PHYSICAL REVIEW A VOLUME 21, NUMBER 6 JUNE 1980

Multipole and overlap integrals over reduced Bessel functions in molecular quantum mechanics

Danko Antolović* and Joseph Delhalle

Laboratoire de Chimie Théorique Appliquée, Facultés Universitaires Notre-Dame de la Paix, Rue de Bruxelles, 61, B-5000 Namur, Belgium

(Received 7 December 1979)

The methods of calculation of overlap integrals over a reduced Bessel-function basis set have been reviewed. Some new results were obtained, and the numerical aspects of existing formulas were investigated. Also, analytical expressions for multipole integrals over reduced Bessel functions have been derived.

I. INTRODUCTION

One of the main obstacles in the application of the HF-Roothaan method to the study of the electronic structure of molecules, polymers, surfaces, and crystals is the evaluation of integrals occurring in the formalism. So far these investigations have been performed mainly with the help of Gaussian-type functions (GTO's). However, these functions are not completely satisfactory since they do not represent the correct behavior of the wave function at the nuclei and at large distances. At the nuclear centers, the exact wave function must fulfill the cusp condition and at large distances it should decrease exponentially. The main reason for using GTO's is to be found in their mathematical and computational conveniences, but to get reliable results one has to include a sufficient number of GTO's which leads also to computational problems. A well-known alternative is provided by the Slater-type orbitals (STO's) which have both the right cusp and exponential decrease characteristics but at the expense of an excessive amount of computer time needed for their evaluation.

Quite recently Steinborn and coworkers[1,2] have pleaded in favor of the reduced Bessel functions (RBF's) which exhibit the same physical properties as STO's but in addition possess convenient mathematical features which yield to easy handling and quite simple matrix elements. Since our group is presently involved in HF-Roothaan calculations of the electronic structure of extended chains (polymers, 1D crystals,...) it was interesting to investigate the usefulness of such functions in this context. Indeed the computational effort in extended systems is basically heavier than in isolated molecules, and it is of continuous importance to search for good compromises between computing time and the quality of the results.

This paper relies strongly upon the theoretical work done previously by Steinborn and coworkers.[1,2,3] Our first aim is to obtain feasible computer algorithms for the calculation of overlap integrals over RBF basis functions. Overlap integrals appear as the building blocks in formulas for other molecular integrals. Therefore, it is necessary to compute them accurately for a relatively wide range of parameters (chiefly quantum numbers).

Again, a short account on the equivalent, older STO basis set is needed. The computational difficulties connected with it have become almost proverbial. The evaluation of integrals over STO's was usually reduced at the evaluation of various auxiliary functions, a procedure that sometimes proved to contain numerical bottlenecks.[4,5] The calculations also involve multiple sums and extensive tabulations of coefficients. At authors' opinion, multiple sums involve numerical risks for higher quantum numbers and are also relatively time-consuming procedures.

In a series of papers, Piela and Delhalle[6,7] have developed a method for calculation of long-range interactions, based on the known multipole expansion for the operator $1/r$. This is a useful tool in the theory of extended systems. Independently of the chosen basis set, this method involves extensive calculation of one-electron multipole integrals. In the present paper analytical formulas are derived for multipole integrals over RBF's. The problem is essentially reduced to the calculation of overlap integrals over reduced Bessel functions. Therefore, the problem of calculation of convolution (overlap) integrals, treated by Steinborn *et al.*, is considered from a computational point of view.

A. Some general aspect of RBF's

We shall follow the notation and definitions given in Ref. 2. The RBF atomic function is given as:

$$B^{M}_{N,L}(\alpha\vec{r}) = [2^{N+L}(N+L)!]^{-1} \times (\alpha r)^{L}\hat{k}_{N-1/2}(\alpha r)Y^{M}_{L}(\theta,\phi)\,, \qquad (1.1)$$

where $\hat{k}_\nu(\alpha r)$, the "reduced Bessel function" is

$$\hat{k}_\nu(\alpha r)=(2/\pi)^{1/2}(\alpha r)^\nu K_\nu(\alpha r)\,.$$

Function $K_\nu(\alpha r)$ is the modified Bessel function of the second kind. Obviously the RBF's for half-integer order are closely related to spherical Bessel functions and have an elementary form:

$$\hat{k}_{N-1/2}(\alpha r)=e^{-\alpha r}\sum_{p=1}^{N}\frac{(2N-p-1)!}{(p-1)!(N-p)!}\times 2^{p-N}(\alpha r)^{p-1}\,. \tag{1.2}$$

It can be seen from the above formula that RBF's constitute a basis equivalent to STO. This fact has been expounded upon in Refs. 8 and 9 by Steinborn and Weniger.

The constant α will be named "scaling parameter". It is related to the screening constant of STO's. Spherical harmonics Y_L^M are defined in Condon-Shortley phases (see Appendix A).

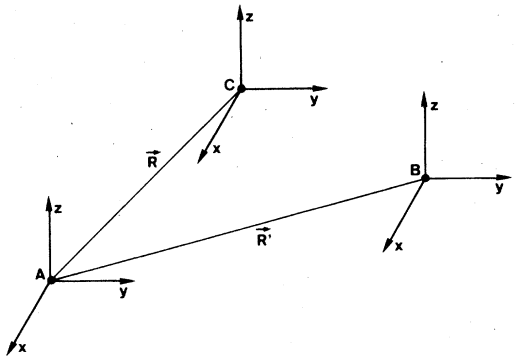

FIG. 1. Coordinate systems used in the multipole expansion.

II. MULTIPOLE INTEGRALS

As we mentioned above, in the multipole expansion method the integrals of the type $\langle\psi|r^l Y_l^m(\theta,\phi)|\psi'\rangle$ appear. The most general case is the one-electron, three-center integral. Coordinate systems used are shown in Fig. 1. Two RBF orbitals are defined with respect to the coordinates on A and B, the operator (regular solid spherical harmonic) is defined on the center C.

First step in evaluation of the integral will be expansion of the harmonic on C in similar functions on A. Such expansions (translation theorems) have been described in literature.[10,11,3] We shall make use of an expansion derived in Ref. 3:

$$r_C^l Y_l^m(\theta_C,\phi_C)=R^l\sum_{\lambda=0}^{l}\sum_{\mu=-\lambda}^{\lambda}(-1)^{l-\lambda}(r_A/R)^\lambda Y_\lambda^\mu(\theta_A,\phi_A)C_{l\lambda}^{m\mu}(\theta_{AR},\phi_{AR})\,,$$
$$C_{l\lambda}^{m\mu}(\theta_{AR},\phi_{AR})=\frac{2\pi^{1/2}[(2l+1)(l+m)!(l-m)!]^{1/2}}{[(2\lambda+1)(\lambda+\mu)!(\lambda-\mu)!(2l-2\lambda+1)(l+m-\lambda-\mu)!(l-m-\lambda+\mu)!]^{1/2}}Y_{l-\lambda}^{m-\mu}(\theta_{AR},\phi_{AR}). \tag{2.1}$$

Utilizing (2.1), we can write

$$I=\langle\psi_A|r_C^l Y_l^m(\theta_C,\phi_C)|\psi_B\rangle=R^l\sum_{\lambda=0}^{l}\sum_{\mu=-\lambda}^{\lambda}(-1)^{l-\lambda}C_{l\lambda}^{m\mu}(\theta_{AR},\phi_{AR})\langle\psi_A|(r_A/R)^\lambda Y_\lambda^\mu(\theta_A,\phi_A)|\psi_B\rangle$$
$$=R^l\sum_{\lambda=0}^{l}(1/R)^\lambda\sum_{\mu=-\lambda}^{\lambda}(-1)^{l-\lambda}C_{l\lambda}^{m\mu}(\theta_{AR},\phi_{AR})K_A\int(\alpha_A r_A)^{L_A}\hat{k}_{N_A-1/2}(\alpha_A r_A)Y_{L_A}^{M_A}{}^*(\Omega_A)r_A^\lambda Y_\lambda^\mu(\Omega_A)\psi_B d\tau\,.$$

Next we use an expansion given in Ref. 1 as formula (6.1):

$$x^t\hat{k}_{n-1/2}(x)=\sum_{p=0}2^p\binom{t/2}{p}\left(\frac{1-2n-t}{2}\right)_p\hat{k}_{t-p+n-1/2}(x)\,. \tag{2.2}$$

here, the brackets with index p denote Pochhammer symbol (Ref. 12, formula 6.1.22). Formula (2.2) is applied to the product

$$(\alpha_A r_A)^{L_A+\lambda-L}\hat{k}_{N_A-1/2}(\alpha_A r_A)\,.$$

Also, the product of spherical harmonics is expanded in the series of harmonics (Appendix A). This yields

$$I=K_A R^l\sum_\lambda(-1)^{l-\lambda}\alpha_A^{-\lambda}R^{-\lambda}\sum_\mu C_{l\lambda}^{m\mu}\sum_L\langle LM|L_A M_A|\lambda\mu\rangle\sum_p 2^p\binom{(L_A+\lambda-L)/2}{p}\left(\frac{1-2N_A-L_A-\lambda+L}{2}\right)_p$$
$$\times 2^{N_A+L_A+\lambda-p}(N_A+L_A+\lambda-p)!$$
$$\times\int B_{N_A+L_A+\lambda-L-p,L}^{M_A*}(\alpha_A\vec{r}_A)B_{N_B L_B}^{M_B}(\alpha_B\vec{r}_B)d\tau\,, \tag{2.3}$$

and finally

$$I=(-1)^l R^l[(N_A+L_A)!\,]^{-1}\sum_{\lambda=0}^{l}2^\lambda(-1)^\lambda\alpha_A^{-\lambda}R^{-\lambda}\sum_{\mu=-\lambda}^{\lambda}C_{l\lambda}^{m\mu}(\theta_{CA},\phi_{CA})$$
$$\times\sum_L\langle LM|L_AM_A|\lambda\mu\rangle\sum_{p=0}^{\Delta L}\binom{\Delta L}{p}(\tfrac{1}{2}-N_A-\Delta L)_p(N_A+L_A+\lambda-p)!$$
$$\times S^{N_BL_BM_B}_{N_A+L_A+\lambda-L-p,\,L,\,M}(\alpha_A,\alpha_B,\vec{R}')\,. \tag{2.4}$$

Here $\Delta L=\frac{1}{2}(L_A+\lambda-L)$.

A. Two-center case $R=0$

For this case, the following simple formula holds:

$$I=\langle\psi_A|r_A^l Y_l^m(\theta_A,\phi_A)|\psi_B\rangle$$
$$=2^l[(N_A+L_A)!\,\alpha_A^l\,]^{-1}\sum_L\langle LM|L_AM_A|lm\rangle\sum_{p=0}^{\Delta L}\binom{\Delta L}{p}$$
$$\times(\tfrac{1}{2}-N_A-\Delta L)_p(N_A+L_A+l-p)!\,S^{N_BL_BM_B}_{N_A+L_A+l-L-p,\,L,\,M}(\alpha_A,\alpha_B,\vec{R}')\,. \tag{2.5}$$

Here $\Delta L=\frac{1}{2}(L_A+l-L)$.

B. Two-center case $R'=0$

For this case the following formula holds:

$$I=(-1)^l[(N_A+L_A)!\,]^{-1}R^l\sum_{\lambda=0}^{l}2^\lambda(-1)^\lambda\alpha_A^{-\lambda}R^{-\lambda}C_{l\lambda}^{m,\,M_B-M_A}(\theta_{CA},\phi_{CA})\langle L_BM_B|L_AM_A|\lambda,M_B-M_A\rangle$$
$$\times\sum_{p=0}^{\Delta L_B}\binom{\Delta L_B}{p}(\tfrac{1}{2}-N_A-\Delta L_B)_p(N_A+L_A+\lambda-p)!\,S^{N_BL_BM_B}_{N_A+L_A+\lambda-L_B-p,\,L_B,\,M_B}(\alpha_A,\alpha_B,0)\,. \tag{2.6}$$

Here $\Delta L_B=\frac{1}{2}(L_A+\lambda-L_B)$.

C. One-center case

For this case the following formula holds:

$$I=2^l[(N_A+L_A)!\,\alpha_A^l\,]^{-1}\langle L_BM_B|L_AM_A|lm\rangle\sum_{p=0}^{\Delta L_B}\binom{\Delta L_B}{p}(\tfrac{1}{2}-N_A-\Delta L_B)_p(N_A+L_A+l-p)!\,S^{N_BL_BM_B}_{N_A+L_A+l-L_B-p,\,L_B,\,M_B}(\alpha_A,\alpha_B,0). \tag{2.7}$$

Here $\Delta L_B=\frac{1}{2}(L_A+l-L_B)$.

III. OVERLAP INTEGRALS

The centerpiece of the theory of RBF's, developed so far, is the convolution theorem. It says that the convolution integral over two atomic RBF's can be represented as an expression closed with respect to the RBF's themselves. The formula has two different forms, for the cases of equal and unequal scaling parameters of orbitals; three formulas for some special cases also exist. The proof of the theorem has been given in Ref. 1 by E. Filter and E. O. Steinborn.

A. Case $\alpha=\beta$

The overlap integral being given by

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,\vec{R})=\int d\vec{r}\,B^{M_1*}_{N_1L_1}(\alpha\vec{r})B^{M_2}_{N_2L_2}[\beta(\vec{r}-\vec{R})]\,, \tag{3.1}$$

the formula for it is (formula 4.3 in Ref. 2) for $\alpha=\beta$

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\alpha,\vec{R})=4\pi\alpha^{-3}(-1)^{L_2}\sum_l\langle L_2M_2|L_1M_1|lm\rangle\sum_t(-1)^t\binom{\Delta l}{t}B^m_{N_1+N_2+L_1+L_2-l-t+1,\,t}(\alpha\vec{R})\,. \tag{3.2}$$

This formula has been cast into a slightly different form for coding purposes:

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\alpha,\vec{R})=\frac{(-1)^{L_2+M_1}(2\pi)^{1/2}}{\alpha^3 2^{N_1+N_2+L_1+L_2}}e^{im\phi}\sum_l \langle lm\,|\,L_2M_2\,|\,L_1,-M_1\rangle[\Phi^m_l(\cos\theta)(\alpha R)^l]\sum_{t=0}^{\Delta l}(-1)^t\binom{\Delta l}{t}\hat{k}_{N_1+N_2+L_1+L_2-l-t+1/2}(\alpha R)$$
$$\times 2^t[(N_1+N_2+L_1+L_2-t+1)!\,]^{-1}. \tag{3.3}$$

Considering the fact that the value of $\hat{k}_N(x)$ increases very quickly as N increases, and having in mind the computational considerations in Sec. III C., we compute a somewhat modified function

$$\kappa_{N-1/2}(x)=\hat{k}_{N-1/2}(x)/N!$$

using the relations

$$\begin{aligned}&\kappa_{-1/2}(x)=e^{-x}/x,\\ &\kappa_{1/2}(x)=e^{-x},\\ &x^2\kappa_{N-1/2}(x)=(N+2)(N+1)\kappa_{N+3/2}(x)-(2N+1)(N+1)\kappa_{N+1/2}(x),\end{aligned} \tag{3.4}$$

which follow directly from the known properties of Bessel functions. For the details concerning Gaunt coefficients and functions $\Phi^m_l(\cos\theta)$, see Appendix A.

B. Case $\alpha\neq\beta$

For this case formulas (4.6) and (4.7) in Ref. 2 hold. We have unified these two expressions into the following working formula:

$$\begin{aligned}S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,\vec{R})=(-1)^{L_2+M_1}2(2\pi)^{1/2}e^{im\phi}\sum_l \langle lm\,|\,L_2M_2\,|\,L_1,-M_1\rangle\Phi^m_l(\cos\theta)\\ \times\Bigg[(\alpha R)^l(-1)^{N_1+L_1}\alpha^{L_2}\beta^{2N_2+L_2-1}(\beta^2-\alpha^2)^{-N_2-L_2-1}\\ \times\sum_{t=0}^{N_1+L_1}(-1)^t P^{(-N_1-\Delta L_2+t,\,N_2+\Delta L_1)}_{N_1+L_1-t}\left(\frac{\beta^2+\alpha^2}{\beta^2-\alpha^2}\right)\hat{k}_{t-l-1/2}(\alpha R)(2^t t!)^{-1}\\ +(\beta R)^l(-1)^{N_2+L_2}\beta^{L_1}\alpha^{2N_1+L_1-1}(\alpha^2-\beta^2)^{-N_1-L_1-1}\\ \times\sum_{t=0}^{N_2+L_2}(-1)^t P^{(-N_2-\Delta L_1+t,\,N_1+\Delta L_2)}_{N_2+L_2-t}\left(\frac{\alpha^2+\beta^2}{\alpha^2-\beta^2}\right)\hat{k}_{t-l-1/2}(\beta R)(2^t t!)^{-1}\Bigg].\end{aligned} \tag{3.5}$$

Here $\Delta L_1=\frac{1}{2}(L_2+l-L_1)$, $\Delta L_2=\frac{1}{2}(L_1+l-L_2)$, $P^{(\nu,\mu)}_N(x)$ are Jacobi polynomials as defined in Ref. 13.

We shall devote some more consideration to an efficient procedure for evaluation of Jacobi polynomials, as a relatively heavy use of this function is made in the above formula. Let us consider the set of polynomials $P^{(-\nu_2-\Delta\lambda_2+t,\,\nu_1+\Delta\lambda_2)}_{\nu_2+\lambda_2-t}(x)$. Both sets of functions needed in the calculation are obtained from this set by obvious substitutions. We introduce the notation

$$\begin{aligned}&\mu=-\nu_2-\Delta\lambda_1+t,\\ &\nu=\nu_1+\Delta\lambda_2,\\ &N=\nu_2+\lambda_2-t.\end{aligned} \tag{3.6}$$

With μ,ν,N considered as coordinates in an affine space (e.g. Euclidean, to simplify the matters), the above equations represent a surface parametrized by variables l,t. Recalling the meaning of the symbol Δ,

$$\begin{aligned}&\Delta\lambda_1=\tfrac{1}{2}(\lambda_2+l-\lambda_1),\\ &\Delta\lambda_2=\tfrac{1}{2}(\lambda_1+l-\lambda_2),\end{aligned} \tag{3.7}$$

two formulas follow immediately:

$$\begin{aligned}&\Delta\lambda_1+\Delta\lambda_2=l,\\ &\Delta\lambda_1-\Delta\lambda_2=\lambda_2-\lambda_1.\end{aligned} \tag{3.8}$$

Elimination of l and t from (3.6) above yields the equation of the surface:

$$(\mu+\nu+N)/(\nu_1+\lambda_1)=1. \tag{3.9}$$

This is the equation of a plane which cuts on the axes three equal segments of length $\nu_1+\lambda_1$. As l,t will be identified with the summation indices in (3.5), we shall consider the part of the plane determined by the conditions

$$\begin{aligned}&0\leq t\leq\nu_2+\lambda_2,\\ &|\lambda_1-\lambda_2|\leq l\leq\lambda_1+\lambda_2.\end{aligned}$$

The second of these conditions is the triangular relation for Gaunt coefficients. Using (3.6), we obtain

$$N = \begin{cases} \nu_2 + \lambda_2, & t = 0 \\ 0, & t = \nu_2 + \lambda_2 . \end{cases}$$

This represents two planes parallel to the μ, ν plane. Introducing $l = \lambda_1 + \lambda_2$ into (3.6), we obtain the equations of a straight line:

$$\mu + N = 0 ,$$

$$\nu = \nu_1 + \lambda_1 .$$

For the lower boundary of l two cases exist:

(i) For $\lambda_1 \geq \lambda_2$ the equations of the borderline are

$$\mu + N = \lambda_2 ,$$

$$\nu = \nu_1 + \lambda_1 - \lambda_2 .$$

(ii) For $\lambda_1 < \lambda_2$ the equations are

$$\mu + N = \nu_2 - \nu_1 + \lambda_1 ,$$

$$\nu = \nu_1 .$$

Thus, the set of functions $P_N^{(\mu,\nu)}(x)$ can be represented by a parallelogram lying in the plane parametrized by l, t. Of course, only the points representing integer l, t are interesting for us. The additional constraint $\lambda_1 + \lambda_2 + l =$ even is also taken into account, so that the three coordinates μ, ν, N always attain integer values. The whole situation is represented graphically on Fig. 2 and in what follows we shall make references to this picture.

Along the edge $t = \nu_2 + \lambda_2$ values of the functions are equal to unity, due to the formula

$$P_0^{(\mu,\nu)}(x) = 1 . \tag{3.10}$$

From the explicit expression for Jacobi polynomials (Ref. 13, Sec. 5.2.2, p. 211), follows the expression

$$P_N^{(-N,\nu)}(x) = \binom{\nu + N}{\nu} \left(\frac{x-1}{2}\right)^N , \tag{3.11}$$

or the recursion

$$P_{N+1}^{(-N-1,\nu)}(x) = \frac{\nu + N + 1}{N+1} \left(\frac{x-1}{2}\right) P_N^{(-N,\nu)}(x) . \tag{3.12}$$

Starting from the point $N = 0$, $\mu = 0$, $\nu = \nu_1 + \lambda_1$, the computation propagates to the left along the edge $l = \lambda_1 + \lambda_2$ using the above recursion.

Let us now consider a known contiguous relation for Jacobi polynomials (Ref. 13, Sec. 5.2.2, p. 213):

$$P_N^{(\mu,\nu-1)}(x) = P_N^{(\mu-1,\nu)}(x) + P_{N-1}^{(\mu,\nu)}(x) . \tag{3.13}$$

Obviously, the points connected by this relation always lie in a plane parallel to the one mentioned above. We see immediately that this relation can be used to generate the row of functions belonging

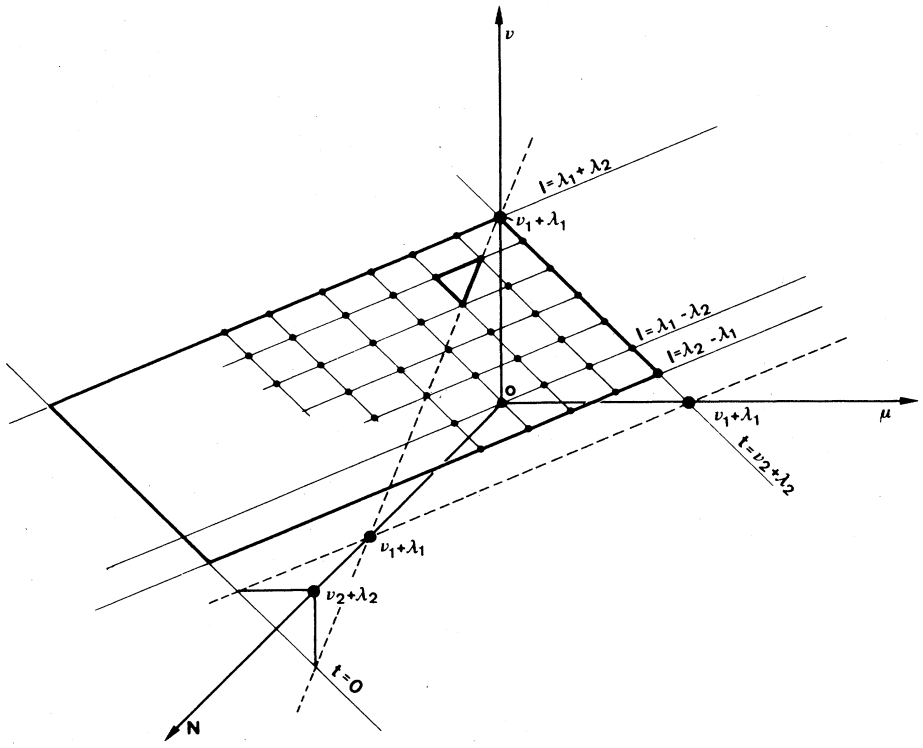

FIG. 2. Graphical representation of the procedure for evaluating Jacobi polynomials.

TABLE I. Values of Jacobi polynomials obtained according to relation (3.13).

$N_1=4 \quad L_1=2$
$N_2=3 \quad L_2=2$
$X=5.000\,000\times10^{-1}$

t	l	N	μ	ν	$P_N^{(\mu,\nu)}(x)$
0	0	5	−3	4	−0.123 046 875
0	2	5	−4	5	0.369 140 625
0	4	5	−5	6	−0.451 171 875
1	0	4	−2	4	$-0.546\,875\,000\times10^{-1}$
1	2	4	−3	5	−0.492 187 500
1	4	4	−4	6	0.820 312 500
2	0	3	−1	4	0.437 500 000
2	2	3	−2	5	0.437 500 000
2	4	3	−3	6	$-0.131\,250\,000\times10^{1}$
3	0	2	0	4	−0.750 000 000
3	2	2	−1	5	0.000 000 000
3	4	2	−2	6	$-0.175\,000\,000\times10^{1}$
4	0	1	1	4	0.250 000 000
4	2	1	0	5	−0.750 000 000
4	4	1	−1	6	$-0.175\,000\,000\times10^{1}$
5	0	0	2	4	$0.100\,000\,000\times10^{1}$
5	2	0	1	5	$0.100\,000\,000\times10^{1}$
5	4	0	0	6	$0.100\,000\,000\times10^{1}$

to $l-1$ if the functions belonging to l are known. That means that the whole parallelogram can be calculated.

We have used this procedure systematically for both double summations over P functions. According to our experience, it is numerically stable and economical. Propagation along the rows has been done simultaneously with the summations and no more than one row of the parallelogram should be kept in the machine memory.

A set of values of Jacobi polynomials obtained by this algorithm is shown in Table I. It has been stated by Filter and Steinborn[1] that the formula (3.5) breaks down for $\alpha=\beta$ and that instabilities occur for very close values of α and β. For these cases alternative formulas are given. Our observation is that (3.5), convenient as it is from analytical aspects, contains a serious numerical bottleneck. Namely, the two terms containing sums over t are in certain cases close in value and opposite in sign. This leads to the cancellation of decimal places during addition of these two terms. Generally speaking, matters become worse for higher quantum numbers and closer values of α and β.

TABLE II. α_{max} values beyond which expression (3.5) is no longer reliable for numerical computation. $0<\alpha\leq\alpha_{max}$; $\theta=45°$; $\phi=45°$.

R \ β	1	2	5	7	10
1	0.6	1	3	5	8
5	0.65	1.4	4	6	8.5
8	0.65	1.5	4	6	8.5

We have checked a relatively wide range of parameters for the numerical reliability of (3.5). N_1 has been varied from 1 to 15, N_2 from 1 to 6, L_1 and L_2 from zero to 5. Working with such high indices, we had in mind subsequent calculation of multipole integrals (see Sec. II). Check has been performed for several values of R, and Table II shows the results. For each β the α is given for which the procedure is still safe. For α nearer to β, a heavy loss of significant figures is encountered for N_1, N_2 greater or equal to 6. As θ, ϕ, M_1, and M_2 do not influence the phenomenon, they have been held constant ($\theta, \phi=45°$, $M_1, M_2=0$). A somewhat less exorbitant example of this numerical difficulty is given in Table III.

C. Case $\alpha\approx\beta$

In order to obtain a stable numerical procedure for the case of nearly equal scaling parameters, Steinborn and Filter have derived a formula (4.9 in Ref. 2) which expresses the overlap integral with different scaling parameters as an infinite series of integrals with equal parameters:

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,\vec{R})=(\alpha/\beta)^{2N_1+L_1-1}\sum_{p=0}^{\infty}\binom{p+N_1+L_1}{p}[1-(\alpha/\beta)^2]^p S^{N_2L_2M_2}_{N_1+p,L_1,M_1}(\beta,\beta,\vec{R}),\quad \beta\geq\alpha\,. \tag{3.14}$$

For the purposes of computation we have used the following working formula, obtained by combining (3.3) and (3.14):

$$\begin{aligned}S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,\vec{R})&=(\alpha/\beta)^{2N_1+L_1-1}(-1)^{L_2+M_1}(2\pi)^{1/2}(\beta^3 2^{N_1+N_2+L_1+L_2})^{-1}\\&\times e^{im\phi}\sum_{p=0}^{\infty}\binom{p+N_1+L_1}{p}\left[\frac{1-(\alpha/\beta)^2}{2}\right]^p\sum_l\langle lm\,|\,L_2M_2\,|\,L_1,-M_1\rangle\Phi_l^m(\cos\theta)\\&\times(\beta R)^l\sum_{t=0}^{\Delta l}(-1)^t\binom{\Delta l}{t}\hat{k}_{N_1+p+N_2+L_1+L_2-l-t+1/2}(\beta R)\\&\times 2^t[(N_1+p+N_2+L_1+L_2-t+1)!\,]^{-1}\,.\end{aligned} \tag{3.15}$$

Instead of $\hat{k}$, the κ function from (3.1) is used in actual computation.

Steinborn and Filter assert that the convergence of the above series is very good and that it could be used for computational purposes even for larger differences between scaling parameters. During our work on this subject, we have found that the series converges rather slowly and that its applicability is severely limited. In Table IV a number of examples is presented, which, in our opinion, illustrate the behavior of this series.

A way has been sought to circumvent this numerical difficulty. We have found that the use of a continued fraction instead of series can be advantageous. For all the underlying theory we refer to the monograph by Wall,[14] chiefly Chap. 11, Sec. 51. The details of the algorithm used are as follows:

(i) Consider the series $P=\sum_{i=0}^{\infty} c_i/z^{i+1}$, with the known coefficients c_i.

(ii) Consider also the fraction

$$J=\cfrac{a_0}{b_1+z-\cfrac{a_1}{b_2+z-\cdots}}.$$

The partial numerators and denominators (and therefrom the approximants) of this fraction are determined by the recursion scheme:

$$\delta_{00}=1, \quad c_0\delta_{00}=a_0, \quad c_1\delta_{00}=h_0, \quad b_1=-c_1/c_0,$$

$$(\delta_{i0}\delta_{i1}\delta_{i2}\cdots\delta_{ii})=(\delta_{i-1,0}\delta_{i-1,1}\cdots\delta_{i-1,i-1})\begin{pmatrix} 1 & b_i & & & & \\ & 1 & b_i & & 0 & \\ & & 1 & b_i & & \\ & & & \ddots & \ddots & \\ & & 0 & & \ddots & \ddots \\ & & & & & 1 \quad b_i \end{pmatrix}-a_i(00\delta_{i-2,0}\delta_{i-2,1}\cdots\delta_{i-2,i-2}),$$

$$(c_{2i}\cdots c_i)\begin{pmatrix}\delta_{i0}\\ \vdots \\ \delta_{ii}\end{pmatrix}=a_1a_2\cdots a_{i+1}=g_i, \quad a_{i+1}=g_i/g_{i-1},$$

$$(c_{2i+1}\cdots c_{i+1})\begin{pmatrix}\delta_{i0}\\ \vdots \\ \delta_{ii}\end{pmatrix}=h_i, \quad b_{i+1}=h_{i-1}/g_{i-1}-h_i/g_i. \tag{3.16}$$

Knowing the quantities a_{i+1}, b_{i+1} and using the fundamental recurrences of continued fractions

$$\begin{aligned} &A_{-1}=1, \quad B_{-1}=0, \\ &A_0=b_0, \quad B_0=1, \\ &A_{i+1}=b_{i+1}A_i+a_{i+1}A_{i-1}, \quad i=0,1,2,3,\ldots \\ &B_{i+1}=b_{i+1}B_i+a_{i+1}B_{i-1}. \end{aligned} \tag{3.17}$$

we can generate the numerators and denominators A, B of the fraction J. As we can see, the computation of the $(i+1)$st approximant A_{i+1}/B_{i+1} involves $2i+1$ terms of the series. It is shown in Ref. 14 that the expansion of the ith approximant in the inverse power series of z coincides with the series P up to at least the term $2i$.

Let us now cast the formula (3.15) in a different form. We introduce the notation:

TABLE III. Illustration of the cancellation of figures upon adding the two terms in expression (3.5).

	$N_1=6$	$L_1=5$	$M_1=4$
	$N_2=6$	$L_2=5$	$M_2=4$
	$\alpha=1$	$\beta=1.5$	
	$R=1$	$\theta=45°$	$\phi=45°$
l	First term		Second term
10	$-0.297\,581\,213\,339\,524\,565\times10^{14}$		$0.297\,581\,213\,339\,524\,645\times10^{14}$
8	$-0.333\,195\,493\,127\,629\,280\times10^{12}$		$0.333\,195\,493\,127\,629\,326\times10^{12}$
6	$-0.608\,855\,622\,486\,082\,444\times10^{10}$		$0.608\,855\,622\,486\,082\,562\times10^{10}$
4	$-0.213\,190\,058\,388\,730\,140\times10^{9}$		$0.213\,190\,058\,388\,730\,178\times10^{9}$
2	$-0.192\,906\,694\,455\,188\,834\times10^{8}$		$0.192\,906\,694\,455\,188\,883\times10^{8}$
0	$-0.822\,627\,070\,788\,225\,667\times10^{7}$		$0.822\,627\,070\,788\,215\,411\times10^{7}$
	$N_1=4$	$L_1=3$	$M_1=1$
	$N_2=5$	$L_2=3$	$M_2=2$
	$\alpha=2$	$\beta=3$	
	$R=2$	$\theta=45°$	$\phi=45°$
l	First term		Second term
6	$-0.341\,633\,755\,217\,602\,620\times10^{-5}$		$0.341\,633\,755\,222\,990\,786\times10^{-5}$
4	$-0.330\,460\,192\,977\,763\,193\times10^{-3}$		$0.330\,460\,192\,721\,257\,681\times10^{-3}$
2	$-0.569\,737\,713\,155\,768\,661\times10^{-1}$		$0.569\,737\,719\,425\,615\,567\times10^{-1}$

$$K=(\alpha/\beta)^{2N_1+L_1-1}(-1)^{L_2+M_1}e^{im\phi}(2\pi)^{1/2}(\beta^3 2^{N_1+N_2+L_1+L_2})^{-1},$$

$$d_p=\binom{p+N_1+L_1}{p}\sum_l\langle lm|L_2M_2|L_1,-M_1\rangle\Phi_l^m(\cos\theta)(\beta R)^l\sum_{t=0}^{\Delta l}(-1)^t\binom{\Delta l}{t}\cdot\hat{k}_{N_1+p+N_2+L_1+L_2-l-t+1/2}(\beta R)$$
$$\times 2^t[(N_1+p+N_2+L_1+L_2-t+1)!]^{-1}, \tag{3.18}$$

$$z=2/[1-(\alpha/\beta)^2],$$

and now (3.15) can be written as

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,\vec{R})=K\left(d_0+\sum_{i=0}^{\infty}\frac{d_{i+1}}{z^{i+1}}\right). \tag{3.19}$$

Identifying c_i with d_{i+1}, we can apply the above algorithm to the series in (3.19).

It turns out that, for a certain range of parameters, the ith approximant of the fraction represents much more than just $2i$ terms of the series. The iteration by the sequence of approximants has been checked for numerical applicability in the same range of parameters as formula (3.5). Generally, this procedure becomes unreliable for greater differences between α and β, and also for high quantum numbers. Again, Table V shows the range of α and β for which the algorithm is applicable. We should emphasize that the term "applicability" in this context means the meeting of rather strong requests (particularly for quantum numbers) and that for common use this procedure might work perfectly for much broader range of α and β. Also, the upper limit to the computation lies in the request that the upper index of binomial coefficients in (3.15) be smaller or equal 40. In Table VI, some sequences of approximants are given.

D. The limiting case $R = 0$

The explicit expression for one-center overlap with equal scaling parameters is given by formula 4.5 in Ref. 2:

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\alpha,0)=\frac{(2L_1+1)!!\,(2N_1+2N_2+2L_1-1)!!}{\alpha^3(2N_1+2N_2+4L_1+2)!!}\delta_{L_1L_2}\delta_{M_1M_2}. \tag{3.20}$$

This elementary expression is quite convenient for all computational purposes. We shall pay some more attention to the case of unequal scaling parameters, given by formula (4.10) in Ref. 2. This formula

TABLE IV. Partial sums over p in expression (3.15).

			p	Partial sums
$N_1=3$	$L_1=2$	$M_1=1$	2	−0.198 426 304 516 741 952
$N_2=4$	$L_2=2$	$M_2=1$	3	−0.280 008 447 445 203 520
$\alpha=1$	$\beta=1.05$		4	−0.300 056 999 440 924 850
$R=1$	$\theta=45°$	$\phi=45°$	5	−0.303 889 604 508 465 450
			6	−0.304 518 972 153 943 537
			7	−0.304 612 286 247 106 997
value of the integral:			8	−0.304 625 144 036 055 534
$0.228\,894\,558\,906\,585\,311\times10^{-3}$			9	−0.304 626 820 952 265 585
			10	−0.304 627 030 527 574 477
			11	−0.304 627 055 845 686 341
			12	−0.304 627 058 821 089 563
			13	−0.304 627 059 162 879 076
			14	−0.304 627 059 201 397 321
			15	−0.304 627 059 205 668 238
			16	−0.304 627 059 206 135 246
			17	−0.304 627 059 206 185 699
			18	−0.304 627 059 206 191 090
			19	−0.304 627 059 206 191 659
			20	−0.304 627 059 206 191 722
			21	−0.304 627 059 206 191 729
			22	−0.304 627 059 206 191 729
$N_1=6$	$L_1=5$	$M_1=3$	2	$0.660\,066\,700\,148\,410\,880\times10^{-1}$
$N_2=5$	$L_2=4$	$M_2=2$	3	0.109 412 994 119 820 335
$\alpha=1.05$	$\beta=1$		4	0.125 390 906 472 157 497
$R=1$	$\theta=45°$	$\phi=45°$	5	0.129 736 837 316 164 733
			6	0.130 711 220 084 705 013
value of the integral:			7	0.130 901 923 535 564 828
$-0.143\,397\,217\,931\,694\,917\times10^{-6}$			8	0.130 935 651 813 754 067
			9	0.130 941 166 394 105 218
			10	0.130 942 013 220 200 631
			11	0.130 942 136 769 832 760
			12	0.130 942 154 044 539 644
			13	0.130 942 156 374 760 355
			14	0.130 942 156 679 605 625
			15	0.130 942 156 718 446 018
			16	0.130 942 156 723 282 108
			17	0.130 942 156 723 872 219
			18	0.130 942 156 723 942 951
			19	0.130 942 156 723 951 295
			20	0.130 942 156 723 952 266
			21	0.130 942 156 723 952 377
			22	0.130 942 156 723 952 391

establishes an interesting connection between overlap integrals and the Gauss hypergeometric function:

$$S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\beta,0)=(\alpha/\beta)^{2N_1+L_1+2}S^{N_2L_2M_2}_{N_1L_1M_1}(\alpha,\alpha,0)$$

$$\times\,{}_2F_1(N_1+L_1+1,N_1+N_2+L_1+\tfrac{1}{2};N_1+N_2+2L_1+2;1-(\alpha/\beta)^2),\quad \beta\geq\alpha\,. \tag{3.21}$$

If we recall the one-center STO overlap formula

$$S=(2\zeta_1)^{N_1+1/2}(2\zeta_2)^{N_2+1/2}(N_1+N_2)!\,[(2N_1)!\,(2N_2)!\,]^{-1/2}(\zeta_1+\zeta_2)^{-N_1-N_2-1}\delta_{L_1L_2}\delta_{M_1M_2},$$

and consider the fact that STO and RBF can be represented as each others' linear combinations (see Sec. 1.1), it becomes obvious that the hypergeometric function in (3.21) represents a special case, expressible in a more elementary form.

However, let us first consider the numerical as aspects of (3.21). Let us use the notation

$$z=1-(\alpha/\beta)^2,$$

$$a=N_1+L_1+1,$$

TABLE V. α_{min} values on this side of which expression (3.19) is no longer safe for numerical purposes. $\alpha_{min} \leq \alpha < \beta$; $\theta = 45°$; $\phi = 45°$.

R \ β	1	2	5	7	10
1	0.9	1.8	4.6	6.4	9.2
5	0.92	1.85	4.7	6.7	9.5
10	0.93	1.9	4.75	6.75	

$$b = N_1 + N_2 + L_1 + \tfrac{1}{2},$$

$$c = N_1 + N_2 + 2L_1 + 2.$$

The following inequalities are easily verified

$$0 \leq z < 1,$$

$$2 \leq a < b < c,$$

a, c being integers; b, half integer. We restrict the domain of indices by $c \leq 30$ and seek for a procedure to evaluate the function

$$F(a, b; c; z).$$

We shall mention, without boring the reader with formulas and tables, that a number of methods has been tested numerically. They are as follows:

(i) Gauss series (directly or turned into a continued fraction);

(ii) recursion schemes (Ref. 12, formulas 15.2.10–15.2.27);

(iii) Chebyshev polynomial expansion and rational approximation.[15]

According to our experience, the most reliable method consists of numerical evaluation of the known integral representation for F (see, e.g., Ref. 12 or Ref. 16):

$$F(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 t^{a-1}(1-t)^{c-a-1} \times (1-tz)^{-b} dt. \tag{3.22}$$

As $c - a - b < 0$, the hypergeometric function will have a singularity at $z = 1$. In the close vicinity of $z = 1$, we use the formula (for the proof and comments see Appendix B):

$$S^{N_2 L_2 M_2}_{N_1 L_1 M_1}(\alpha, \beta, 0) = (-1)^{N_1} \alpha^{2N_1 + L_1 - 1} \beta^{2N_2 + 3L_1} (\beta^2 - \alpha^2)^{-N_1 - N_2 - 2L_1 - 1} \times \left[P^{(N_1 - 1/2,\, -N_1 - N_2 - 2L_1 - 1)}_{N_2 + L_1}\left(\frac{\beta^2 - 2\alpha^2}{\beta^2}\right) - \left(\frac{\beta}{\alpha}\right)^{2N_1 - 1} P^{(-N_1 + 1/2,\, -N_1 - N_2 - 2L_1 - 1)}_{N_1 + L_1}\left(\frac{\beta^2 - 2\alpha^2}{\beta^2}\right) \right]. \tag{3.23}$$

Here $P_N^{(\mu,\nu)}(x)$ are Jacobi polynomials, discussed in the Sec. III B. For the evaluation of individual Jacobi polynomials, the recurrence in N given in Ref. 13 (p. 213) is entirely satisfactory.

Formula (3.23) has the same disadvantages as (3.5): a cancellation occurs for z considerably smaller than unity, but in the neighborhood of $z = 1$, it is a very valuable numerical tool. Finally, the algorithm for one-center overlap is as follows:

$0 \leq z < 0.8$, Gauss-Legendre quadrature, 50 points

TABLE VI. Examples of sequences of successive approximants obtained in the continued fraction approach (3.19).

			Successive approximants
$N_1 = 3$	$L_1 = 2$	$M_1 = 1$	$0.793\,874\,463\,212\,941\,756 \times 10^{-1}$
$N_2 = 4$	$L_2 = 2$	$M_2 = 1$	$0.793\,874\,405\,821\,512\,557 \times 10^{-1}$
$\alpha = 1$	$\beta = 1.05$		$0.793\,874\,405\,847\,102\,643 \times 10^{-1}$
$R = 1$	$\theta = 45°$	$\phi = 45°$	$0.793\,874\,405\,847\,099\,888 \times 10^{-1}$
			$0.793\,874\,405\,847\,099\,867 \times 10^{-1}$
Value of the integral:			$0.793\,874\,405\,847\,099\,867 \times 10^{-1}$
$0.228\,894\,558\,906\,584\,777 \times 10^{-3}$			
$N_1 = 6$	$L_1 = 5$	$M_1 = 3$	$0.649\,355\,577\,366\,388\,984 \times 10^{-1}$
$N_2 = 5$	$L_2 = 4$	$M_2 = 2$	$0.649\,354\,866\,155\,016\,884 \times 10^{-1}$
$\alpha = 1.05$	$\beta = 1$		$0.649\,354\,867\,091\,729\,605 \times 10^{-1}$
$R = 1$	$\theta = 45°$	$\phi = 45°$	$0.649\,354\,867\,091\,112\,841 \times 10^{-1}$
			$0.649\,354\,867\,091\,113\,029 \times 10^{-1}$
Value of the integral:			$0.649\,344\,867\,091\,113\,029 \times 10^{-1}$
$-0.143\,397\,217\,931\,694\,914 \times 10^{-6}$			

$0.8 \leq z < 0.9$, Gauss-Legendre quadrature, 2×50 points

$0.9 \leq z < 0.95$, Gauss-Legendre quadrature, 4×50 points

$0.95 \leq z < 1$, formula (3.23).

E. Comments

Concluding this chapter, we would like to discuss generally the calculations performed. The reduced Bessel functions prove to be much more advantageous than STO's, at least with respect to the overlap integrals. Compactness of the convolution formulas renders the whole matter accessible for a numerical investigation. This is certainly not the case with STO's. Furthermore, special functions appearing in these formulas are well investigated, which makes improvements of the formulas possible and also simplifies the computation.

However, it should be pointed out that numerical difficulties mentioned above (Sec. III B and III C) restrict the use of convolution theorem quite seriously. As it can be seen from Tables II, III, IV, and VI ranges of parameters exist for which the given formulas do not provide a satisfactory numerical path. Since the overlap integrals appear as the building blocks in Coulomb as well as in multipole integrals, some further procedures for their evaluation must be sought.

ACKNOWLEDGMENTS

One of us (D.A.) is very much indebted to Professor J. M. André for the kind invitation and to the Facultés Universitaires de Namur for a fellowship.

APPENDIX A

Surface spherical harmonics used in this paper are defined as:

$$Y_l^m(\theta,\phi) = (2\pi)^{-1/2} \mathcal{P}_l^m(\cos\theta)\, e^{im\phi},$$

$$\mathcal{P}_l^m(\cos\theta) = (-1)^m \left(\frac{(2l+1)(l-m)!}{2(l+m)!}\right)^{1/2} \times P_l^m(\cos\theta). \quad \text{(A1)}$$

Here $\mathcal{P}_l^m(x)$ are the associated Legendre functions.[3] The above choice of phase is known as the Condon-Shortley phase. The functions $\mathcal{P}_l^m(x)$, appearing in the formulas in this paper are calculated by a recursion relation derived from the Bonnet recursion for the associated Legendre functions:

$$\mathcal{P}_{l+1}^m(x) = \left(\frac{2l+3}{(l-m+1)(l+m+1)}\right)^{1/2} \times \left[(2l+1)^{1/2} x\, \mathcal{P}_l^m(x) - \left(\frac{(l-m)(l+m)}{2l-1}\right)^{1/2} \mathcal{P}_{l-1}^m(x)\right]. \quad \text{(A2)}$$

The starting values are

$$\mathcal{P}_{m-1}^m(x) = 0,$$

$$\mathcal{P}_m^m(x) = (-1)^m \left(\frac{(2m+1)!!}{2(2m)!!}\right)^{1/2} (1-x^2)^{m/2}. \quad \text{(A3)}$$

The Gaunt coefficients are defined:

$$\langle LM | l_1 m_1 | l_2 m_2 \rangle = \int Y_L^M{}^*(\Omega)\, Y_{l_1}^{m_1}(\Omega)\, Y_{l_2}^{m_2}(\Omega)\, d\Omega. \quad \text{(A4)}$$

We shall mention a relation closely connected with Gaunt coefficients; this relation is used in the chapter on multipole integrals:

$$Y_{l_1}^{m_1}(\Omega)\, Y_{l_2}^{m_2}(\Omega) = \sum_L \langle LM | l_1 m_1 | l_2 m_2 \rangle\, Y_L^M(\Omega). \quad \text{(A5)}$$

A good account on the subject of Gaunt coefficients and spherical harmonics can be found in F. E. Harris's book.[4] We shall only mention that the individual coefficients have been calculated by the Racah formula, a procedure that proved to be sufficiently reliable for our purposes.

APPENDIX B

This appendix deals in some more detail with the hypergeometric function encountered in Sec. III D. First, a proof of formula (3.23) will be given. Consider the identity which holds for hypergeometric functions (Ref. 12, formula 15.3.6)

$$F(a,b;c;z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} F(a,b;a+b-c+1;1-z) + (1-z)^{c-a-b} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} F(c-a,c-b;c-a-b+1;1-z). \quad \text{(B1)}$$

To each function on the right-hand side of (B1) the following transformation is applied (Ref. 12, 15.3.3):

$$F(a,b;c;z)=(1-z)^{c-a-b}F(c-a,c-b;c;z). \tag{B2}$$

This yields

$$F(a,b;c;z)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\,z^{1-c}F(b-c+1,a-c+1;\,a+b-c+1;\,1-z)$$
$$+(1-z)^{c-a-b}\,\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\,z^{1-c}F(-b+1,-a+1;\,c-a-b+1;\,1-z). \tag{B3}$$

It should be noticed that both functions in (B3) represent polynomials, since $a-c+1$ and $-a+1$ always attain negative integer values. Let us now use the formula for Jacobi polynomials (Ref. 12, 15.4.6):

$$F(-n,\alpha+1+\beta+n;\,\alpha+1;\,x)=\frac{n!}{(\alpha+1)_n}\,P_n^{(\alpha,\beta)}(1-2x). \tag{B4}$$

Combination of (B3) and (B4) yields, after some elementary substitutions and rearrangements:

$$F(a,b;c;z)=\frac{(c-1)!\,\Gamma(c-a-b)\Gamma(a+b-c+1)}{\Gamma(c-b)\Gamma(b)\,z^{c-1}}$$
$$\times[P_{c-a-1}^{(a+b-c,\,-c+1)}(2z-1)-(1-z)^{c-a-b}\,P_{a-1}^{(c-a-b,\,-c+1)}(2z-1)]. \tag{B5}$$

The parameter b will attain half-integer values only. Substituting now (B5) into (3.21) and performing some straightforward rearrangements, we obtain the formula (3.23).

By systematic investigation of various forms of 24 Kummer's solutions and by the use of linear relations between them, fifteen more formulas of type (B5) can be obtained. We shall give the list without derivation. It follows similar lines as above, and for further details we refer to Ref. 16:

$$F(a,b;c;z)=\frac{(c-1)!\,\Gamma(a+b-c+1)\Gamma(c-a-b)}{\Gamma(c-b)\Gamma(b)z^{c-1}}$$
$$\times[P_{c-a-1}^{(a+b-c,\,-c+1)}(2z-1)-z^{a-1}(1-z)^{c-a-b}\,P_{a-1}^{(c-a-b,\,b-a)}\left(\frac{2-z}{z}\right) \tag{B6}$$

$$=\frac{(c-1)!\,\Gamma(a+b-c+1)\Gamma(c-a-b)}{\Gamma(c-b)\Gamma(b)z^{c-1}}$$
$$\times\left[z^{c-a-1}\,P_{c-a-1}^{(a+b-c,\,a-b)}\left(\frac{2-z}{z}\right)-(1-z)^{c-a-b}\,P_{a-1}^{(c-a-b,\,-c+1)}(2z-1)\right] \tag{B7}$$

$$=\frac{(c-1)!\,\Gamma(a+b-c+1)\Gamma(c-a-b)}{\Gamma(c-b)\Gamma(b)z^{c-1}}\cdot$$
$$\times\left[z^{c-a-1}\,P_{c-a-1}^{(a+b-c,\,a-b)}\left(\frac{2-z}{z}\right)-z^{a-1}(1-z)^{c-a-b}\,P_{a-1}^{(c-a-b,\,b-a)}\left(\frac{2-z}{z}\right)\right] \tag{B8}$$

$$=\frac{(c-1)!\,\Gamma(a-b+1)\Gamma(b-a)}{\Gamma(c-b)\Gamma(b)z^{c-1}}\,(-1)^a$$
$$\times\left[z^{c-a-1}\,P_{c-a-1}^{(a-b,\,a+b-c)}\left(\frac{z-2}{z}\right)-(-1)^c\,z^{a-1}(1-z)^{c-a-b}\,P_{a-1}^{(b-a,\,c-a-b)}\left(\frac{z-2}{z}\right)\right] \tag{B9}$$

$$=\frac{(c-1)!\,\Gamma(a-b+1)\Gamma(b-a)}{\Gamma(c-b)\Gamma(b)z^{c-1}}$$
$$\times\left[(-1)^a\,z^{c-a-1}\,P_{c-a-1}^{(a-b,\,a+b-c)}\left(\frac{z-2}{z}\right)+(-1)^c(1-z)^{c-b-1}\,P_{a-1}^{(b-a,\,-c+1)}\left(\frac{z+1}{z-1}\right)\right] \tag{B10}$$

$$=\frac{(c-1)!\,\Gamma(a-b+1)\Gamma(b-a)}{\Gamma(b)z^{c-1}}\,(-1)^{c-1}(1-z)^{c-a-1}$$
$$\times\left[\frac{1}{\Gamma(-b)}\,P_{c-a-1}^{(a-b,\,-c+1)}\left(\frac{z+1}{z-1}\right)+(-1)^a\,z^{a-1}\,\frac{(1-z)^{1-b}}{\Gamma(c-b)}\,P_{a-1}^{(b-a,\,c-a-b)}\left(\frac{z-2}{z}\right)\right] \tag{B11}$$

$$= \frac{(c-1)!\,\Gamma(a-b+1)\Gamma(b-a)}{\Gamma(b)z^{c-1}}(-1)^{c-1}(1-z)^{c-a-1}$$

$$\times\left[\frac{1}{\Gamma(-b)}P_{c-a-1}^{(a-b,-c+1)}\left(\frac{z+1}{z-1}\right)-(1-z)^{a-b}\frac{1}{\Gamma(c-b)}P_{a-1}^{(b-a,-c+1)}\left(\frac{z+1}{z-1}\right)\right] \tag{B12}$$

$$= \frac{(c-1)!\,\Gamma(1-b)}{\Gamma(c-b)z^{c-1}}$$

$$\times\left[z^{c-a-1}P_{c-a-1}^{(a-b,a+b-c)}\left(\frac{z-2}{z}\right)+(-1)^{c-a}(1-z)^{c-a-b}P_{a-1}^{(c-a-b,-c+1)}(2z-1)\right] \tag{B13}$$

$$= \frac{(c-1)!\,\Gamma(1-b)}{\Gamma(c-b)z^{c-1}}$$

$$\times\left[z^{c-a-1}P_{c-a-1}^{(a-b,a+b-c)}\left(\frac{z-2}{z}\right)+(-1)^{c-a}z^{a-1}(1-z)^{c-a-b}P_{a-1}^{(c-a-b,b-a)}\left(\frac{2-z}{z}\right)\right] \tag{B14}$$

$$= \frac{(c-1)!\,\Gamma(1-b)}{z^{c-1}}(1-z)^{c-a-1}(-1)^{c+a+1}$$

$$\times\left[\frac{1}{\Gamma(-b)}P_{c-a-1}^{(a-b,-c+1)}\left(\frac{z+1}{z-1}\right)-\frac{(1-z)^{1-b}}{\Gamma(c-b)}P_{a-1}^{(c-a-b,-c+1)}(2z-1)\right] \tag{B15}$$

$$= \frac{(c-1)!\,\Gamma(1-b)}{z^{c-1}}(-1)^{c+a+1}(1-z)^{c-a-1}$$

$$\times\left[\frac{1}{\Gamma(-b)}P_{c-a-1}^{(a-b,-c+1)}\left(\frac{z+1}{z-1}\right)-z^{a-1}\frac{(1-z)^{1-b}}{\Gamma(c-b)}P_{a-1}^{(c-a-b,b-a)}\left(\frac{2-z}{z}\right)\right] \tag{B16}$$

$$= \frac{(c-1)!\,\Gamma(b-c+1)}{\Gamma(b)z^{c-1}}$$

$$\times\left[(-1)^{a}P_{c-a-1}^{(a+b-c,-c+1)}(2z-1)+z^{a-1}(1-z)^{c-a-b}P_{a-1}^{(b-a,c-a-b)}\left(\frac{z-2}{z}\right)\right] \tag{B17}$$

$$= (-1)^{a}\frac{(c-1)!\,\Gamma(b-c+1)}{\Gamma(b)z^{c-1}}$$

$$\times\left[P_{c-a-1}^{(a+b-c,-c+1)}(2z-1)-(1-z)^{c-b-1}P_{a-1}^{(b-a,-c+1)}\left(\frac{z+1}{z-1}\right)\right] \tag{B18}$$

$$= \frac{(c-1)!\,\Gamma(b-c+1)}{\Gamma(b)z^{c-1}}$$

$$\times\left[(-1)^{a}z^{c-a-1}P_{c-a-1}^{(a+b-c,a-b)}\left(\frac{2-z}{z}\right)+z^{a-1}(1-z)^{c-a-b}P_{a-1}^{(b-a,c-a-b)}\left(\frac{z-2}{z}\right)\right] \tag{B19}$$

$$= (-1)^{a}\frac{(c-1)!\,\Gamma(b-c+1)}{\Gamma(b)z^{c-1}}$$

$$\times\left[z^{c-a-1}P_{c-a-1}^{(a+b-c,a-b)}\left(\frac{2-z}{z}\right)-(1-z)^{c-b-1}P_{a-1}^{(b-a,-c+1}\left(\frac{z+1}{z-1}\right)\right]. \tag{B20}$$

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*Present address: Chemistry Department, The Johns Hopkins University, Baltimore, Maryland 21218.

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