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Method of variation of constants for difference equations and its application to the calculation of atomic integrals

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In this paper we extend the method for numerically stable calculation of the atomic integrals suggested in our previous paper for the *S*-states of two-electron atoms to the states with arbitrary total angular momenta. The extension consists in finding numerically stable forms of the solution of difference equations appearing in the calculation of the radial part of the atomic integrals. These equations become for some value of the independent variable homogenous and their solution in that region is described by one of the two linearly independent solutions. Modification of the method of the variation of constants for this special type of linear second order inhomogenous difference equations is suggested and applied. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1849811]

I. INTRODUCTION

This work grew out from the search for a numerically stable method of the solution of linear inhomogenous second order difference equations appearing in the calculation of the radial part of the atomic integrals.[1] Generally, once we know one of the two linearly independent solutions of the homogenous equation, the second solution can be obtained by the method of the reduction of order.[2] The solution of the inhomogenous equation is then obtained by the method of the variation of constants.[2] However, it turns out that for the difference equations appearing in the calculation of the atomic integrals this general well-known procedure is of little use in its standard form. The reason is that these difference equations become for certain values of the independent variable homogenous and their solution in that region is described by one of the two linearly independent solutions. This behavior results from the general formula by several cancellations of large numbers. If these cancellations are left on the computer working, for example, in double precision arithmetics, totally wrong results are obtained.

Therefore, a general method for obtaining a numerically stable solution of this type of difference equation is given in this paper. The method is applied to the special case of difference equations appearing in the calculation of the radial part of the atomic integrals. Thus, the method suggested in our previous paper for the *S*-states of the two-electron atoms is extended here to the states with arbitrary total angular momenta. Since in general there are at most two-electron interactions, these results can be extended to all atoms and more generally to all one-center integrals.

The paper is organized as follows. In Sec. II we briefly summarize the calculation of the atomic integrals via the multipole expansion of Coulomb potential. Here, we proceed along the lines of our previous paper.[1] After integrating out angular degrees of freedom, we use analog of the Wigner–Eckart theorem for the radial functions. This reduces the integration over four radial functions to the integration over two radial functions. Then we write down a generalization of the difference equations for the reduced radial integrals derived in Ref. 1 for the *S*-states to the states of arbitrary total angular momenta of the electrons. The main difference is the fact that for the states of the nonzero total angular momentum the difference equations are inhomogenous. In Sec. III we discuss solutions of these equations. We present results of numerical experiments that show

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that the difference equations are in a region where they are homogenous described by just one of the two linearly independent solutions. In Sec. IV we first briefly summarize general methods of the reduction of order and the variation of constants. We modify the method of the variation of constants for the cases when the second of the two linearly independent solutions of homogenous equations is obtained by the method of the reduction of order. The form proposed by us is more suitable for computational purposes. We then turn our attention to the special type of equations appearing in the calculation of the atomic integrals and derive numerically stable forms of their solution. In Sec. V we apply the general method of Sec. IV to the difference equations for the reduced radial integrals and test it for the case of very large quantum numbers. In Sec. VI, a summary of the achieved results and perspectives of their further applications are given. In the Appendix computationally suitable forms of the hypergeometric functions needed in Secs. II and III are given.

II. CALCULATION OF THE ATOMIC INTEGRALS

In this section we derive the difference equations for the reduced radial part of the atomic integrals. The derivation of these equations was given in great detail in Ref. 1 for the *S*-states of two-electron atoms. What is difficult in the extension of the method described in Ref. 1 for the *S*-states to the general state is the *solution* of these difference equations, not their derivation. Therefore, we shall proceed very briefly.

We search for the exact two-electron wave function by the expansion into the symmetry adapted products of the one-electron wave functions

$$|i\rangle = 2^{-(1+\delta_{l_{i1},l_{i2}}\delta_{n_{i1},n_{i2}})/2}[R_{n_{i1},l_{i1}}(r_1)R_{n_{i2},l_{i2}}(r_2)|(l_{i1},l_{i2})L\rangle \pm R_{n_{i2},l_{i2}}(r_1)R_{n_{i1},l_{i1}}(r_2)|(l_{i2},l_{i1})L\rangle]. \tag{1}$$

Here, the states $|(l_1,l_2)L\rangle$ are the eigenfunctions of the square and the third component of the sum of the angular momenta of two electrons

$$|(l_1,l_2)L\rangle = \sum_{m_1=-l_1}^{l_1} (l_1,m_1,l_2,M-m_1|L,M)|l_1,m_1\rangle^{(1)}|l_2,M-m_1\rangle^{(2)}, \tag{2}$$

where $(\,|\,)$ denotes Clebsch–Gordan coefficients. Their explicit form is given, for example, in Refs. 3–5. The radial functions $R_{n,l}$ are eigenfuctions of one of the generators of the so(2,1) algebra[1] and will be described in greater detail later.

A. Multipole expansion

The matrix elements of the Coulomb interaction, i.e., repulsion integrals, are calculated by means of the multipole expansion of the operator r_{12}^{-1},

$$r_{12}^{-1} = \frac{1}{r_>}\sum_{l=0}^{\infty}\left(\frac{r_<}{r_>}\right)^l P_l(\vec{n}_1 \,.\, \vec{n}_2), \tag{3}$$

where $r_< = \min(r_1,r_2)$ and $r_> = \max(r_1,r_2)$, $P_l(x)$ denotes the Legendre polynomials. With the usual definition of the inner product (to avoid confusion we note that the inner product used in Ref. 1 differs from the usual one by the factor r^{-1}) and multipole expansion (3) the matrix elements of the operator r_{12}^{-1} between the states (1) can be written as

$$\langle i|r_{12}^{-1}|j\rangle = 2^{-(\delta_{n_{i1},n_{i2}}\delta_{l_{i1},l_{i2}}+\delta_{n_{j1},n_{j2}}\delta_{l_{j1},l_{j2}})/2}\left[\sum_{l=\max(|l_{i1}-l_{j1}|,|l_{i2}-l_{j2}|)}^{\min(l_{i1}+l_{j1},l_{i2}+l_{j2})} \theta_{l_{i1},l_{i2},l_{j1},l_{j2},l} X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}} \right.$$
$$\left. \pm \sum_{l=\max(|l_{i1}-l_{j2}|,|l_{j1}-l_{i2}|)}^{\min(l_{i1}+l_{j2},l_{j1}+l_{i2})} \theta_{l_{i1},l_{i2},l_{j2},l_{j1},l} X^{l_{i1},l_{i2},l_{j2},l_{j1},l}_{n_{i1},n_{i2},n_{j2},n_{j1}} \right], \tag{4}$$

where l in the summation increases by 2.

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The angular part $\theta_{l_{i1},l_{i2},l_{j1},l_{j2},l}$ corresponds to the matrix elements of the Legendre polynomials $P_l(\vec{n}_1.\vec{n}_2)$ between the coupled states (2),

$$\begin{aligned}\theta_{l_{i1},l_{i2},l_{j1},l_{j2},l} &= \langle (l_{i1},l_{i2})L|P_l(\vec{n}_1\,.\,\vec{n}_2)|(l_{j1},l_{j2})L\rangle \\ &= (-1)^{L+l+l_{i1}-l_{j1}+l_{i2}-l_{j2}}\frac{\sqrt{(2l_{i1}+1)(2l_{i2}+1)(2l_{j1}+1)(2l_{j2}+1)}}{2l+1} \\ &\quad\times W(l_{i1},l_{j1},l_{i2},l_{j2},l,L)(l_{i1},0,l_{j1},0|l,0)(l_{i2},0,l_{j2},0|l,0),\end{aligned} \tag{5}$$

where $W(a,b,c,d;e,f)$ are the so-called Racah coefficients and their explicit form is given, for example, in Refs. 4 and 5. The Clebch–Gordan coefficients $(a,0,b,0|c,0)$ are zero unless a, b, and c satisfy the triangle inequality $|a-b|\leqslant c\leqslant a+b$ and $a+b+c$ is even. This reduces the infinite sum in Eq. (3) to the finite number of terms in Eq. (4).

The radial part of the integration reads

$$\begin{aligned}X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}} &= \int_0^\infty \mathrm{d}r_1\int_0^\infty \mathrm{d}r_2\, r_1^2 r_2^2 R_{n_{i1},l_{i1}}(r_1)R_{n_{i2},l_{i2}}(r_2)\frac{r_<^l}{r_>^{l+1}}R_{n_{j1},l_{j1}}(r_1)R_{n_{j2},l_{j2}}(r_2) \\ &= \int_0^\infty \mathrm{d}r_1\, R_{n_{i1},l_{i1}}(r_1)R_{n_{j1},l_{j1}}(r_1)r_1^{l+2}\int_{r_1}^\infty \mathrm{d}r_2\, R_{n_{i2},l_{i2}}(r_2)R_{n_{j2},l_{j2}}(r_2)r_2^{-l+1} \\ &\quad+\int_0^\infty \mathrm{d}r_1\, R_{n_{i1},l_{i1}}(r_1)R_{n_{j1},l_{j1}}(r_1)r_1^{-l+1}\int_0^{r_1} \mathrm{d}r_2\, R_{n_{i2},l_{i2}}(r_2)R_{n_{j2},l_{j2}}(r_2)r_2^{l+2}.\end{aligned} \tag{6}$$

B. Reduction of the radial integrals

Using the analog of the Wigner–Eckart theorem for so(2,1) algebra[1] we can write the integrals over four radial functions as a linear combination of the integrals over two radial functions

$$\begin{aligned}X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}} &= 2^{-2}A^{l_{i1},l_{j1}}_{n_{i1},n_{j1}}A^{l_{i2},l_{j2}}_{n_{i2},n_{j2}}\sum_{n_1=-1}^{n_{i1}+n_{j1}-l_{i1}-l_{j1}-2} c^{l_{i1},l_{j1}}_{n_{i1},n_{j1},n_1}\sum_{n_2=-1}^{n_{i2}+n_{j2}-l_{i2}-l_{j2}-2} c^{l_{i2},l_{j2}}_{n_{i2},n_{j2},n_2} \\ &\quad\times \tilde{Q}^{l_{i1}+l_{j1},l_{i2}+l_{j2},l}_{n_{i1}+n_{j1}-1-n_1,n_{i2}+n_{j2}-1-n_2},\end{aligned} \tag{7}$$

where the multiplicative factor $A^{l_i,l_j}_{n_i,n_j}$ equals

$$A^{l_i,l_j}_{n_i,n_j} = \frac{2^{1-n_i-n_j}(n_i+n_j-l_i-l_j-2)!(n_i+l_i+n_j+l_j)!}{(n_i-l_i-1)!(n_j-l_j-1)!}\sqrt{\frac{(n_i-l_i-1)!}{(n_i+l_i)!}}\sqrt{\frac{(n_j-l_j-1)!}{(n_j+l_j)!}}. \tag{8}$$

The coefficients $c^{l_i,l_j}_{n_i,n_j,n}$ of the linear combination read

$$c^{l_i,l_j}_{n_i,n_j,n} = C^{l_i,l_j}_{n_i,n_j,n} - \frac{(n_i+n_j-l_i-l_j-2-n)}{(n_i+n_j+l_i+l_j-n-1)}C^{l_i,l_j}_{n_i,n_j,n+1}, \tag{9}$$

where the coefficients $C^{l_i,l_j}_{n_i,n_j,n}$ are given as

$$C^{l_i,l_j}_{n_i,n_j,n} = \frac{F(-n_i+l_i+1,-n;-n_i-n_j+l_i+l_j+2;2)F(-n_i-l_i,-n;-n_i-n_j-l_i-l_j;2)}{(n_i+l_i+n_j+l_j-n-1)!n!} \tag{10}$$

for $n\geqslant 0$ and equal zero otherwise. Here, $F(\alpha,\beta;\gamma;z)$ denotes the hypergeometric function (see, e.g., Refs. 6–8). We note that Eq. (43) in Ref. 1 is incorrect.

$\tilde{Q}^{L_1,L_2,l}_{N_1,N_2}$ denotes the integrals over two radial functions

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$$\tilde{Q}^{L_1,L_2,l}_{N_1,N_2} = \tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} + \tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2}. \tag{11}$$

Here,

$$\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = \int_0^\infty \mathrm{d}r_1\, \tilde{R}_{N_1,L_1}(2r_1) r_1^{l+1} \int_{r_1}^\infty \mathrm{d}r_2\, \tilde{R}_{N_2,L_2}(2r_2) r_2^{-l} \tag{12}$$

and

$$\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2} = \int_0^\infty \mathrm{d}r_1\, \tilde{R}_{N_1,L_1}(2r_1) r_1^{-l} \int_0^{r_1} \mathrm{d}r_2\, \tilde{R}_{N_2,L_2}(2r_2) r_2^{l+1}, \tag{13}$$

where $\tilde{R}_{N,L}(r)$ differs from $R_{N,L}(r)$ by the normalization factor

$$\tilde{R}_{N,L}(r) = 2\sqrt{\frac{(N+L)!}{(N-L-1)!}} R_{N,L}(r). \tag{14}$$

We note that due to the selection rules for the Clebsch–Gordan coefficients mentioned earlier the difference $|L_1 - L_2|$ is always even. Moreover, the sum $L_1 + L_2 + l$ must be even as well.

C. Difference equations for the reduced integrals

Proceeding in complete analogy with the considerations made in Ref. 1 we obtain the following difference equations for the integrals $\tilde{Q}^{\pm,L_1,L_2,l}_{N_1,N_2}$,

$$(N_2 - L_2)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2+1} - (N_2 + L_2)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2-1} - 2l\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = -p^{L_1,L_2}_{N_1,N_2} \tag{15}$$

and

$$(N_1 - L_1)\tilde{Q}^{+,L_1,L_2,l}_{N_1+1,N_2} - (N_1 + L_1)\tilde{Q}^{+,L_1,L_2,l}_{N_1-1,N_2} + 2(l+1)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = p^{L_1,L_2}_{N_1,N_2}. \tag{16}$$

The values of $\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2}$ are obtained from the relation[1]

$$\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2} = \tilde{Q}^{+,L_2,L_1,l}_{N_2,N_1}. \tag{17}$$

Here, the right-hand side of equations $p^{L_1,L_2}_{N_1,N_2}$ equals

$$p^{L_1,L_2}_{N_1,N_2} = \int_0^\infty \mathrm{d}r\, r^2 \tilde{R}_{N_1,L_1}(2r)\tilde{R}_{N_2,L_2}(2r). \tag{18}$$

Using the explicit form of the radial functions,[9]

$$\tilde{R}_{n,l}(r) = 2^2 e^{-r}(2r)^l L^{2l+1}_{n-l-1}(2r), \tag{19}$$

and the expression for the generalized Laguerre polynomials (see, e.g., Refs. 6–8)

$$L^\alpha_K(r) = \frac{1}{K!} e^r r^{-\alpha} \frac{d^K}{\mathrm{d}r^K}(e^{-r} r^{K+\alpha}), \tag{20}$$

we obtain for $L_1 > L_2 + 1$ integrating by parts (see, e.g., Ref. 5),

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$$p_{N_1,N_2}^{L_1,L_2} = \frac{(L_1+L_2+2)!}{2} \sum_{q=\max(0,N_2-L_1-2)}^{\min(N_1-L_1-1,N_2-L_2-1)} (-1)^{N_2-L_2-1-q} \times \binom{N_1-L_2-q-3}{L_1-L_2-2} \binom{L_1+L_2+2+q}{L_1+L_2+2} \binom{L_1-L_2+1}{N_2-L_2-1-q} \tag{21}$$

for $N_2 \leqslant N_1+1$ and

$$p_{N_1,N_2}^{L_1,L_2} = 0 \tag{22}$$

otherwise. The values of $p_{N_1,N_2}^{L_1,L_2}$ for $L_2 > L_1+1$ are obtained from the obvious symmetry $p_{N_1,N_2}^{L_1,L_2} = p_{N_2,N_1}^{L_2,L_1}$, see Eq. (18).

Using difference equations (15) and (16) the integrals are reduced to the integrals over nodeless functions that can be calculated analytically,[1]

$$\tilde{Q}_{L_1+1,L_2+1}^{+,L_1,L_2,l} = 2^{-1}(L_1+L_2+1)!F(1,-L_2+l;-L_1-L_2-1;2). \tag{23}$$

The difference equations (15) and (16) were programmed in MAPLE in form of the recursive algorithm and solved both in rational and 16 digit arithmetics. From these numerical experiments we found that for large quantum numbers N_1, N_2, L_1, and L_2 numerical instabilities appear. Moreover, after some time the recursive algorithm took so much computer memory that further computation was not feasible.

Therefore, we search for the explicit solution of Eqs. (15) and (16). This is done in the following section.

III. SOLUTION OF DIFFERENCE EQUATIONS

In this section we discuss the explicit solution of Eqs. (15) and (16). We argue that the method of variation of constants cannot be used in its standard form and discuss the result of our numerical experiments. These experiments show that Eqs. (15) and (16) are in the region where they are homogenous described by just one of the two linearly independent solutions.

A. The extension of the method given in Ref. 1

In our previous paper[1] we solved Eqs. (15) and (16) for the *S*-states. It follows from the properties of the Clebsch–Gordan coefficients that we must consider the only case $L_1=L_2=L$. In such a case the situation is simplified by virtue of the fact that the right-hand side $p_{N_1,N_2}^{L,L}$ vanishes whenever $|N_1-N_2|>1$.[1] That means that Eqs. (15) and (16) are for most of the values N_1 and N_2 homogenous. Therefore, it was sufficient to find two linearly independent solutions (fundamental system) of homogenous equations (15) and (16) for $l<L$. The two linearly independent solutions of homogenous equation (15) are

$$a_{N_2} = (-1)^{N_2-L_2-1}F(N_2-L_2,-L_2+l;-2L_2;2) \tag{24}$$

and

$$b_{N_2} = F(N_2-L_2,-L_2-l;-2L_2;2). \tag{25}$$

The two linearly independent solutions of the homogenous equation (16) are

$$a_{N_1} = F(N_1-L_1-1,-L_1+l+1;-2L_1;2) \tag{26}$$

and

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$$b_{N_1} = (-1)^{N_1-L_1-1} F(N_1 - L_1, -L_1 - l - 1; -2L_1, 2). \tag{27}$$

For $l=L$, behavior of Eqs. (15) and (16) was so simple that it was possible to guess the result directly from the numerical analysis.

The task of solving Eqs. (15) and (16) is therefore twofold.

First, to determine two linearly independent solutions of homogenous equations (15) and (16) in the cases when $l=\min(L_1,L_2)$. In these cases solutions are not hypergeometric functions. In the Appendix we give a method for finding the solution of Eqs. (15) and (16) in terms of the power series in N_1 or N_2. For $l<\min(L_1,L_2)$ we obtain in this way an alternative expression for the hypergeometric functions. For $l=\min(L_1,L_2)$ this method yields at least one of the two linearly independent solutions. The second solution is found by the method of the reduction of order described in Sec. IV A below.

Second, the fundamental system is used for the solution of inhomogenous equations by the method of the variation of constants. One possibility is to apply this method to Eq. (16) and fix constants on the values $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,N_2}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,N_2}$. Then we apply the method first to Eq. (15) for $N_1=L_1+1$ and fix constants on the values of $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,L_2+1}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,L_2+2}$. Second, we apply the method to Eq. (16) for $N_1=L_1+2$ and fix constants on the values of $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,L_2+1}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,L_2+2}$. Such solution, however, is neither fast nor numerically stable. The reason is that solution of Eqs. (15) and (16) is simplified by virtue of the fact that these equations become homogenous for $L_1<L_2$ and $N_1>N_2+1$ or $L_1>L_2$ and $N_2>N_1+1$, see Eq. (22). Further simplifications were found from numerical experiments given below. All these simplifications must be carefully examined and taken into account to get numerically stable formulas.

B. Numerical experiments

We found that Eq. (15) can be for $L_1>L_2$ and $N_2>N_1+1$ described by just one of the two linearly independent solutions,

$$Q^{+,L_1,L_2,l}_{N_1,N_2} = K(N_1,L_1,L_2,l) a_{N_2}, \tag{28}$$

where a_{N_2} is given by Eq. (24). This equation holds for $l<L_2$. For $l=L_2$ the dependence of $Q^{+,L_1,L_2,L_2}_{N_1,N_2}$ on N_2 can be described as

$$Q^{+,L_1,L_2,L_2}_{N_1,N_2} = K(N_1,L_1,L_2)(-1)^{N_2-L_2-1}. \tag{29}$$

Equation (16) behaves in the same way for $L_2>L_1$ and $N_1>N_2+1$,

$$Q^{+,L_1,L_2,l}_{N_1,N_2} = K(N_2,L_1,L_2,l) a_{N_1}, \tag{30}$$

where a_{N_1} is given by Eq. (26). This equation holds for $l<L_1$. For $l=L_1$ and $N_1>N_2$ we found

$$Q^{+,L_1,L_2,L_1}_{N_1,N_2} = 0. \tag{31}$$

These results show that Eq. (15) is for $L_1>L_2$ and $N_2>N_1+1$ described by just *one* of the two linearly independent solutions. Equation (16) behaves in this way for $L_1<L_2$ and $N_1>N_2+1$. A consequence of this is that although Eqs. (15) and (16) are three term recursion relations we need in the case of Eq. (15) for $L_1>L_2$ and in the case of Eq. (16) for $L_1<L_2$ just *one* initial condition instead of two. In the case of Eq. (16) for $L_1<L_2$ and $l=L_1$ we do not need initial conditions at all. From numerical experiments given in Sec. V below, we were able to determine these initial conditions, that means to determine behavior of $\tilde{Q}^{+,L_1,L_2,l}_{N_1,L_2+1}$ for $L_1>L_2$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,N_2}$ for $L_1<L_2$ and $l<L_1$.

This simplifies the situation tremendously because it means that *instead of solving both Eqs. (16) and (15) simultaneously, we must solve only Eq. (16) for $L_1<L_2$ and Eq. (15) for $L_1>L_2$.*

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As it is clear from the above discussion we need modification of the method of the variation of constants for the case when one of the solutions is obtained by the method of the reduction of order [the case $l=\min(L_1,L_2)$] and for special types of equations when for some value of independent variable equations become homogenous and their solution in that region is described by one of the two linearly independent solutions [Eq. (16) for $L_1<L_2$ and Eq. (15) for $L_1>L_2$]. A general theory of the variation of constants for these cases is given in the following section.

IV. GENERAL THEORY

In this section a general modification of the method of variation of constants is described. We consider general linear second order inhomogenous difference equations for the discrete function f_n,

$$f_{n+1} + q_n f_n + r_n f_{n-1} = s_n. \tag{32}$$

We assume that $f_n=0$ for $n<L+1$ where L is integer and that $s_n=0$ for all $n>M+1$. Equation (15) is obtained from this general equation by setting $n=N_2$, $L=L_2$, $M=N_1$, and $f_{N_2}=\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2}$. Equation (16) is obtained from this general equation by setting $n=N_1$, $L=L_1$, $M=N_2$, and $f_{N_1}=\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2}$. With these assignments we have for both cases

$$r_n = -\frac{n+L}{n-L}. \tag{33}$$

We first show the method of the reduction of order. This is not new, but for the sake of further considerations we describe it in greater detail. Then we summarize the method of the variation of constants and modify it for the cases when one of the solutions was obtained by the reduction of order and for special types of equations appearing in the calculation of atomic integrals.

A. Reduction of order

Let a_n be a solution of the homogenous equation

$$a_{n+1} + q_n a_n + r_n a_{n-1} = 0. \tag{34}$$

The second linearly independent solution can be found by the method of the reduction of order. We search for it in the form

$$b_n = (x_n - x_L)a_n. \tag{35}$$

Inserting it into homogenous equation (32) (with $s_n=0$) and using Eq. (34) we obtain after some manipulation

$$d_{n+1} = r_n \frac{a_{n-1}}{a_{n+1}} d_n, \tag{36}$$

where

$$d_n = x_n - x_{n-1}. \tag{37}$$

Considering the last equation successively for descending n we get

$$x_j - x_n = \sum_{i=n+1}^{j} d_i. \tag{38}$$

Considering Eq. (36) successively for descending n we get

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$$d_n = \prod_{k=n-m}^{n-1} r_k \frac{a_{n-m}a_{n-m-1}}{a_n a_{n-1}} d_{n-m}. \tag{39}$$

Since $a_n=0$ for $n<L+1$ we set $n-m-1=L+1$ in the last equation. Then we obtain for d_n,

$$d_n = \frac{\prod_{k=L+2}^{n-1} r_k}{a_n a_{n-1}} a_{L+2}a_{L+1}d_{L+2}. \tag{40}$$

Inserting this equation into Eq. (38) we get finally

$$x_j - x_n = a_{L+2}a_{L+1}d_{L+2} \sum_{i=n+1}^{j} \frac{\prod_{k=L+2}^{i-1} r_k}{a_i a_{i-1}}. \tag{41}$$

B. Variation of constants

Having two linearly independent solutions a_n and b_n of the homogenous equation a general solution of the inhomogenous equation (32) is obtained by the method of variation of constants[2]

$$f_n = c_1 a_n + c_2 b_n + \sum_{j=L+2}^{n-1} T_j (b_j a_n - a_j b_n). \tag{42}$$

Here, T_j denotes the ratio

$$T_j = \frac{s_j}{W_j}, \tag{43}$$

where W_j is the Wronskian of the solutions

$$W_j = a_{j+1}b_j - a_j b_{j+1}. \tag{44}$$

The constants c_1 and c_2 in Eq. (42) are fixed by the initial values f_{L+1} and f_{L+2}.

For further considerations we derive an alternative form of the Wronskian W_j, see also Ref. 2. Inserting b_j from Eq. (35) we rewrite Eq. (44) into the form

$$W_j = -a_{j+1}a_j(x_{j+1} - x_j). \tag{45}$$

Inserting the difference $x_{j+1}-x_j$ from Eq. (41) into the last equation we obtain

$$W_j = -a_{L+2}a_{L+1}d_{L+2} \prod_{k=L+2}^{j} r_k. \tag{46}$$

Since

$$W_{L+1} = -a_{L+2}a_{L+1}d_{L+2} \tag{47}$$

we can write

$$W_j = W_{L+1} \prod_{k=L+2}^{j} r_k. \tag{48}$$

By means of Eq. (47) we can rewrite also Eq. (41) into the form

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$$x_j - x_n = -W_{L+1} \sum_{i=n+1}^{j} \frac{\prod_{k=L+2}^{i-1} r_k}{a_i a_{i-1}}. \tag{49}$$

We note that, quite generally, formula (42) can be set into an alternative form. Inserting b_n from Eq. (35) we get

$$f_n = a_n[c_1 + c_2(x_n - x_L) + \sum_{j=L+2}^{n-1} T_j a_j (x_j - x_n)], \tag{50}$$

where the difference $x_j - x_n$ is given by Eq. (49). This form of the solution is likely to be less numerically unstable than the form (42), especially in the cases where one of the solutions was obtained by the method of the reduction of order. The reason is that in Eq. (42) we subtract the numbers $b_j a_n$ and $a_j b_n$. Inserting b_j from Eq. (35) we see that we subtract in fact $a_j a_n (x_j - x_L)$ and $a_j a_n (x_n - x_L)$. These two numbers can be very large especially for large n and j. Therefore their subtraction can cause a loss of significant digits. The advantage of Eq. (50) is that we directly calculate the *result* of the subtraction.

C. Special type of equations

Until now, our considerations were quite general. Now we turn to the special type of Eq. (32) for which $s_n = 0$ for all $n > M+1$ where M is integer and the solution of Eq. (32) in this region is fully described by just *one* of the two linearly independent solutions of the homogenous equation

$$f_n = K a_n, \tag{51}$$

where K is independent on n. Comparing Eqs. (50) and (51) we get

$$K = c_1 + (x_n - x_L)c_2 + \sum_{j=L+2}^{M+1} T_j a_j (x_j - x_n) \tag{52}$$

for arbitrary $n > M+1$. Since this equation holds for $n > M+1$ independently on the value of n we get

$$c_1 - x_L c_2 + \sum_{j=L+2}^{M+1} T_j a_j x_j = K \tag{53}$$

and

$$c_2 - \sum_{j=L+2}^{M+1} T_j a_j = 0. \tag{54}$$

The last two equations are a source of numerical instabilities if constants c_1 and c_2 are determined from the initial values f_{L+1} and f_{L+2}. To avoid these instabilities *we use Eqs. (53) and (54) as equations determining constants* c_1 *and* c_2. If we do so and insert the result into Eq. (50) we obtain

$$f_n = a_n \left[K - \sum_{j=n}^{M+1} T_j a_j (x_j - x_n) \right]. \tag{55}$$

Considering this equation for $n = L+1$ we determine the constant K,

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$$K = \frac{f_{L+1}}{a_{L+1}} + \sum_{j=L+1}^{M+1} T_j a_j (x_j - x_{L+1}). \tag{56}$$

Inserting this back into Eq. (55) we obtain finally

$$f_n = a_n \left[\frac{f_{L+1}}{a_{L+1}} + \sum_{j=L+2}^{n-1} T_j a_j (x_j - x_{L+1}) + \sum_{j=n}^{M+1} T_j a_j (x_n - x_{L+1}) \right]. \tag{57}$$

Alternatively, we can use Eq. (35) and rewrite Eq. (57) in terms of a_n and b_n,

$$f_n = \frac{a_n}{a_{L+1}} \left[f_{L+1} - \sum_{j=L+2}^{M+1} T_j a_j b_{L+1} \right] + a_n \sum_{j=L+2}^{n-1} T_j b_j + b_n \sum_{j=n}^{M+1} T_j a_j. \tag{58}$$

The last two equations are likely to be more convenient for computational purposes than Eq. (42) since there are no cancellations of large numbers in these equations. The possible exception is the subtraction in the square brackets in Eq. (58), but for the special case of interest (see Sec. V) we avoid this difficulty.

V. APPLICATION OF THE METHOD

General theory outlined in the preceding section will be applied to the difference equations (15) and (16). To do so, we need to calculate T_j from Eq. (43).

A. Calculation of T_j

First we calculate Wronskian (44) from Eq. (48). Inserting r_k from Eq. (33) into this equation we get that Wronskian behaves for both Eqs. (15) and (16) as

$$W_j = (-1)^{j-L-1} \frac{(j+L)!}{(j-L)!} \frac{W_{L+1}}{(2L+1)!}, \tag{59}$$

where we set either $L=L_2$ or $L=L_1$. We note that W_{L+1} is the only quantity in this equation that depends on the concrete form of a_j and b_j.

Second, we take the right-hand side s_j of Eq. (32) equal to

$$s_j = -\frac{p_{N_1,j}^{L_1,L_2}}{j - L_2} \tag{60}$$

in case of Eq. (15) and

$$s_j = \frac{p_{N_2,j}^{L_2,L_1}}{j - L_1} \tag{61}$$

in case of Eq. (16).

Equations (59), (60), and (61) can be used to simplify formula (43). By inserting Eq. (59) with $L=L_2$ and Eq. (60) into Eq. (43) we get in the case of Eq. (15),

$$T_j = -\frac{P_{N_1,j}^{L_1,L_2}}{W_{L_2+1}}. \tag{62}$$

Analogously, by inserting Eq. (59) with $L=L_1$ and Eq. (61) into Eq. (43) we get in the case of Eq. (16),

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$$T_j = \frac{P_{N_2,j}^{L_2,L_1}}{W_{L_1+1}}. \tag{63}$$

Here, $P_{N_1,N_2}^{L_1,L_2}$ denotes

$$P_{N_1,N_2}^{L_1,L_2} = \frac{p_{N_1,N_2}^{L_1,L_2} W_{L_2+1}}{(N_2 - L_2) W_{N_2}}. \tag{64}$$

This quantity was introduced because of the symmetry

$$P_{N_1,N_2}^{L_1,L_2} = P_{N_2,N_1}^{L_2,L_1} \tag{65}$$

[see the notes after Eqs. (22) and (59)]. By combining Eqs. (21) and (59) we can write for $L_1 > L_2+1$,

$$P_{N_1,N_2}^{L_1,L_2} = \frac{(L_1 - L_2 + 1)!(2L_2 + 1)!}{2} \sum_{q=\max(0,N_2-L_1-2)}^{\min(N_1-L_1-1,N_2-L_2-1)} (-1)^q \times \binom{N_1 - L_2 - q - 3}{L_1 - L_2 - 2} \binom{N_2 - L_2 - 1}{q} \binom{L_1 + L_2 + 2 + q}{N_2 + L_2}. \tag{66}$$

The case $L_2 > L_1+1$ is calculated by means of Eq. (65).

B. Numerical experiments and final formulas

1. Case $l < \min(L_1, L_2)$

By numerical experiments we found that the initial values f_{L+1} for Eq. (15) with $L_1 > L_2$ and $l < L_2$ and for Eq. (16) with $L_1 < L_2$ and $l < L_1$ are given as

$$f_{L+1} = (a_{L+1} + b_{L+1}) \sum_{j=L+1}^{M+1} T_j a_j. \tag{67}$$

In the case of Eq. (15) this equation holds with $L = L_2$, $M = N_1$, $f_{L+1} = \tilde{Q}_{N_1,L_2+1}^{+,L_1,L_2,l}$ and with a_j, b_j, and T_j given by Eqs. (24), (25), and (62). In the case of Eq. (16) this equation holds with $L = L_1$, $M = N_2$, $f_{L+1} = \tilde{Q}_{L_1+1,N_2}^{+,L_1,L_2,l}$ and with a_j, b_j, and T_j given by Eqs. (26), (27), and (63).

Then Eq. (58) can be brought to the form

$$f_n = a_n \sum_{j=L+1}^{n-1} T_j (a_j + b_j) + (a_n + b_n) \sum_{j=n}^{M+1} T_j a_j. \tag{68}$$

2. Case $l = L_2$

It follows from Eq. (29) that in this case one of the two linearly independent solutions is

$$a_{N_2} = (-1)^{N_2 - L_2 - 1}. \tag{69}$$

The second one is determined by the reduction of order. We use Eq. (57) for $f_{N_2} = \tilde{Q}_{N_1,N_2}^{+,L_1,L_2,L_2}$ with $n = N_2$, $L = L_2$, $M = N_1$, and T_j given by Eq. (62). The value of f_{L+1} was found from numerical analysis to be

$$\tilde{Q}_{N_1,L_2+1}^{+,L_1,L_2,L_2} = \frac{(L_1 + L_2 + 1)!(N_1 - L_2 - 2)!}{2(L_1 - L_2 - 1)!(N_1 - L_1 - 1)!}. \tag{70}$$

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3. Case $l=L_1$

It follows from Eq. (31) that the constant K in Eq. (51) is equal to zero, so we can use Eq. (55) for $f_{N_1}=\tilde{Q}^{+,L_1,L_2,L_1}_{N_1,N_2}$ with $n=N_1$, $L=L_1$, $M=N_2$, and T_j calculated from Eq. (63).

One of the two linearly independent solutions of homogenous equation (16) is given by Eq. (A6) of the Appendix with $J=2L_1+1$,

$$a_{N_1}=(-1)^{N_1-L_1-1}\sum_{j=0}^{2L_1+1} h_j(N_1-L_1)^j, \tag{71}$$

where h_j are given by Eq. (A11) and where $h_{2L_1+1}=1$.

Using Eqs. (33) and (49) we can write Eq. (55) for the case considered as

$$f_n=-a_n\frac{W_{L+1}}{(2L+1)!}\sum_{j=n+1}^{M+1} T_j a_j \sum_{k=n+1}^{j}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}. \tag{72}$$

This expression is still not entirely satisfactory. We found that there is residual instability for n close to $L+1$. To eliminate it we rewrite the double summation in the last equation

$$f_n=-a_n\frac{W_{L+1}}{(2L+1)!}\sum_{k=n+1}^{M+1}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}\sum_{j=k}^{M+1} T_j a_j. \tag{73}$$

The source of instability for n close to $L+1$ is an interesting identity,

$$\sum_{j=L+1}^{M+1} T_j a_j=0. \tag{74}$$

Therefore, we use this identity in Eq. (73) and rewrite this equation to the form

$$f_n=a_n\frac{W_{L+1}}{(2L+1)!}\sum_{k=n+1}^{M+1}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}\sum_{j=L+1}^{k-1} T_j a_j. \tag{75}$$

This equation is stable for all n from $L+1$ to M. For $n>M$, it yields zero as it should.

C. Numerical tests

We tested derived formulas numerically for very large quantum numbers. First we set $L_1=16$ and $L_2=14$, second we considered $L_1=20$ and $L_2=10$. We took $N_1=50$ and varied N_2 from L_2+1 to 70 and l from 2 to L_2. Then we reversed the role of L_1 and L_2 and also N_1 and N_2. These tests are rather severe; in normal calculation one encounters much more favorable situations. The formulas were run in double precision arithmetics and compared with the exact solutions of Eqs. (15) and (16) programmed in MAPLE in the form of the recursive algorithm run in rational arithmetics. For $l<\min(L_1,L_2)$, the hypergeometric functions (24)–(27) were calculated from the MAPLE subroutine. The numerical stable way of their calculations is given in the Appendix. For $|L_1-L_2|=2$ the relative error of the derived formulas was typically of order 10^{-15}. For the case $|L_1-L_2|=10$ the relative error was typically two orders higher. This shows that numerical stability of formulas slightly deteriorates with increasing difference $|L_1-L_2|$. However, one can expect that with increasing difference of the angular momenta of the electrons the contributions of the terms with large numbers of nodes to the energy is relatively small. Therefore, the achieved numerical stability is sufficient for all practical purposes.

VI. CONCLUSIONS

In this paper we extended the method of numerically stable calculation of the atomic integrals suggested in our previous paper[1] for the S-states of two-electron atoms to the states of arbitrary

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total angular momenta. Thus, in these two papers the complete solution of the numerically stable calculation of the atomic integrals is given. In the first paper[1] we succeeded in transformation of the problem of the numerical stable calculation of the atomic integrals to the problem of the numerical stable solution of the difference equations. In this paper we completed our program by solving the latter problem in required generality. To achieve this aim we suggested a computationally stable method for the solution of inhomogenous difference equations that for certain values of the discrete independent variable become homogenous and in that region are described by just one of the two linearly independent solutions. The method was applied to the difference equations appearing in the radial part of the atomic integrals and tested for very large quantum numbers. These tests show high numerical stability of the suggested method. The stability slightly decreases with increasing difference of the angular momenta of the electrons.

The method suggested in these two papers can be used for the calculation of the radial part of the Coulomb interaction between electrons whose orbitals are expanded from the same center. This covers all atoms and the simplest molecules. The results obtained in these papers can be directly used for the configuration interaction calculation of the excited states of two electron atoms. This will be reported elsewhere.

Because of the potential importance of the achieved results it would be desirable to put them on a rigorous basis. The paper is based on the observation that Eqs. (15) and (16) can be in the region where they become homogenous described by just *one* of the two linearly independent solutions. Although we are certain about this observation, one should see *why* equations behave in this way. The same applies to our guesses (67), (70), and (74), and for Eq. (A17) in the Appendix.

Therefore, we believe that the results achieved in this paper are of some interest from the point of view of atomic physics as well as pure mathematics.

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APPENDIX

In this appendix we suggest a solution of the homogenous equations (15) and (16). Since this solution is given in terms of the hypergeometric function $F(a,b,c,2)$ we find a particularly useful form of these functions that can be used also in Eq. (10).

Let us rewrite homogenous equations (15) and (16) into a general form,

$$(n-L)g_{n+1}-(n+L)g_{n-1}-2(J-L)g_n=0. \tag{A1}$$

This equation is obtained from the original homogenous equation (16),

$$(n-L)f_{n+1}-(n+L)f_{n-1}+2(l+1)f_n=0, \tag{A2}$$

by setting either $f_n=g_n$ and $J=L-l-1$ or $f_n=(-1)^n g_n$ and $J=L+l+1$. Equation (A1) is obtained also from homogenous equation (15),

$$(n-L)f_{n+1}-(n+L)f_{n-1}-2lf_n=0, \tag{A3}$$

by setting either $f_n=g_n$ and $J=L+l$ or $f_n=(-1)^n g_n$ and $J=L-l$. Due to the selection rules for Clebsch–Gordan coefficients mentioned after Eq. (5), the difference $L-l$ is always even. Therefore, the parameter J is odd in the case of Eq. (16) and even in the case of Eq. (15).

For $J<L-1$ the solution of Eq. (A1) is given by the hypergeometric function

$$g_n=F(n-L,-J;-2L;2). \tag{A4}$$

Let us remind the form of the hypergeometric function $F(a,b,c,z)$ here,

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$$F(a,b,c,z) = 1 + \frac{ab}{c}z + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \cdots . \tag{A5}$$

It turns out that this form of the hypergeometric functions is useful only for a close to zero, i.e., only for n close to L. For larger n, a more suitable form is needed.

Since we want to get expression also for the hypergeometric functions appearing in Eq. (10), we allow L to be half-integral and n to be half-integral and smaller than $L+1$.

We search for the solution of Eq. (A1) in the form of the series

$$g_n = \sum_{j=0}^{J} h_j (n-L)^j . \tag{A6}$$

Later on, it will be clear why we choose the upper bound of summation J. The advantage of this expansion is that the coefficients h_j do not change the sign. Therefore, for n larger than L this way of calculating the hypergeometric functions is numerically stable and can be used for the hypergeometric functions appearing in Eqs. (24)–(27).

Since J must be a non-negative integer, for $L=l$ we obtain only one solution in the form (A6). If $l<L$, we obtain in this way two linearly independent solutions.

The remaining hypergeometric functions to be calculated are those appearing in Eq. (10). For these functions argument a in the definition (A5) is always negative. As it is clear from Eq. (A4) it corresponds to the situation when $n<L$. The use of Eq. (A6) is not advantageous in this case, because for negative value of $n-L$ we get in (A6) the sum of terms with changing signs. When n is close to L, the best way is to calculate the hypergeometric functions from the definition (A5). For n more distant from L we calculate the hypergeometric functions from the series

$$g_n = \sum_{j=0}^{J} c_j n^j . \tag{A7}$$

It appears that for even J the coefficients c_j with odd j equal zero and for odd J the coefficients c_j with even j equal zero. From this fact it immediately follows that

$$F(-n-L,-J;-2L;2) = (-1)^J F(n-L,-J;-2L,2). \tag{A8}$$

Using this equation we can always raise the value of the parameter a over $-L$.

In the following we first show how to calculate the coefficients h_j in the expansion (A6), then we calculate the coefficients c_j in the expansion (A7).

Expansion around $n=L$

We make substitution $N=n-L$ in Eq. (A1). Then Eq. (A1) reads

$$Ng_{N+1} - (N+2L)g_{N-1} - 2(J-L)g_N = 0. \tag{A9}$$

Inserting the expansion (A6) and using the binomial formula we obtain after some manipulation

$$\sum_{j=0}^{J}\left[\sum_{k=0}^{j}\binom{j}{k}N^{k+1}(1-(-1)^{j-k}) - 2L\sum_{k=0}^{j}N^k(-1)^{j-k} - 2(J-L)N^j\right]h_j = 0. \tag{A10}$$

Comparing now terms with the same powers of N we get for the highest power N^J identically zero. It means that the coefficient h_J is free for the normalization of the solution. This is the reason why we chose in Eq. (A6) the upper bound of the summation equal to J. Going then successively to the lower powers of N we obtain recurrence relations for the coefficients h_j,

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$$\frac{h_{J-j}}{h_J} = \frac{1}{j(J-j)!}\sum_{p=0}^{j-1}\frac{(J-p)!}{(1+j-p)!}\left[\frac{1-(-1)^{j-p-1}}{2}(J-j) - L(1+j-p)(-1)^{j-p}\right]\frac{h_{J-p}}{h_J}. \quad \text{(A11)}$$

Normalization of the series (A6) to the hypergeometric function is done by comparing Eqs. (A4) and (A6) for some value of n. The best choice is $n=L$ since then we have

$$1 = h_J\frac{h_0}{h_J}, \quad \text{(A12)}$$

where we used the identity $F(0,-J;-2L;2)=1$. The ratio h_0/h_J is calculated from Eq. (A11).

Expansion around $n=0$

We proceed along the same lines as in the derivation of recurrence relations for the coefficients h_j. We insert the expansion (A7) into Eq. (A1), use binomial formula and compare the terms with the same powers of n. After some manipulation we obtain

$$\frac{c_{J-2p}}{c_J} = \frac{1}{2p(J-2p)!}\sum_{j=0}^{p-1}\frac{c_{J-2j}}{c_J}\frac{(J-2j)!}{(2p-2j+1)!}[J-2p-L(2p-2j+1)] \quad \text{(A13)}$$

for p running from 1 to $J/2$ for J even and to $(J-1)/2$ for J odd. The coefficients c_{J-2p-1} equal zero.

The coefficient c_J is determined by comparing series (A7) and the hypergeometric function (A4) for some n. Setting $n=L$ we obtain

$$1 = c_J\sum_{j=0}^{J}\frac{c_j}{c_J}L^j, \quad \text{(A14)}$$

where we used the identity $F(0,-J;-2L;2)=1$. For practical purposes, however, this form is not very convenient, since there is a cancellation of large numbers in the sum on the right-hand side. For this reason the use of series (A7) is not suitable for calculation of the hypergeometric functions with n comparable or greater than L. Instead we determine the constant c_J as follows.

For even values of $J=2P$ the constant c_{2P} is found by comparing Eqs. (A4) and (A7) for $n=0$,

$$F(-L,-2P;-2L;2) = c_{2P}\frac{c_0}{c_{2P}}, \quad \text{(A15)}$$

where the ratio c_0/c_{2P} is calculated from Eq. (A13). The values of $F(-L,-2P;-2L,2)$ were found from the numerical experiments to be

$$F(-L,-2P,-2L,2) = \prod_{p=0}^{P-1}\frac{2p+1}{2L-2p-1}. \quad \text{(A16)}$$

For odd values of $J=2P+1$, comparison of Eqs. (A4) and (A7) yields for $n=0$ nothing, since both sides are identically equal to zero. However, the constant c_{2P+1} can be calculated from remarkable identity

$$c_{2P+1} = \frac{c_{2P}}{L-P} \quad \text{(A17)}$$

found by numerical experiments.

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