations are of a hypergeometric type and coincide with difference equations for special dual Hahn polynomials [11], [14], [16] (see also appendix A), are given in the next section.
3. Transformations of Relativistic Coulomb Integrals

The integrals $A_p$, $B_p$, and $C_p$ can be evaluated in terms of two linearly independent $3F_2$ functions, which are related to the special dual Hahn polynomials that can be thought of as difference analogs of the Laguerre polynomials in explicit formulas for the radial wave functions (see [17] and [27] for a detailed tutorial on solution of the relativistic Coulomb problem). This fact has been partially explored in [25] and we elaborate on this connection here. Two different representations of the expectation values are available in a complete analogy with the well-known structure of the relativistic wave functions.

Analogs of the traditional forms are as follows

$$2 (p + 1) a \mu (2a \beta)^p \frac{\Gamma (2\nu + 1)}{\Gamma (2\nu + p + 1)} A_p$$

$$= (\mu + a\kappa) (a (2\varepsilon \kappa + p + 1) - 2\varepsilon \mu)$$
$$\times 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right)$$
$$+ (\mu - a\kappa) (a (2\varepsilon \kappa + p + 1) + 2\varepsilon \mu)$$
$$\times 3F_2 \left( \begin{array}{c} -n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right),$$

(3.1)

$$2 (p + 1) a \mu (2a \beta)^p \frac{\Gamma (2\nu + 1)}{\Gamma (2\nu + p + 1)} B_p$$

$$= (\mu + a\kappa) (a (2\kappa + \varepsilon (p + 1)) - 2\mu)$$
$$\times 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right)$$
$$+ (\mu - a\kappa) (a (2\kappa + \varepsilon (p + 1)) + 2\mu)$$
$$\times 3F_2 \left( \begin{array}{c} -n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right),$$

(3.2)

$$4\mu (2a \beta)^p \frac{\Gamma (2\nu + 1)}{\Gamma (2\nu + p + 1)} C_p$$

$$= a (\mu + a\kappa) 3F_2 \left( \begin{array}{c} 1 - n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right)$$
$$- a (\mu - a\kappa) 3F_2 \left( \begin{array}{c} -n, -p, p + 1 \\ 2\nu + 1, 1 \end{array} \right).$$

(3.3)

The averages of $r^p$ for the relativistic hydrogen atom were evaluated in the late 1930s by Davis [6] as a sum of certain three $3F_2$ functions. But it has been realized only recently that these series are, in fact, linearly dependent and related to the Chebyshev polynomials of a discrete variable [25]. Our formulas here present the final result (we use the standard definition of the generalized hypergeometric series throughout the paper [3], [7]).
Analogs of the Nikiforov and Uvarov form of the relativistic radial functions [17], [27] are given by

\begin{align}
4 (p + 1) \varepsilon \mu \nu (2a \beta)^p \ A_p & = a (\varepsilon \kappa + \nu) (2 (\varepsilon \kappa - \nu) + p + 1) \\
& \times \frac{\Gamma (2 \nu + p + 3)}{\Gamma (2 \nu + 2)} \ 3\!\!F_2 \left( \begin{array}{c}
1 - n, p + 2, -p - 1 \\
2\nu + 2, 1
\end{array} \right) \\
& - a (\varepsilon \kappa - \nu) (2 (\varepsilon \kappa + \nu) + p + 1) \\
& \times \frac{\Gamma (2 \nu + p + 1)}{\Gamma (2 \nu)} \ 3\!\!F_2 \left( \begin{array}{c}
-n, p + 2, -p - 1 \\
2\nu, 1
\end{array} \right),
\end{align}

\begin{align}
4 \mu \nu (2a \beta)^p \ B_p & = a (\varepsilon \kappa + \nu) \frac{\Gamma (2 \nu + p + 3)}{\Gamma (2 \nu + 2)} \ 3\!\!F_2 \left( \begin{array}{c}
1 - n, p + 2, -p - 1 \\
2\nu + 2, 1
\end{array} \right) \\
& - a (\varepsilon \kappa - \nu) \frac{\Gamma (2 \nu + p + 1)}{\Gamma (2 \nu)} \ 3\!\!F_2 \left( \begin{array}{c}
-n, p + 2, -p - 1 \\
2\nu, 1
\end{array} \right),
\end{align}

\begin{align}
8 (p + 1) \varepsilon \mu^2 \nu (2a \beta)^p \ C_p & = a (\varepsilon \kappa + \nu) (2 \kappa (\varepsilon \kappa - \nu) + (p + 1) (\kappa - \varepsilon \nu)) \\
& \times \frac{\Gamma (2 \nu + p + 3)}{\Gamma (2 \nu + 2)} \ 3\!\!F_2 \left( \begin{array}{c}
1 - n, p + 2, -p - 1 \\
2\nu + 2, 1
\end{array} \right) \\
& - a (\varepsilon \kappa - \nu) (2 \kappa (\varepsilon \kappa + \nu) + (p + 1) (\kappa + \varepsilon \nu)) \\
& \times \frac{\Gamma (2 \nu + p + 1)}{\Gamma (2 \nu)} \ 3\!\!F_2 \left( \begin{array}{c}
-n, p + 2, -p - 1 \\
2\nu, 1
\end{array} \right).
\end{align}

These representations simplify Eqs. (3.7)–(3.9) of [25] with the help of the linear relation (1.4) (the calculation details are left to the reader).

It is important noting in this paper, that formulas (3.1)–(3.3) and (3.4)–(3.6) provide explicit examples (of inverses) of the linear transformations (2.21) that reduce the original three-term recurrence relations (2.8)–(2.9) to the difference equations of the corresponding dual Hahn polynomials in a complete analogy with the case of the relativistic radial wave functions (see, for example, [17] and [27]). One may choose any two of three linearly dependent integrals \( A_p, B_p, \) and \( C_p \) and take the corresponding renormalized dual Hahn polynomials as \( X_p \) and \( Y_p \).

For example, by choosing \( A_p \) and \( B_p \) as the independent integrals and introducing

\begin{align}
X_p & = \ 3\!\!F_2 \left( \begin{array}{c}
1 - n, -p, p + 1 \\
2\nu + 1, 1
\end{array} \right), \quad (3.7) \\
Y_p & = \ 3\!\!F_2 \left( \begin{array}{c}
-n, -p, p + 1 \\
2\nu + 1, 1
\end{array} \right),
\end{align}
from (3.1)–(3.2) we arrive at the following transformation matrix

\[
T_p = \left( \frac{(2a\beta)^p}{2a^2} \frac{\Gamma(2\nu + 1)}{\Gamma(2\nu + p + 1)} \right) \times \begin{pmatrix}
\frac{a(2\kappa + \varepsilon(p + 1)) + 2\mu}{\mu + a\kappa} & -\frac{a(2\varepsilon\kappa + p + 1) + 2\varepsilon\mu}{\mu + a\kappa} \\
\frac{-a(2\kappa + \varepsilon(p + 1)) - 2\mu}{\mu - a\kappa} & \frac{a(2\varepsilon\kappa + p + 1) - 2\varepsilon\mu}{\mu - a\kappa}
\end{pmatrix}
\] (3.8)

with

\[
\det T_p = \left( \frac{(2a\beta)^p}{2a^2} \frac{\Gamma(2\nu + 1)}{\Gamma(2\nu + p + 1)} \right)^2 \frac{\mu(p + 1)}{a(\mu^2 - a^2\kappa^2)}. \quad (3.9)
\]

Then

\[
\tilde{S}_p = T_p S_p T_p^{-1} = \left( a^2 p (2\nu + p) \right)^{-1} \times \begin{pmatrix}
-a^2 p^2 + 2a\varepsilon\mu p - 2(\mu^2 - a^2\kappa^2) & 2(\mu^2 - a^2\kappa^2) \\
-2(\mu^2 - a^2\kappa^2) & a^2 p^2 + 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)
\end{pmatrix}
\] (3.10)

with the help of the matrix identity (B.1) and

\[
\tilde{\Delta}_p = \det \tilde{S}_p = \frac{2\nu - p}{2\nu + p}. \quad (3.11)
\]

The new system (2.23) takes much simpler form

\[
X_p = -\frac{a^2 p^2 - 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} X_{p-1} + \frac{2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} Y_{p-1}
\] (3.12)

and

\[
Y_p = -\frac{2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} X_{p-1} + \frac{a^2 p^2 + 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} Y_{p-1}
\] (3.13)

with the initial data

\[
\begin{pmatrix} X_0 \\ Y_0 \end{pmatrix} = T_0 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}
\] (3.14)

\[
= \frac{1}{2a^2} \begin{pmatrix}
\frac{a(2\kappa + \varepsilon) + 2\mu}{\mu + a\kappa} & -\frac{a(2\varepsilon\kappa + 1) + 2\varepsilon\mu}{\mu + a\kappa} \\
\frac{-a(2\kappa + \varepsilon) - 2\mu}{\mu - a\kappa} & \frac{a(2\varepsilon\kappa + 1) - 2\varepsilon\mu}{\mu - a\kappa}
\end{pmatrix} \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\]

After this transformation, the three-term recurrence relations (2.30)–(2.31) coincide with the difference equations for the corresponding special dual Hahn polynomials (A.7) (one should use the spectral identity \(\varepsilon\mu = a(\nu + n)\), further computational details are left to the reader). Our consideration shows how the relativistic Coulomb expectation values \(A_p\) and \(B_p\) can be independently
obtained in their closed forms (3.1)–(3.2), when solving the original system (1.5)–(1.6) by the methods of the theory of difference equations developed in the previous section and without explicit evaluation of the integrals. A striking similarity with the structure of the radial wave functions provides a guidance in this approach. A similar analysis of the case (3.4)–(3.5) is left to the reader.

On the second hand, our equations (3.1)–(3.3) and (3.4)–(3.6) imply the following linear relations:

\[
\begin{align*}
\mathbf{3}_2 F_2 \left( \begin{array}{c}
1 - n, -p, p + 1 \\
2\nu + 1, 1
\end{array} \right) &= \frac{(2\nu + n)(2\nu + p + 1)(2\nu + p + 2)(2n + p + 1)}{4\nu(2\nu + 1)(\nu + n)(p + 1)} \\
&\times \mathbf{3}_2 F_2 \left( \begin{array}{c}
1 - n, p + 2, -p - 1 \\
2\nu + 2, 1
\end{array} \right) \\
&- \frac{n(4\nu + 2n + p + 1)}{2(\nu + n)(p + 1)} \mathbf{3}_2 F_2 \left( \begin{array}{c}
-n, p + 2, -p - 1 \\
2\nu, 1
\end{array} \right)
\end{align*}
\]

and

\[
\begin{align*}
\mathbf{3}_2 F_2 \left( \begin{array}{c}
-n, -p, p + 1 \\
2\nu + 1, 1
\end{array} \right) &= \frac{n(4\nu + 2n - p - 1)(2\nu + p + 1)(2\nu + p + 2)}{4\nu(2\nu + 1)(\nu + n)(p + 1)} \\
&\times \mathbf{3}_2 F_2 \left( \begin{array}{c}
1 - n, p + 2, -p - 1 \\
2\nu + 2, 1
\end{array} \right) \\
&- \frac{(2\nu + n)(2n - p - 1)}{2(\nu + n)(p + 1)} \mathbf{3}_2 F_2 \left( \begin{array}{c}
-n, p + 2, -p - 1 \\
2\nu, 1
\end{array} \right)
\end{align*}
\]

between two pairs of the generalized hypergeometric series under consideration. As required, only one dimensionless parameter is involved in the transformations. Details of these elementary but rather tedious calculations are left to the reader.

In addition, from (3.7) of [25] and (3.4) of this paper one gets

\[
\begin{align*}
\frac{p(p + 1)}{2\nu + n} \mathbf{3}_2 F_2 \left( \begin{array}{c}
1 - n, p + 1, -p \\
2\nu + 1, 2
\end{array} \right) &= \frac{(p - 2\nu)(2\nu + p + 1)}{2(2\nu + 1)(\nu + n)} \mathbf{3}_2 F_2 \left( \begin{array}{c}
1 - n, p + 1, -p \\
2\nu + 2, 1
\end{array} \right) \\
&+ \frac{\nu}{\nu + n} \mathbf{3}_2 F_2 \left( \begin{array}{c}
-n, p + 1, -p \\
2\nu, 1
\end{array} \right)
\end{align*}
\]
which complements relation (3.12) of [25]:

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

reproduced here for completeness. One needs to derive transformations (3.15)–(3.17) directly from the advanced theory of generalized hypergeometric functions [3], [7].

It is worth noting, in conclusion, that explicit solutions of the systems of the first order difference equations with variable coefficients are not widely available in mathematical literature. This is why, it is important to investigate in detail a remarkable structure of the expectation values pointed out in this paper for a classical problem of the relativistic quantum mechanics, such as spectra of high-Z hydrogenlike ions.

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**Appendix A. Laguerre and Dual Hahn Polynomials**

The Laguerre polynomials are [7], [16], [17]

\[
L_m^\alpha(x) = \frac{\Gamma(\alpha + m + 1)}{m! \Gamma(\alpha + 1)} \binom{1}{1} F_1 \left( \begin{array}{c}
-m \\
\alpha + 1 ; x
\end{array} \right).
\]

(A.1)

The dual Hahn polynomials are given by [16]

\[
w_m^{(c)} (s(s+1), a, b) = \frac{(1 + a - b)_m (1 + a + c)_m}{m!} \\
\times 3 F_2 \left( \begin{array}{c}
-m, a - s, a + s + 1 \\
1 + a - b, 1 + a + c ; 1
\end{array} \right).
\]

(A.2)

In (3.1)–(3.3) and (3.4)–(3.6) of this paper, we are dealing only with the following special cases:

\[
m = n, n - 1 \text{ and } a = b = 0, c = 2\nu, s = p \text{ and } a = b = 0, c = 2\nu \pm 1, s = p + 1, \text{ respectively.}
\]

The difference equation for the dual Hahn polynomials has the form

\[
\sigma(s) \frac{\Delta}{\nabla x_1(s)} \left( \frac{\nabla y(s)}{\nabla x(s)} \right) + \tau(s) \frac{\Delta y(s)}{\Delta x(s)} + \lambda_m y(s) = 0,
\]

(A.3)

where

\[
\Delta f(s) = \nabla f(s+1) - f(s), x(s) = s(s+1), x_1(s) = x(s+1/2), \text{ and}
\]

\[
\sigma(s) = (s - a)(s + b)(s - c),
\]

(A.4)

\[
\sigma(s) + \tau(s) \nabla x_1(s) = \sigma(-s - 1)
\]

(A.5)

\[
= (a + s + 1)(b - s - 1)(c + s + 1),
\]
\( \lambda_m = m. \) (A.6)

It can be rewritten as the three-term recurrence relation

\[
\begin{align*}
\sigma (-s - 1) \nabla x (s) y (s + 1) + \sigma (s) \Delta x (s) y (s - 1) \\
+ \left( \lambda_m \Delta x (s) \nabla x (s) \nabla x_1 (s) - \sigma (-s - 1) \nabla x (s) - \sigma (s) \Delta x (s) \right) y (s) = 0.
\end{align*}
\] (A.7)

See [11], [14] and [16] for more details on the properties of the dual Hahn polynomials.

Appendix B. Matrix Identity

The required matrix identity

\[
\begin{pmatrix}
\frac{a(2\kappa + \varepsilon (p + 1)) + 2\mu}{\mu + a\kappa} & \frac{a(2\varepsilon + p + 1) + 2\varepsilon\mu}{\mu + a\kappa} \\
\frac{a(2\kappa + \varepsilon (p + 1)) - 2\mu}{\mu - a\kappa} & \frac{a(2\varepsilon + p + 1) - 2\varepsilon\mu}{\mu - a\kappa}
\end{pmatrix}
\times
\begin{pmatrix}
- p(4\nu^2 \varepsilon + 2\kappa (p + 1) + \varepsilon p(2\kappa + p + 1)) & 4\mu^2 (p + 1) + p(2\kappa + p)(2\kappa + p + 1) \\
- p(4\nu^2 + 2\kappa (2p + 1) + \varepsilon^2 p(p + 1)) & 4\mu^2 \varepsilon (p + 1) + p(2\kappa + p)(2\kappa + \varepsilon (p + 1)) \end{pmatrix}
\times
\begin{pmatrix}
(\mu + a\kappa) (a(2\varepsilon + p) - 2\varepsilon\mu) & (\mu - a\kappa) (a(2\varepsilon + p) + 2\varepsilon\mu) \\
(\mu + a\kappa)(a(2\kappa + \varepsilon p) - 2\mu) & (\mu - a\kappa)(a(2\kappa + \varepsilon p) + 2\mu)
\end{pmatrix}
\]

\[
= 8a^2 \mu^2 (p + 1)
\begin{pmatrix}
-a^2 p^2 + 2a\varepsilon\mu p - 2(\mu^2 - a^2\kappa^2) & 2(\mu^2 - a^2\kappa^2) \\
-2(\mu^2 - a^2\kappa^2) & a^2 p^2 + 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)
\end{pmatrix},
\]

provided \( a^2 = 1 - \varepsilon^2 \) and \( \mu^2 = \kappa^2 - \nu^2 \), can be verified with the help of a computer algebra system.

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