Mathematical structure of relativistic Coulomb integrals

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(Received 10 December 2009; published 9 March 2010)

We show that the diagonal matrix elements $\langle Or^p \rangle$, where $O = \{1, \beta, i\alpha\mathbf{n}\beta\}$ 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.

DOI: 10.1103/PhysRevA.81.032110 PACS number(s): 03.65.Pm

I. INTRODUCTION

Recent experimental and theoretical progress has renewed interest in quantum electrodynamics of atomic hydrogenlike systems (see, for example, Refs. [9,10,13,14,16,23,25] and references therein). In the past 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 [23] and numerical calculations of QED effects in heavy ions were performed with excellent agreement to current experimental data [9,10,25]. 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, Refs. [1,22,24,26] and references therein). These expectation values can be used in calculations with hydrogenlike wave functions when a high precision is required.

In the previous article [26], we have evaluated the relativistic Coulomb integrals of the radial functions,

$$A_p = \int_0^\infty r^{p+2}[F^2(r) + G^2(r)]\, dr, \tag{1}$$

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

$$C_p = \int_0^\infty r^{p+2} F(r)G(r)\, dr, \tag{3}$$

for all admissible powers p, in terms of three special generalized hypergeometric ${}_3F_2$ series related to the Chebyshev polynomials of a discrete variable [17] (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:

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

(see, for example, Refs. [1,20,21,26] 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 article [see (43)–(45) and (46)–(48)].

The integrals (1)–(3) satisfy numerous recurrence relations in p, which provide an effective way of their evaluation for small p (see Refs. [1,20,21,26] and references therein). The two-term recurrence relations were derived by Shabaev [20,21] on the basis of a hypervirial theorem and by a different method using relativistic versions of the Kramers-Pasternack three-term recurrence relations in Ref. [27]. In our notations,

$$A_{p+1} = -(p+1)\frac{4\nu^2\varepsilon + 2\kappa(p+2) + \varepsilon(p+1)(2\kappa\varepsilon + p + 2)}{4(1-\varepsilon^2)(p+2)\beta\mu} A_p + \frac{4\mu^2(p+2) + (p+1)(2\kappa\varepsilon + p + 1)(2\kappa\varepsilon + p + 2)}{4(1-\varepsilon^2)(p+2)\beta\mu} B_p, \tag{5}$$

$$B_{p+1} = -(p+1)\frac{4\nu^2 + 2\kappa\varepsilon(2p+3) + \varepsilon^2(p+1)(p+2)}{4(1-\varepsilon^2)(p+2)\beta\mu} A_p + \frac{4\mu^2\varepsilon(p+2) + (p+1)(2\kappa\varepsilon + p + 1)[2\kappa + \varepsilon(p+2)]}{4(1-\varepsilon^2)(p+2)\beta\mu} B_p \tag{6}$$

and

$$A_{p-1} = \beta\frac{4\mu^2\varepsilon(p+1) + p(2\kappa\varepsilon + p)[2\kappa + \varepsilon(p+1)]}{\mu(4\nu^2 - p^2)p} A_p - \beta\frac{4\mu^2(p+1) + p(2\kappa\varepsilon + p)(2\kappa\varepsilon + p + 1)}{\mu(4\nu^2 - p^2)p} B_p, \tag{7}$$

$$B_{p-1} = \beta\frac{4\nu^2 + 2\kappa\varepsilon(2p+1) + \varepsilon^2 p(p+1)}{\mu(4\nu^2 - p^2)} A_p - \beta\frac{4\nu^2\varepsilon + 2\kappa(p+1) + \varepsilon p(2\kappa\varepsilon + p + 1)}{\mu(4\nu^2 - p^2)} B_p, \tag{8}$$

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respectively. Throughout this article,

$$\kappa = \pm(j+1/2), \quad \nu = \sqrt{\kappa^2-\mu^2},$$
$$\mu = \alpha Z = Ze^2/\hbar c, \quad a = \sqrt{1-\varepsilon^2}, \tag{9}$$
$$\varepsilon = E/mc^2, \quad \beta = mc/\hbar$$

with the total angular momentum $j = 1/2, 3/2, 5/2, \ldots$ (see Refs. [26,28] for more details).

These recurrence relations are complemented by the symmetries of the integrals A_p, B_p, and C_p under reflections $p \to -p-1$ and $p \to -p-3$ found in Ref. [26] (see also Ref. [2]). For example,

$$A_{-p-3} = (2a\beta)^{2p+3}\,\frac{\Gamma(2\nu-p-2)}{\Gamma(2\nu+p+3)} \times\left[-(p+1)\frac{4\nu^2+2\varepsilon\kappa(2p+3)-(p+2)^2}{p+2}\,A_p + 2\kappa(2\varepsilon\kappa-1)\frac{2p+3}{p+2}\,B_p\right], \tag{10}$$

$$B_{-p-3} = (2a\beta)^{2p+3}\,\frac{\Gamma(2\nu-p-2)}{\Gamma(2\nu+p+3)}\{\varepsilon(p+1)(2p+3)\,A_p + [4\nu^2-2\varepsilon\kappa(2p+3)-(p+1)^2]\,B_p\}, \tag{11}$$

for independent convergent integrals A_p and B_p.

In this article, we would like to draw the reader's attention to an interesting analogy between the explicit solutions of the first-order system of difference equations (5)–(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, Refs. [5,6,11,18,19,28] 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)–(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 as a by-product.

II. 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 Ref. [27]. A more general setting is as follows. Let us rewrite (5)–(6) and (7)–(8) in the matrix form

$$\begin{pmatrix} A_p \\ B_p \end{pmatrix} = S_p \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}, \quad \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} = S_p^{-1} \begin{pmatrix} A_p \\ B_p \end{pmatrix} \tag{12}$$

and denote

$$S_p = \begin{pmatrix} a_p & b_p \\ c_p & d_p \end{pmatrix}, \quad S_p^{-1} = \frac{1}{\Delta_p}\begin{pmatrix} d_p & -b_p \\ -c_p & a_p \end{pmatrix} \tag{13}$$

with

$$a_p = -p\,\frac{4\nu^2\varepsilon + 2\kappa(p+1) + \varepsilon p(2\kappa\varepsilon + p + 1)}{4(1-\varepsilon^2)(p+1)\beta\mu}, \tag{14}$$

$$b_p = \frac{4\mu^2(p+1) + p(2\kappa\varepsilon + p)(2\kappa\varepsilon + p + 1)}{4(1-\varepsilon^2)(p+1)\beta\mu}, \tag{15}$$

$$c_p = -p\,\frac{4\nu^2 + 2\kappa\varepsilon(2p+1) + \varepsilon^2 p(p+1)}{4(1-\varepsilon^2)(p+1)\beta\mu}, \tag{16}$$

$$d_p = \frac{4\mu^2\varepsilon(p+1) + p(2\kappa\varepsilon + p)[2\kappa + \varepsilon(p+1)]}{4(1-\varepsilon^2)(p+1)\beta\mu} \tag{17}$$

and

$$\Delta_p = \det S_p = \frac{(4\nu^2 - p^2)p}{(2a\beta)^2(p+1)}. \tag{18}$$

Eliminating A_p and B_p, respectively, from the system (12), we arrive at the following three-term recurrence equations for the independent integrals

$$A_{p+1} = \left(a_{p+1} + \frac{b_{p+1}}{b_p}d_p\right)\,A_p - \frac{b_{p+1}}{b_p}\Delta_p\,A_{p-1}, \tag{19}$$

$$B_{p+1} = \left(d_{p+1} + \frac{c_{p+1}}{c_p}a_p\right)\,B_p - \frac{c_{p+1}}{c_p}\Delta_p\,B_{p-1}, \tag{20}$$

which seem are missing in the available literature.

In general, one can easily verify that the following vector three-term recurrence relation holds:

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = M_p \begin{pmatrix} A_p \\ B_p \end{pmatrix} + N_p \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} \tag{21}$$

for two matrices M_p and N_p provided that

$$S_{p+1} = M_p + N_p S_p^{-1}. \tag{22}$$

Our equations (19)–(20) provide a diagonal matrix solution. According to (12), (21), and (22), a simple identity

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = \left(S_{p+1} - N_p S_p^{-1}\right)\begin{pmatrix} A_p \\ B_p \end{pmatrix} + N_p \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} \tag{23}$$

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 (12) and two more explicit solutions have been found in Ref. [27]. 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 λ_p and μ_p. A new convenient relations are as follows

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = \begin{pmatrix} a_{p+1} + b_{p+1}\dfrac{d_p}{b_p} & 0 \\ 0 & d_{p+1} + c_{p+1}\dfrac{a_p}{c_p} \end{pmatrix}\begin{pmatrix} A_p \\ B_p \end{pmatrix} - \Delta_p \begin{pmatrix} b_{p+1}/b_p & 0 \\ 0 & c_{p+1}/c_p \end{pmatrix}\begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}, \tag{24}$$

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = \begin{pmatrix} a_{p+1} + b_{p+1}\dfrac{c_p}{a_p} & 0 \\ 0 & d_{p+1} + c_{p+1}\dfrac{b_p}{d_p} \end{pmatrix}\begin{pmatrix} A_p \\ B_p \end{pmatrix} + \Delta_p \begin{pmatrix} 0 & b_{p+1}/a_p \\ c_{p+1}/d_p & 0 \end{pmatrix}\begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}, \tag{25}$$

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = \begin{pmatrix} 0 & b_{p+1} + a_{p+1}\dfrac{b_p}{d_p} \\ c_{p+1} + d_{p+1}\dfrac{c_p}{a_p} & 0 \end{pmatrix} \begin{pmatrix} A_p \\ B_p \end{pmatrix} + \Delta_p \begin{pmatrix} a_{p+1}/d_p & 0 \\ 0 & d_{p+1}/a_p \end{pmatrix} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}, \quad (26)$$

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = \begin{pmatrix} 0 & b_{p+1} + a_{p+1}\dfrac{a_p}{c_p} \\ c_{p+1} + d_{p+1}\dfrac{d_p}{b_p} & 0 \end{pmatrix} \begin{pmatrix} A_p \\ B_p \end{pmatrix} - \Delta_p \begin{pmatrix} 0 & a_{p+1}/c_p \\ d_{p+1}/b_p & 0 \end{pmatrix} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix}. \quad (27)$$

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

$$A_{p+1} = \frac{\mu P(p)}{a^2\beta[4\mu^2(p+1) + p(2\varepsilon\kappa + p)(2\varepsilon\kappa + p + 1)](p+2)} A_p - \frac{(4\nu^2 - p^2)[4\mu^2(p+2) + (p+1)(2\varepsilon\kappa + p + 1)(2\varepsilon\kappa + p + 2)]p}{(2a\beta)^2[4\mu^2(p+1) + p(2\varepsilon\kappa + p)(2\varepsilon\kappa + p + 1)](p+2)} A_{p-1}, \quad (28)$$

$$B_{p+1} = \frac{\varepsilon\mu Q(p)}{a^2\beta[4\nu^2 + 2\varepsilon\kappa(2p+1) + \varepsilon^2 p(p+1)](p+2)} B_p - \frac{(4\nu^2 - p^2)[4\nu^2 + 2\varepsilon\kappa(2p+3) + \varepsilon^2(p+1)(p+2)](p+1)}{(2a\beta)^2[4\nu^2 + 2\varepsilon\kappa(2p+1) + \varepsilon^2 p(p+1)](p+2)} B_{p-1}, \quad (29)$$

where

$$P(p) = 2\varepsilon p(p+2)(2\varepsilon\kappa + p)(2\varepsilon\kappa + p + 1) + \varepsilon\{4(\varepsilon^2\kappa^2 - \nu^2) - p[4\varepsilon^2\kappa^2 + p(p+1)]\} + (2p+1)[4\varepsilon^2\kappa + 2(p+2)(2\varepsilon\mu^2 - \kappa)], \quad (30)$$

$$Q(p) = (2p+3)[4\nu^2 + 2\varepsilon\kappa(2p+1) + p(p+1)] - a^2(2p+1)(p+1)(p+2). \quad (31)$$

In comparison with other articles (see Refs. [1,2,20,21,26,27] and references therein), our consideration provides an alternative way of the recursive evaluation of the special values A_p and B_p, when we deal separately with one of these integrals only. The corresponding initial data $A_0 = 1$, $B_{-1} = a^2\beta/\mu$ can be found in Ref. [26]. It is important emphasizing, for the purpose of this article, 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, Refs. [18,28]).

If one wants to solve equations (28)–(29) 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 [3,17]. The following consideration helps. A linear transformation

$$\begin{pmatrix} X_p \\ Y_p \end{pmatrix} = T_p \begin{pmatrix} A_p \\ B_p \end{pmatrix}, \quad (32)$$

where

$$T_p = \begin{pmatrix} \alpha_p & \beta_p \\ \gamma_p & \delta_p \end{pmatrix}, \quad \det T_p = \alpha_p\delta_p - \beta_p\gamma_p \neq 0, \quad (33)$$

results in a new system of the first-order difference equations

$$\begin{pmatrix} X_p \\ Y_p \end{pmatrix} = \widetilde{S}_p \begin{pmatrix} X_{p-1} \\ Y_{p-1} \end{pmatrix}, \quad (34)$$

where the corresponding similar matrix is given by

$$\widetilde{S}_p = T_p S_p T_{p-1}^{-1} = \begin{pmatrix} \widetilde{a}_p & \widetilde{b}_p \\ \widetilde{c}_p & \widetilde{d}_p \end{pmatrix} \quad (35)$$

with

$$\det T_{p-1}\, \widetilde{a}_p = \alpha_p\delta_{p-1}a_p - \alpha_p\gamma_{p-1}b_p + \beta_p\delta_{p-1}c_p - \beta_p\gamma_{p-1}d_p, \quad (36)$$

$$\det T_{p-1}\, \widetilde{b}_p = -\alpha_p\beta_{p-1}a_p + \alpha_p\alpha_{p-1}b_p - \beta_p\beta_{p-1}c_p + \beta_p\alpha_{p-1}d_p, \quad (37)$$

$$\det T_{p-1}\, \widetilde{c}_p = \gamma_p\delta_{p-1}a_p - \gamma_p\gamma_{p-1}b_p + \delta_p\delta_{p-1}c_p - \delta_p\gamma_{p-1}d_p, \quad (38)$$

$$\det T_{p-1}\, \widetilde{d}_p = -\gamma_p\beta_{p-1}a_p + \gamma_p\alpha_{p-1}b_p - \delta_p\beta_{p-1}c_p + \delta_p\alpha_{p-1}d_p, \quad (39)$$

and

$$\widetilde{\Delta}_p = \det \widetilde{S}_p = \det S_p \frac{\det T_p}{\det T_{p-1}} \neq 0. \quad (40)$$

The new separated three-term recurrence equations take the similar forms

$$X_{p+1} = \left(\widetilde{a}_{p+1} + \frac{\widetilde{b}_{p+1}}{\widetilde{b}_p}\widetilde{d}_p\right) X_p - \frac{\widetilde{b}_{p+1}}{\widetilde{b}_p}\widetilde{\Delta}_p X_{p-1}, \quad (41)$$

$$Y_{p+1} = \left(\widetilde{d}_{p+1} + \frac{\widetilde{c}_{p+1}}{\widetilde{c}_p}\widetilde{a}_p\right) Y_p - \frac{\widetilde{c}_{p+1}}{\widetilde{c}_p}\widetilde{\Delta}_p Y_{p-1}. \quad (42)$$

As in the case of the radial wave functions in Refs. [18] and [28], there are several possibilities to choose the matrix T_p in order to simplify the original equations (28)–(29). Examples of such transformations, when the resulting equations are of a hypergeometric type and coincide with difference equations for special dual Hahn polynomials [12,15,17] (see also Appendix A), are given in the next section.

III. 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 Refs. [18,28] for a detailed tutorial on solution of the relativistic Coulomb problem). This fact has been partially explored in Ref. [26] 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

$$\begin{aligned}2(p+1)a\mu(2a\beta)^p\,\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\,A_p &= (\mu+a\kappa)[a(2\varepsilon\kappa+p+1)-2\varepsilon\mu]\\ &\quad\times{}_3F_2\left(\begin{matrix}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right)\\ &\quad+(\mu-a\kappa)[a(2\varepsilon\kappa+p+1)+2\varepsilon\mu]\\ &\quad\times{}_3F_2\left(\begin{matrix}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right),\end{aligned}\tag{43}$$

$$\begin{aligned}2(p+1)a\mu(2a\beta)^p\,\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\,B_p &= (\mu+a\kappa)[a\big(2\kappa+\varepsilon(p+1)\big)-2\mu]\\ &\quad\times{}_3F_2\left(\begin{matrix}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right)\\ &\quad+(\mu-a\kappa)[a\big(2\kappa+\varepsilon(p+1)\big)+2\mu]\\ &\quad\times{}_3F_2\left(\begin{matrix}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right),\end{aligned}\tag{44}$$

$$\begin{aligned}4\mu(2a\beta)^p\,\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\,C_p &= a(\mu+a\kappa)\,{}_3F_2\left(\begin{matrix}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right)\\ &\quad-a(\mu-a\kappa)\,{}_3F_2\left(\begin{matrix}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right).\end{aligned}\tag{45}$$

The averages of r^p for the relativistic hydrogen atom were evaluated in the late 1930s by Davis [7] 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 [26]. Here, the most compact version of the final result is presented (we use the standard definition of the generalized hypergeometric series throughout the article [4,8]).

Analogs of the Nikiforov and Uvarov form of the relativistic radial functions [18,28] are given by

$$\begin{aligned}4(p+1)\varepsilon\mu\nu(2a\beta)^p\,A_p &= a(\varepsilon\kappa+\nu)[2(\varepsilon\kappa-\nu)+p+1]\\ &\quad\times\frac{\Gamma(2\nu+p+3)}{\Gamma(2\nu+2)}\,{}_3F_2\left(\begin{matrix}1-n,\ p+2,\ -p-1\\ 2\nu+2,\quad 1\end{matrix}\right)\\ &\quad-a(\varepsilon\kappa-\nu)[2(\varepsilon\kappa+\nu)+p+1]\\ &\quad\times\frac{\Gamma(2\nu+p+1)}{\Gamma(2\nu)}\,{}_3F_2\left(\begin{matrix}-n,\ p+2,\ -p-1\\ 2\nu,\quad 1\end{matrix}\right),\end{aligned}\tag{46}$$

$$\begin{aligned}4\mu\nu(2a\beta)^p\,B_p &= a(\varepsilon\kappa+\nu)\frac{\Gamma(2\nu+p+3)}{\Gamma(2\nu+2)}\,{}_3F_2\left(\begin{matrix}1-n,\ p+2,\ -p-1\\ 2\nu+2,\quad 1\end{matrix}\right)\\ &\quad-a(\varepsilon\kappa-\nu)\frac{\Gamma(2\nu+p+1)}{\Gamma(2\nu)}\,{}_3F_2\left(\begin{matrix}-n,\ p+2,\ -p-1\\ 2\nu,\quad 1\end{matrix}\right),\end{aligned}\tag{47}$$

$$\begin{aligned}8(p+1)\varepsilon\mu^2\nu(2a\beta)^p\,C_p &= a(\varepsilon\kappa+\nu)[2\kappa(\varepsilon\kappa-\nu)+(p+1)(\kappa-\varepsilon\nu)]\\ &\quad\times\frac{\Gamma(2\nu+p+3)}{\Gamma(2\nu+2)}\,{}_3F_2\left(\begin{matrix}1-n,\ p+2,\ -p-1\\ 2\nu+2,\quad 1\end{matrix}\right)\\ &\quad-a(\varepsilon\kappa-\nu)[2\kappa(\varepsilon\kappa+\nu)+(p+1)(\kappa+\varepsilon\nu)]\\ &\quad\times\frac{\Gamma(2\nu+p+1)}{\Gamma(2\nu)}\,{}_3F_2\left(\begin{matrix}-n,\ p+2,\ -p-1\\ 2\nu,\quad 1\end{matrix}\right).\end{aligned}\tag{48}$$

These representations simplify Eqs. (3.7)–(3.9) of Ref. [26] with the help of the linear relation (4) (the calculation details are left to the reader).

It is important noting in this article that formulas (43)–(45) and (46)–(48) provide explicit examples (of inverses) of the linear transformations (32) that reduce the original three-term recurrence relations (19)–(20) 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, Refs. [18,28]). 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

$$X_p={}_3F_2\left(\begin{matrix}1-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right),\qquad Y_p={}_3F_2\left(\begin{matrix}-n,\ -p,\ p+1\\ 2\nu+1,\quad 1\end{matrix}\right),\tag{49}$$

from (43)–(44) we arrive at the following transformation matrix

$$T_p=\frac{(2a\beta)^p}{2a^2}\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\times\begin{pmatrix}\dfrac{a[2\kappa+\varepsilon(p+1)]+2\mu}{\mu+a\kappa} & -\dfrac{a(2\varepsilon\kappa+p+1)+2\varepsilon\mu}{\mu+a\kappa}\\ -\dfrac{a[2\kappa+\varepsilon(p+1)]-2\mu}{\mu-a\kappa} & \dfrac{a(2\varepsilon\kappa+p+1)-2\varepsilon\mu}{\mu-a\kappa}\end{pmatrix}\tag{50}$$

with

$$\det T_p=\left[(2a\beta)^p\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)}\right]^2\frac{\mu(p+1)}{a(\mu^2-a^2\kappa^2)}.\tag{51}$$

Then

$$\widetilde{S}_p = T_p S_p T_{p-1}^{-1} = [a^2 p(2\nu + p)]^{-1} \times \begin{pmatrix} -a^2p^2 + 2a\varepsilon\mu p - 2(\mu^2 - a^2\kappa^2) & 2(\mu^2 - a^2\kappa^2) \\ -2(\mu^2 - a^2\kappa^2) & a^2p^2 + 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2) \end{pmatrix} \tag{52}$$

with the help of the matrix identity (B1) and

$$\widetilde{\Delta}_p = \det \widetilde{S}_p = \frac{2\nu - p}{2\nu + p}. \tag{53}$$

The new system (34) takes much simplier form

$$X_p = -\frac{a^2p^2 - 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} X_{p-1} + \frac{2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} Y_{p-1} \tag{54}$$

and

$$Y_p = -\frac{2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} X_{p-1} + \frac{a^2p^2 + 2a\varepsilon\mu p + 2(\mu^2 - a^2\kappa^2)}{a^2 p(2\nu + p)} Y_{p-1} \tag{55}$$

with the initial data

$$\begin{pmatrix} X_0 \\ Y_0 \end{pmatrix} = T_0 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \frac{1}{2a^2} \begin{pmatrix} \dfrac{a(2\kappa + \varepsilon) + 2\mu}{\mu + a\kappa} & -\dfrac{a(2\varepsilon\kappa + 1) + 2\varepsilon\mu}{\mu + a\kappa} \\ -\dfrac{a(2\kappa + \varepsilon) - 2\mu}{\mu - a\kappa} & \dfrac{a(2\varepsilon\kappa + 1) - 2\varepsilon\mu}{\mu - a\kappa} \end{pmatrix} \times \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{56}$$

After this transformation, the three-term recurrence relations (41)–(42) become:

$$X_{p+1} = \frac{(2p+1)[2(\nu + n) - 1]}{(p+1)(2\nu + p + 1)} X_p - \frac{p(2\nu - p)}{(p+1)(2\nu + p + 1)} X_{p-1}, \tag{57}$$

$$Y_{p+1} = \frac{(2p+1)[2(\nu + n) + 1]}{(p+1)(2\nu + p + 1)} Y_p - \frac{p(2\nu - p)}{(p+1)(2\nu + p + 1)} Y_{p-1} \tag{58}$$

and coincide with the difference equations for the corresponding special dual Hahn polynomials (A7) [one should use the spectral identity $\varepsilon\mu = a(\nu + n)$ and the initial conditions $X_0 = Y_0 = 1$, 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 found in their closed forms (43)–(44), when solving the original system (5)–(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. In addition, use of the single recurrence relation in (57)–(58) gives an effective way of simultaneous numerical evaluation of all three integrals (43)–(45) (see also Ref. [2]).

Analysis of the case (46)–(47) is similar. Denoting

$$\widetilde{X}_p = {}_3F_2 \begin{pmatrix} 1-n, & p+2, & -p-1 \\ 2\nu + 2, & & 1 \end{pmatrix}, \tag{59}$$

$$\widetilde{Y}_p = {}_3F_2 \begin{pmatrix} -n, & p+2, & -p-1 \\ 2\nu, & & 1 \end{pmatrix}, \tag{60}$$

we obtain the following system:

$$\widetilde{X}_p = (2\nu - p)\frac{(a^2\nu^2 + \varepsilon^2\mu^2)(p+1) + 2\nu(a^2\nu^2 - \varepsilon^2\mu^2)}{2a\varepsilon\mu\nu(p + 2\nu + 2)(p+1)} \widetilde{X}_{p-1} - \frac{(2\nu + 1)(a^2\nu^2 - \varepsilon^2\mu^2)}{a\varepsilon\mu(p + 2\nu + 2)(p+1)} \widetilde{Y}_{p-1} \tag{61}$$

and

$$\widetilde{Y}_p = (p - 2\nu)\frac{[(p+1)^2 - 4\nu^2](a^2\nu^2 - \varepsilon^2\mu^2)}{4a\varepsilon\mu\nu^2(2\nu + 1)(p+1)} \widetilde{X}_{p-1} + \frac{(a^2\nu^2 + \varepsilon^2\mu^2)(p+1) - 2\nu(a^2\nu^2 - \varepsilon^2\mu^2)}{2a\varepsilon\mu\nu(p+1)} \widetilde{Y}_{p-1} \tag{62}$$

[one can start from the new system (54)–(55) instead of (5)–(6) and use another matrix identity (B2)]. Then equations (41)–(42) for the corresponding dual Hahn polynomials are given by

$$\widetilde{X}_{p+1} = \frac{2(\nu + n)(2p+3)}{(2\nu + p + 3)(p+2)} \widetilde{X}_p - \frac{(2\nu - p)(p+1)}{(2\nu + p + 3)(p+2)} \widetilde{X}_{p-1}, \tag{63}$$

$$\widetilde{Y}_{p+1} = \frac{2(\nu + n)(2p+3)}{(2\nu + p + 1)(p+2)} \widetilde{Y}_p - \frac{(2\nu - p - 2)(p+1)}{(2\nu + p + 1)(p+2)} \widetilde{Y}_{p-1} \tag{64}$$

with $\widetilde{X}_{-1} = \widetilde{Y}_{-1} = 1$. Further details are left to the reader.

It is worth noting, in conclusion, that the explicit solutions of systems of the first-order difference equations with variable coefficients are not widely available in mathematical literature. This is why, it is important to study in detail a remarkable structure of the expectation values pointed out in this article for a classical problem of quantum mechanics, such as spectra of high-Z hydrogenlike ions. After more than 80 years of a thorough investigation, the relativistic Coulomb problem keeps generating some mathematical challenges.

IV. RELATED TRANSFORMATIONS OF GENERALIZED HYPERGEOMETRIC SERIES

On the second hand, our equations (43)–(45) and (46)–(48) imply the following linear relations:

$$
\begin{aligned}
&{}_3F_2\left(\begin{matrix}1-n, & -p, & p+1\\ 2\nu+1, & & 1\end{matrix}\right) \\
&\quad=\frac{(2\nu+n)(2\nu+p+1)(2\nu+p+2)(2n+p+1)}{4\nu(2\nu+1)(\nu+n)(p+1)} \\
&\qquad\times {}_3F_2\left(\begin{matrix}1-n, & p+2, & -p-1\\ 2\nu+2, & & 1\end{matrix}\right) \\
&\qquad-\frac{n(4\nu+2n+p+1)}{2(\nu+n)(p+1)}\,{}_3F_2\left(\begin{matrix}-n, & p+2, & -p-1\\ 2\nu, & & 1\end{matrix}\right)
\end{aligned} \tag{65}
$$

and

$$
\begin{aligned}
&{}_3F_2\left(\begin{matrix}-n, & -p, & p+1\\ 2\nu+1, & & 1\end{matrix}\right) \\
&\quad=\frac{n(4\nu+2n-p-1)(2\nu+p+1)(2\nu+p+2)}{4\nu(2\nu+1)(\nu+n)(p+1)} \\
&\qquad\times {}_3F_2\left(\begin{matrix}1-n, & p+2, & -p-1\\ 2\nu+2, & & 1\end{matrix}\right) \\
&\qquad-\frac{(2\nu+n)(2n-p-1)}{2(\nu+n)(p+1)}\,{}_3F_2\left(\begin{matrix}-n, & p+2, & -p-1\\ 2\nu, & & 1\end{matrix}\right)
\end{aligned} \tag{66}
$$

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 Ref. [26] and (46) of this article one obtains

$$
\begin{aligned}
&\frac{p(p+1)}{2\nu+n}\,{}_3F_2\left(\begin{matrix}1-n, & p+1, & -p\\ 2\nu+1, & & 2\end{matrix}\right) \\
&\quad=\frac{(p-2\nu)(2\nu+p+1)}{2(2\nu+1)(\nu+n)}\,{}_3F_2\left(\begin{matrix}1-n, & p+1, & -p\\ 2\nu+2, & & 1\end{matrix}\right) \\
&\qquad+\frac{\nu}{\nu+n}\,{}_3F_2\left(\begin{matrix}-n, & p+1, & -p\\ 2\nu, & & 1\end{matrix}\right),
\end{aligned} \tag{67}
$$

which complements relation (3.12) of Ref. [26]:

$$
\begin{aligned}
&\frac{p(p+1)}{n+2\nu}\,{}_3F_2\left(\begin{matrix}1-n, & -p, & p+1\\ 2\nu+1, & & 2\end{matrix}\right) \\
&\quad=\frac{p(p+1)}{2\nu+1}\,{}_3F_2\left(\begin{matrix}1-n, & 1-p, & p+2\\ 2\nu+2, & & 2\end{matrix}\right) \\
&\quad={}_3F_2\left(\begin{matrix}-n, & -p, & p+1\\ 2\nu+1, & & 1\end{matrix}\right)-{}_3F_2\left(\begin{matrix}1-n, & -p, & p+1\\ 2\nu+1, & & 1\end{matrix}\right)
\end{aligned} \tag{68}
$$

reproduced here for completeness. One needs to derive transformations (65)–(67) directly from the advanced theory of generalized hypergeometric functions [4,8].

ACKNOWLEDGMENTS

I thank Carlos Castillo-Chávez, Hal Smith, and Vladimir Zakharov for valuable discussions and encouragement.

APPENDIX A: LAGUERRE AND DUAL HAHN POLYNOMIALS

The Laguerre polynomials are [8,17,18]

$$L_m^{\alpha}(x)=\frac{\Gamma(\alpha+m+1)}{m!\,\Gamma(\alpha+1)}\,{}_1F_1\left(\begin{matrix}-m\\ \alpha+1\end{matrix};\,x\right). \tag{A1}$$

The dual Hahn polynomials are given by [17]

$$
\begin{aligned}
w_m^{(c)}[s(s+1),a,b]&=\frac{(1+a-b)_m(1+a+c)_m}{m!} \\
&\quad\times {}_3F_2\left(\begin{matrix}-m, & a-s, & a+s+1\\ 1+a-b, & & 1+a+c\end{matrix};\,1\right).
\end{aligned} \tag{A2}
$$

In (43)–(45) and (46)–(48) of this article, we are dealing only with the following special cases: $m=n-1,n$ and $a=b=0,\ c=2\nu,\ s=p$ and $a=b=0,\ c=2\nu\pm1,\ s=p+1$, respectively.

The difference equation for the dual Hahn polynomials has the form

$$\sigma(s)\frac{\Delta}{\nabla x_1(s)}\left[\frac{\nabla y(s)}{\nabla x(s)}\right]+\tau(s)\frac{\Delta y(s)}{\Delta x(s)}+\lambda_m y(s)=0, \tag{A3}$$

where $\Delta f(s)=\nabla f(s+1)=f(s+1)-f(s)$, $x(s)=s(s+1)$, $x_1(s)=x(s+1/2)$, and

$$\sigma(s)=(s-a)(s+b)(s-c), \tag{A4}$$

$$
\begin{aligned}
\sigma(s)+\tau(s)\nabla x_1(s)&=\sigma(-s-1) \\
&=(a+s+1)(b-s-1)(c+s+1),
\end{aligned} \tag{A5}
$$

$$\lambda_m=m. \tag{A6}$$

It can be rewritten as the three-term recurrence relation

$$
\begin{aligned}
&\sigma(-s-1)\nabla x(s)y(s+1)+\sigma(s)\Delta x(s)y(s-1) \\
&\quad+[\lambda_m\Delta x(s)\nabla x(s)\nabla x_1(s)-\sigma(-s-1)\nabla x(s) \\
&\quad-\sigma(s)\Delta x(s)]y(s)=0.
\end{aligned} \tag{A7}
$$

See Refs. [12,15,17] for more details on the properties of the dual Hahn polynomials.

APPENDIX B: MATRIX IDENTITIES

The required matrix identity

$$\begin{pmatrix} \frac{a[2\kappa+\varepsilon(p+1)]+2\mu}{\mu+a\kappa} & -\frac{a(2\varepsilon\kappa+p+1)+2\varepsilon\mu}{\mu+a\kappa} \\ -\frac{a[2\kappa+\varepsilon(p+1)]-2\mu}{\mu-a\kappa} & \frac{a(2\varepsilon\kappa+p+1)-2\varepsilon\mu}{\mu-a\kappa} \end{pmatrix}$$
$$\times \begin{pmatrix} -p\left[4\nu^2\varepsilon+2\kappa(p+1)+\varepsilon p(2\kappa\varepsilon+p+1)\right] & 4\mu^2(p+1)+p(2\kappa\varepsilon+p)(2\kappa\varepsilon+p+1) \\ -p\left[4\nu^2+2\kappa\varepsilon(2p+1)+\varepsilon^2 p(p+1)\right] & 4\mu^2\varepsilon(p+1)+p(2\kappa\varepsilon+p)\left[2\kappa+\varepsilon(p+1)\right] \end{pmatrix}$$
$$\times \begin{pmatrix} (\mu+a\kappa)\left[a(2\varepsilon\kappa+p)-2\varepsilon\mu\right] & (\mu-a\kappa)\left[a\left(2\varepsilon\kappa+p\right)+2\varepsilon\mu\right] \\ (\mu+a\kappa)\left[a\left(2\kappa+\varepsilon p\right)-2\mu\right] & (\mu-a\kappa)\left[a\left(2\kappa+\varepsilon p\right)+2\mu\right] \end{pmatrix}$$
$$= 8a^2\mu^2(p+1)\begin{pmatrix} -a^2p^2+2a\varepsilon\mu p-2(\mu^2-a^2\kappa^2) & 2(\mu^2-a^2\kappa^2) \\ -2(\mu^2-a^2\kappa^2) & a^2p^2+2a\varepsilon\mu p+2(\mu^2-a^2\kappa^2) \end{pmatrix}, \tag{B1}$$

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

Another convenient matrix relation

$$\begin{pmatrix} a(\varepsilon\mu+a\nu)(p+1)-2(\varepsilon^2\mu^2-a^2\nu^2) & a(\varepsilon\mu-a\nu)(p+1)+2(\varepsilon^2\mu^2-a^2\nu^2) \\ a(\varepsilon\mu-a\nu)(p+1)-2(\varepsilon^2\mu^2-a^2\nu^2) & a(\varepsilon\mu+a\nu)(p+1)+2(\varepsilon^2\mu^2-a^2\nu^2) \end{pmatrix}$$
$$\times \begin{pmatrix} -a^2p^2+2a\varepsilon\mu p-2(\varepsilon^2\mu^2-a^2\nu^2) & 2(\varepsilon^2\mu^2-a^2\nu^2) \\ -2(\varepsilon^2\mu^2-a^2\nu^2) & a^2p^2+2a\varepsilon\mu p+2(\varepsilon^2\mu^2-a^2\nu^2) \end{pmatrix}$$
$$\times \begin{pmatrix} a(a\nu+\varepsilon\mu)p+2(\varepsilon^2\mu^2-a^2\nu^2) & a(a\nu-\varepsilon\mu)p-2(\varepsilon^2\mu^2-a^2\nu^2) \\ a(a\nu-\varepsilon\mu)p+2(\varepsilon^2\mu^2-a^2\nu^2) & a(a\nu+\varepsilon\mu)p-2(\varepsilon^2\mu^2-a^2\nu^2) \end{pmatrix}$$
$$= 2a^4p^2 \times \begin{pmatrix} \frac{(a^2\nu^2+\mu^2\varepsilon^2)(p+1)+2\nu(a^2\nu^2-\mu^2\varepsilon^2)}{(2\nu-p)^{-1}} & -(p+2\nu)(p+2\nu+1)(a^2\nu^2-\mu^2\varepsilon^2) \\ (p-2\nu)(p-2\nu+1)(a^2\nu^2-\mu^2\varepsilon^2) & \frac{(a^2\nu^2+\mu^2\varepsilon^2)(p+1)-2\nu(a^2\nu^2-\mu^2\varepsilon^2)}{(p+2\nu)^{-1}} \end{pmatrix}, \tag{B2}$$

when $\varepsilon^2\kappa^2-\nu^2 = \mu^2-a^2\kappa^2 = \varepsilon^2\mu^2-a^2\nu^2$, can be derived in a similar fashion.

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