Relativistic Coulomb Integrals and Zeilberger's Holonomic Systems Approach II

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Abstract. We derive the recurrence relations for relativistic Coulomb integrals directly from the integral representations with the help of computer algebra methods. In order to manage the computational complexity of this problem, we employ holonomic closure properties in a sophisticated way.

Keywords: Coulomb integral, holonomic systems approach, creative telescoping, holonomic closure property, operator algebra, annihilating ideal

1 Introduction

This work was originally motivated by experimental and theoretical progress in checking Quantum Electrodynamics in strong fields [5, 6, 16, 18] (see also the references therein). A study of the expectation values of the Dirac matrix operators multiplied by the powers of the radius between the bound-state relativistic Coulomb wave functions was initiated in [19, 20] and continued, from computer algebra point-of-view, in [11].

We present the radial wave functions F and G in the following form:

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = E(r) \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} L_{n-1}^{(2\nu)}(2a\beta r) \\ L_n^{(2\nu)}(2a\beta r) \end{pmatrix} \tag{1}$$

where the prefactor E is given by

$$E(r) = a^2 \beta^{3/2} \sqrt{\frac{n!}{\gamma\,\Gamma(n+2\nu)}}\,(2a\beta r)^{\nu-1} e^{-a\beta r}$$

and where $L_n^{(\lambda)}(x)$ denotes the Laguerre polynomials. The quantities α_1, α_2, β_1, and β_2 are given by the following expressions:

$$\alpha_{1,2} = \pm\sqrt{1+\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon} \pm \mu\sqrt{1-\varepsilon}\right), \tag{2}$$

$$\beta_{1,2} = \sqrt{1-\varepsilon}\left((\kappa-\nu)\sqrt{1+\varepsilon} \pm \mu\sqrt{1-\varepsilon}\right). \tag{3}$$

The symbols a, n, β, ε, κ, μ, and ν denote physical constants and they are connected by the following relations:

$$\kappa^2 = \mu^2 + \nu^2, \tag{4}$$

$$a^2 = 1 - \varepsilon^2, \tag{5}$$

$$\varepsilon\mu = a(\nu + n). \tag{6}$$

We are interested in computing the relativistic Coulomb integrals of the radial wave functions where p is a non-negative integer:

$$A_p = \int_0^\infty r^{p+2}\left(F(r)^2 + G(r)^2\right)\mathrm{d}r, \tag{7}$$

$$B_p = \int_0^\infty r^{p+2}\left(F(r)^2 - G(r)^2\right)\mathrm{d}r, \tag{8}$$

$$C_p = \int_0^\infty r^{p+2}\left(F(r)G(r)\right)\mathrm{d}r. \tag{9}$$

The title of the present paper bears the attribute "II" which refers the reader to our first study of applying the holonomic systems approach to relativistic Coulomb integrals: in [11] the desired recurrences for the integrals A_p, B_p, and C_p were derived starting from hypergeometric series representations [11, (8)-(10)] of these integrals. In order to obtain such representations, in our case as sums of three ${}_3F_2$ series, human insight and experience is needed — not to mention manipulatorial skills and computational perseverance. Consequently, the question, whether it is possible to derive the recurrences *directly from the integrals*, is a quite natural one.

We want to stress the point that the algorithmic theory is sufficiently developed to carry out this task *in principle*; namely, by applying holonomic closure properties as introduced below. But for the integrals in question the computational complexity of this approach turns out to be prohibitively expensive. Nevertheless, there is an algorithmic workaround which we describe in Section 3. This workaround might be useful also in other problems, and this is the reason why we wrote this short note.

The software we use is the package `HolonomicFunctions` [10], developed by the first-named author in the computer algebra system Mathematica in the frame of his PhD thesis [8]. We start our investigations by loading this package into the Mathematica system:

In[1]:= << **HolonomicFunctions.m**

HolonomicFunctions package by Christoph Koutschan, RISC-Linz, Version 1.6 (12.04.2012)

2   The Holonomic Systems Approach

In order to state, in an algebraic language, the concepts that are introduced in this section, and for writing mixed difference-differential equations in a concise way, the following operator notation is employed: let D_x denote the partial derivative operator with respect to x (x is then called a *continuous variable*) and S_n the forward shift operator with respect to n (n is then called a *discrete variable*); they act on a function f by

$$D_x f = \frac{\partial f}{\partial x} \quad \text{and} \quad S_n f = f\big|_{n \to n+1}.$$

They allow us to write linear homogeneous difference-differential equations in terms of operators, e.g.,

$$\frac{\partial}{\partial x} f(k, n+1, x, y) + n\frac{\partial}{\partial y} f(k, n, x, y) + xf(k+1, n, x, y) - f(k, n, x, y) = 0$$

turns into

$$\big(D_x S_n + nD_y + xS_k - 1\big) f(k, n, x, y) = 0;$$

in other words, such equations are represented by polynomials in the operator symbols D_x, S_n, etc., with coefficients in some field $\mathbb{F}$ which we assume to be of characteristic 0. Typically, $\mathbb{F}$ is a rational function field in the variables x, n, etc. Note that in general the polynomial ring $\mathbb{F}\langle D_x, S_n, \dots \rangle$ is not commutative (this fact is indicated by the angle brackets) in the following sense: its coefficients from $\mathbb{F}$ do not commute with the polynomial variables D_x, S_n, etc. For instance, multiplication with $a(x, n) \in \mathbb{F}$ is subject to the rules

$$D_x \cdot a(x, n) = a(x, n) \cdot D_x + \frac{\partial}{\partial x} a(x, n) \quad \text{and} \quad S_n \cdot a(x, n) = a(x, n+1) \cdot S_n.$$

Such non-commutative rings of operators are called *Ore algebras*, denoted by $\mathbb{O}$; concise definitions and specifications of the properties of such algebras, for instance, can be found in [8].

We define the *annihilator* (with respect to some Ore algebra $\mathbb{O}$) of a function f by:

$$\mathrm{Ann}_{\mathbb{O}}(f) := \{P \in \mathbb{O} \mid Pf = 0\}.$$

It can easily be seen that $\mathrm{Ann}_{\mathbb{O}}(f)$ is a left ideal in $\mathbb{O}$. Every left ideal $I \subseteq \mathrm{Ann}_{\mathbb{O}}(f)$ is called an *annihilating ideal* for f.

Definition 1. *Let $\mathbb{O} = \mathbb{F}\langle \dots \rangle$ be an Ore algebra. A function f is called ∂-finite w.r.t. $\mathbb{O}$ if $\mathbb{O}/\mathrm{Ann}_{\mathbb{O}}(f)$ is a finite-dimensional $\mathbb{F}$-vector space. The dimension of this vector space is called the* rank *of f w.r.t. $\mathbb{O}$.*

In the holonomic systems approach, the representing data structures of functions are (generators of) annihilating ideals (plus initial values). When working with (left) ideals, we use *(left) Gröbner bases* [2, 7] which are an important tool

for executing certain operations (e.g., the ideal membership test) in an algorithmic way.

Without proof we state the following theorem about *closure properties* of ∂-finite functions; its proof can be found in [8, Chap. 2.3]. We remark that all of them are algorithmically executable, and the algorithms work with the above mentioned data structure.

Theorem 1. *Let $\mathbb{O}$ be an Ore algebra and let f and g be ∂-finite w.r.t. $\mathbb{O}$ of rank r and s, respectively. Then*

(i) *$f + g$ is ∂-finite of rank $\leqslant r + s$.*

(ii) *$f \cdot g$ is ∂-finite of rank $\leqslant rs$.*

(iii) *f^2 is ∂-finite of rank $\leqslant r(r + 1)/2$.*

(iv) *Pf is ∂-finite of rank $\leqslant r$ for any $P \in \mathbb{O}$.*

(v) *$f|_{x \to A(x,y,\dots)}$ is ∂-finite of rank $\leqslant rd$ if $x, y, \dots$ are continuous variables and if the algebraic function A satisfies a polynomial equation of degree d.*

(vi) *$f|_{n \to A(n,k,\dots)}$ is ∂-finite of rank $\leqslant r$ if A is an integer-linear expression in the discrete variables $n, k, \dots$.*

Note that in most examples the bounds on the rank are sharp. In Section 3, we exploit the fact that the rank does not grow when applying closure properties (iv) or (vi).

Example 1. Consider the family of Laguerre polynomials $L_n^{(a)}(x)$ as an example of a ∂-finite function w.r.t. $\mathbb{O} = \mathbb{Q}(n, a, x)\langle S_n, S_a, D_x \rangle$. The left ideal $I = \mathrm{Ann}_{\mathbb{O}}(L_n^{(a)}(x))$ is generated by the following three operators that can be easily obtained with the `HolonomicFunctions` package:

In[2]:= **Annihilator[LaguerreL[n, a, x], {S[n], S[a], Der[x]}]**

Out[2]= $\{S_a + D_x - 1, (n + 1)S_n - xD_x + (-a - n + x - 1), xD_x^2 + (a - x + 1)D_x + n\}$

These operators represent well-known identities for Laguerre polynomials. Moreover, they are a left Gröbner basis of I with respect to the degree-lexicographic order. Thus from the leading monomials (S_a, S_n, and D_x^2) one can easily read off that the dimension of the $\mathbb{Q}(n, a, x)$-vector space $\mathbb{O}/I$ is two, in other words: $L_n^{(a)}(x)$ is ∂-finite w.r.t. $\mathbb{O}$ of rank 2.

If we want to consider integration and summation problems, then the function in question needs to be *holonomic*, a concept that is closely related to ∂-finiteness. The precise definition is a bit technical and therefore skipped here; the interested reader can find it, e.g., in [22, 4, 8]. All functions that appear in this paper are both ∂-finite and holonomic. The following theorem establishes the closure of holonomic functions with respect to sums and integrals; for its proof, we once again refer to [22, 8].

Theorem 2. *Let the function f be holonomic w.r.t. D_x (resp. S_n). Then also $\int_a^b f \, dx$ (resp. $\sum_{n=a}^b f$) is holonomic.*

If a function is ∂-finite and holonomic then Chyzak's algorithm [3] can be used to compute an annihilating ideal for the integral (resp. sum), see Section 3.3. In the following we apply this algorithm to the Coulomb integrals presented in Section 1.

3   The Coulomb Integrals

We now turn to the relativistic Coulomb integrals from Section 1. According to (1) the wave functions are of the form

$$F = \big(\alpha_1 L_{n-1} + \alpha_2 L_n\big)E \quad \text{and} \quad G = \big(\beta_1 L_{n-1} + \beta_2 L_n\big)E$$

where $L_n = L_n^{(2\nu)}(2a\beta r)$. Thus the expressions $F^2 \pm G^2$ that appear in the integrands of A_p and B_p, respectively, can be written as follows:

$$F^2 \pm G^2 = \big((\alpha_1^2 \pm \beta_1^2)L_{n-1}^2 + 2(\alpha_1\alpha_2 \pm \beta_1\beta_2)L_{n-1}L_n + (\alpha_2^2 \pm \beta_2^2)L_n^2\big)E^2. \quad (10)$$

Similarly, for the integrand of C_p we get

$$F \cdot G = \big(\alpha_1\beta_1 L_{n-1}^2 + \alpha_2\beta_2 L_n^2\big)E^2 \qquad (11)$$

since $\alpha_1\beta_2 + \alpha_2\beta_1 = 0$ by (2) and (3). In this section we show how to derive linear recurrence equations in p for the Coulomb integrals.

3.1   Standard Closure Properties

In order to treat the integral A_p with the holonomic systems approach, one first has to transform the input, i.e., the integrand, into the required data structure for ∂-finite functions: given generators for the annihilating ideals of L_n, E, and all other functions appearing in the right-hand side of (10), an annihilating ideal for $F^2 + G^2$ can be computed by the closure properties addition, multiplication, and squaring. Considering only the operator D_r, Theorem 1 (i,ii,iii) states that in this case the rank of the result is at most $(1\cdot3+1\cdot2\cdot2+1\cdot3)\cdot1 = 10$, since L_n is of rank 2 (see Example 1) and E is hyperexponential in r, i.e., satisfies a first-order differential equation in r. Recall that the remaining coefficients are free of r and therefore also of rank 1. It turns out that the bound in this case is sharp, so that applying the closure property algorithms implemented in `HolonomicFunctions` to the expression (10) yield an annihilating ideal of rank 10 which is generated by a very large Ore polynomial in D_r. The situation is exactly the same for B_p. For the integrand of C_p, the bound for the rank is 6 by a similar reasoning. Given these annihilating ideals as input, it seems hopeless that the integration step via creative telescoping, see Section 3.3, can be completed in reasonable time.

3.2   Annihilating Ideals for the Integrands

Fortunately, there is a workaround as announced in the Introduction. Namely, we can find annihilating ideals of smaller rank by using different closure properties: application of an operator (iv) and discrete substitution (vi) in Theorem 1. We first demonstrate this idea on the expression $\alpha_1\beta_1 L_{n-1}^2 + \alpha_2\beta_2 L_n^2$ that appears in C_p, see (11). Instead of applying the closure property addition, this expression can also be perceived as the operator $\alpha_1\beta_1 + \alpha_2\beta_2 S_n$ applied to L_{n-1}^2. As a consequence of entry (iv) of Theorem 1 one obtains an annihilating ideal of rank 3, compared to rank 6 when closure properties are employed in standard fashion. We start the computation by determining an annihilating ideal of L_{n-1}^2:

In[3]:= **annL2 = Annihilator[LaguerreL[$n-1, 2\nu, 2a\beta r$]^2, {S[n], Der[r], S[p]}]**

Out[3]= $\{S_p - 1, -r^2 D_r^2 + 2n^2 S_n + (6a\beta r^2 - 2nr - 6\nu r - r)D_r + (-8a^2\beta^2 r^2 + 4a\beta nr + 16a\beta\nu r + 4a\beta r - 8\nu^2 - 2n^2 - 8\nu n), -nr S_n D_r + 2n^2 S_n + (-nr - 2\nu r)D_r + (4a\beta nr + 8a\beta\nu r - 8\nu^2 - 2n^2 - 8\nu n), (n^3 + 2n^2 + n)S_n^2 + (-4a^2\beta^2 nr^2 + 8a\beta n^2 r + 8a\beta\nu nr + 4a\beta nr - 4n^3 - 8\nu n^2 - 4n^2 - 4\nu^2 n - 4\nu n - n)S_n + (-2a\beta nr^2 - 4a\beta\nu r^2 + 2n^2 r + 6\nu nr + nr + 4\nu^2 r + 2\nu r)D_r + (8a^2\beta^2 nr^2 + 16a^2\beta^2\nu r^2 - 12a\beta n^2 r - 40a\beta\nu nr - 4a\beta nr - 32a\beta\nu^2 r - 8a\beta\nu r + 16\nu^3 + 8\nu^2 + 3n^3 + 16\nu n^2 + 2n^2 + 28\nu^2 n + 8\nu n)\}$

Next, we have to apply the operator $\alpha_1\beta_1 + \alpha_2\beta_2 S_n$ to the ∂-finite function L_{n-1}^2. In order to keep the intermediate expressions small, we replace the coefficients of the operator by simpler ones: $c_1 + c_2 S_n$. Additionally, we divide the integrand by $c_1 = \alpha_1\beta_1$; this does not change the recurrence since α_1 and β_1 depend neither on r nor on p, but we can get rid of one parameter. The operator we want to apply to L_{n-1}^2 then reads $1 + q_2 S_n$ with $q_2 = \alpha_2\beta_2/(\alpha_1\beta_1)$. Still, the results we get are somewhat large, so we suppress (by ending the input line with a semicolon) the output of the following computations:

In[4]:= **annFG = DFiniteOreAction[annL2, 1 + q2 * S[n]];**

To complete the derivation of an annihilating ideal for the integrand of C_p, we have to include the prefactor E (squared) and the additional factor r^{p+2}, according to (9) and (11):

In[5]:= **prefactor =**
        a^2 β^(3/2) Sqrt[$n!/\gamma$/Gamma[$n + 2\nu$]] (2aβr)^($\nu - 1$)Exp[$-a\beta r$];
In[6]:= **annIntC = DFiniteTimes[**
        Annihilator[prefactor^2 * r^($p + 2$), {S[n], Der[r], S[p]}], annFG];
In[7]:= **UnderTheStaircase[annIntC]**

Out[7]= $\{1, D_r, S_n\}$

The last output shows that the rank is 3 (the number of monomials under the staircase of the Gröbner basis), as expected.

Next we turn to the Coulomb integral A_p, where the main part of its integrand is given by (10). Analogously to before, the key idea is to rewrite the expression slightly as to interpret it as an operator applied to some function, namely to the product of two Laguerre polynomials. The only hurdle is that the indices of the Laguerre polynomials need to be shifted separately: in order to produce $L_n L_{n-1}$ from $L_{n-1} L_{n-1}$, for example, a mechanism is needed that shifts only the n in the first Laguerre polynomial. This problem can be overcome by introducing a

slack variable, say m, which afterwards is set to n. The latter step is a discrete substitution as it is described in part (vi) of Theorem 1, and which corresponds to the computation of the diagonal of a bivariate sequence. Thus one obtains

$$\frac{F^2 + G^2}{E^2} = \left((\alpha_1^2 + \beta_1^2) + 2(\alpha_1\alpha_2 + \beta_1\beta_2)S_n + (\alpha_2^2 + \beta_2^2)S_m S_n \right) \left(L_{m-1} L_{n-1} \right) \Big|_{m \to n}$$

and from Theorem 1, items (iv) and (vi), it is clear that the rank of the corresponding annihilating ideal is at most 4; our computations show that, once again, the bound is sharp. Similar to C_p above, the following commands yield an annihilating ideal for the integrand of A_p. The only difference is that at the beginning we introduce the slack variable m (and the corresponding operator S_m), which later is substituted by n. Again, we introduce new variables for the coefficients of the operator in order to reduce the number of parameters: we use $1 + q_1 S_n + q_2 S_m S_n$ with

$$q_1 = 2(\alpha_1\alpha_2 + \beta_1\beta_2)/(\alpha_1^2 + \beta_1^2), \tag{12}$$

$$q_2 = (\alpha_2^2 + \beta_2^2)/(\alpha_1^2 + \beta_1^2). \tag{13}$$

Changing all plus signs to minus signs gives the substitutions for B_p, so that the result of the following calculations can be used both for A_p and B_p.

In[8]:= **annLL = Annihilator[**
       LaguerreL[m − 1, 2ν, 2aβr] LaguerreL[n − 1, 2ν, 2aβr],
       {S[m], S[n], Der[r], S[p]}]

Out[8]= $\{S_p - 1, mS_m + nS_n - rD_r + (4a\beta r - m - 4\nu - n), 2nrS_nD_r - r^2D_r^2 + (4\nu n - 4a\beta nr)S_n + (6a\beta r^2 - 2nr - 6\nu r - r)D_r + (-8a^2\beta^2r^2 - 2a\beta mr + 6a\beta nr + 16a\beta\nu r + 4a\beta r - 8\nu^2 - 4\nu n), (n+1)S_n^2 + (2a\beta r - 2\nu - 2n - 1)S_n + (2\nu + n), r^2D_r^3 + (-6a\beta r^2 + 6\nu r + 3r)D_r^2 + (4a\beta mn - 4a\beta n^2)S_n + (8a^2\beta^2r^2 + 2a\beta mr + 6a\beta nr - 16a\beta\nu r - 16a\beta r + 8\nu^2 + 6\nu + 1)D_r + (-16a^2\beta^2nr + 16a^2\beta^2r - 16a\beta\nu - 4a\beta + 2a\beta m - 4a\beta mn + 4a\beta n^2 + 16a\beta\nu n + 2a\beta n)\}$

In[9]:= **ann1 = DFiniteOreAction[annLL, 1 + q1 ∗ S[n] + q2 ∗ S[m] ∗ S[n]];**

In[10]:= **annF2G2 = DFiniteSubstitute[ann1, {m → n},**
        Algebra → OreAlgebra[Der[r], S[p]]];

In[11]:= **annIntA = DFiniteTimes[**
        Annihilator[prefactor^2 ∗ r^(p + 2), {Der[r], S[p]}], annF2G2];

In[12]:= **UnderTheStaircase[annIntA]**

Out[12]= $\{1, D_r, D_r^2, D_r^3\}$

3.3   Creative Telescoping

In the previous section, annihilating ideals for the three integrands in (7)–(9) were derived. Taking these as input, the task is now to compute annihilating ideals for the integrals themselves. This goal can be achieved by the method of *creative telescoping* [23]. To explain the key idea we restrict ourselves to the situation we are confronted with, i.e., a single integral with respect to r which contains a discrete parameter p (but everything can be stated in more general

terms): find an operator P in the annihilating ideal I of the integrand $f(p, r)$ of the form

$$P(p, r, S_p, D_r) = T(p, S_p) + D_r \cdot C(p, r, S_p, D_r). \tag{14}$$

The part T is called the *telescoper* and C is called the *certificate*. Since $P \in I$ it follows that $Pf = 0$; integrating this equation and applying the fundamental theorem of calculus yields

$$T\left(\int_0^\infty f(p, r)\,\mathrm{d}r\right) + \left[C\big(f(p, r)\big)\right]_{r=0}^{r=\infty} = 0.$$

This is the desired recurrence equation for the integral which, if necessary, can be brought into homogeneous form; this is easily done in practice. In terms of annihilating ideals, we observe that $\mathbb{Q}(p)\langle S_p \rangle$ is a principal ideal domain, and therefore the annihilator A of the integral is generated by a single element. Trivially, the singleton $\{T\}$ is already a left Gröbner basis. From the theory of holonomic modules [4] it follows that an operator of the form P always exists, provided the integrand f is holonomic. But in general, it need not be the case that there exists a $P \in I$ whose telescoper coincides with the unique generator of A. In other words, this method indeed succeeds in computing a recurrence for the integral, but it may not be able to deliver one of *minimal order*.

A first algorithm to compute creative telescoping operators was given in [22]; it is based on elimination techniques and not very efficient in practice. Around the same time the algorithms [21, 1] were published; they are more efficient, but restrict the input to terminating hypergeometric series and hyperexponential functions, respectively. These two algorithms were later generalized in [3], and in [9] a heuristic approach was presented which, in practice, completes the task very quickly. All above-mentioned algorithms are implemented in the package `HolonomicFunctions` [10]. Concretely, we apply the method [9] to the Coulomb integrals (7)–(9).

Starting with the annihilating ideal I (computed in the command line In[11] above) of the integrand of A_p, the following command computes operators T and C such that $T + D_r C$ is in I. The results are too large to be printed here, so only their sizes are displayed.

In[13]:= **{{annA}, {certA}} = FindCreativeTelescoping[annIntA, Der[r]];**
In[14]:= **ByteCount /@ {annA, certA}**

Out[14]= $\{75504, 6682440\}$

The following command gives the support of the computed operator in the annihilating ideal A of the integral A_p, which shows that the recurrence for the integral is of order 2.

In[15]:= **Support[annA]**

Out[15]= $\{S_p^2, S_p, 1\}$

The final step consists in replacing the temporarily introduced parameters by their actual values. Using (12), (13), (2), (3), and (4)–(6) one obtains

$$q_1 = \frac{2\varepsilon\nu - 2\varepsilon^2\kappa}{a\mu - \varepsilon\nu + \kappa},$$

$$q_2 = \frac{-a\mu - \varepsilon\nu + \kappa}{a\mu - \varepsilon\nu + \kappa}.$$

Futher simplifications of the recurrence with relations (4)–(6) lead to the result given in [20, 11]:

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

where

$$P(p) = 2\varepsilon p(p+2)(2\varepsilon\kappa + p)(2\varepsilon\kappa + p + 1) +$$
$$\varepsilon\big(4\big(\varepsilon^2\kappa^2 - \nu^2\big) - p\big(4\varepsilon^2\kappa^2 + p(p+1)\big)\big) +$$
$$(2p+1)\big(4\varepsilon^2\kappa + 2(p+2)(2\varepsilon\mu^2 - \kappa)\big).$$

We do not show the calculations for the integrals B_p and C_p since they can be done in an analogous way.

4 Conclusion

We studied the relativistic Coulomb integrals from the viewpoint of the holonomic systems approach; in particular, we showed how these integrals can be treated by computer algebra methods. It is our hope that our exposition is sufficiently instructive and puts the reader into the position to apply these methods to his/her own benefit. Additionally, we discussed several algorithmic workarounds to reduce the complexity of the computations, as it turned out that the integrals under consideration resist a naive application of our software. We want to stress that the overall computing time for the integrals (7)–(9) does not exceed a few minutes on a standard laptop.

Our next challenge is to study the off-diagonal matrix elements that are important in applications [12–15, 17] (see also the references therein). For the radial functions $F_{n,\kappa}(r)$ and $G_{n,\kappa}(r)$ given by (1) in terms of the Laguerre polynomials, one needs to investigate the following four integrals:

$$\int_0^\infty r^{p+2}\big(F_{n_1,\kappa_1}F_{n_2,\kappa_2} \pm G_{n_1,\kappa_1}G_{n_2,\kappa_2}\big)\,\mathrm{d}r,$$
$$\int_0^\infty r^{p+2}\big(F_{n_1,\kappa_1}G_{n_2,\kappa_2} \pm G_{n_1,\kappa_1}F_{n_2,\kappa_2}\big)\,\mathrm{d}r$$

as off-diagonal extensions of (7)–(9). The first-order (4×4 matrix) recurrence relations in p among these integrals are derived in [12] from a virial theorem.

A straightforward consideration requires multiple evaluations of the following integrals:

$$\int_0^\infty L_{n_1}^{(\lambda_1)}(k_1 x) L_{n_2}^{(\lambda_2)}(k_2 x) \, x^{\mu+s} e^{-x} \, \mathrm{d}x,$$

while it is almost impossible to simplify the lengthy end results. Computer algebra methods and, in particular, the holonomic systems approach suggest another path which will be pursued elsewhere.

Acknowledgment

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