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Derivatives of any order of the Gaussian hypergeometric function ${}_2F_1(a, b, c; z)$ with respect to the parameters a, b and c

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Abstract

The derivatives to any order of the Gaussian hypergeometric function ${}_2F_1\,(a, b, c; z)$ with respect to the parameters a, b and c are expressed in terms of generalizations of multivariable Kampé de Fériet functions. Several properties are presented. In an application to the two-body Coulomb scattering problem, the usefulness of these derivatives is illustrated with the study of the charge dependence of Pollaczek-*like* polynomials.

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1. Introduction

The Gaussian hypergeometric function ${}_2F_1\,(a, b, c; z)$ has been studied extensively from its mathematical point of view [1]. This is probably, in part, due to its many applications on a large variety of physical and mathematical problems. In quantum mechanics, the solution of the Schrödinger equation for some systems is expressed in terms of ${}_2F_1$ functions, as for example when solving the Pöschl-Teller, Wood-Saxon or Hulthén potentials [2]. Another very important case is related to the angular momentum theory, since the eigenfunctions of the angular momentum operators are written in terms of ${}_2F_1$ functions [3]. These eigenfunctions depend parametrically on the angular momentum quantum number l, and its analytical extension to the complex plane of l is often necessary [4–7]. Generally, the physical parameters (like l or the magnitude of the mentioned potentials) appear in one or several of the mathematical parameters a, b or c. The dependence on the physical parameters is therefore related to the study of the solutions as a function of a, b or c, rather than z. One important tool is then provided by the derivatives of the ${}_2F_1$ function with respect to these parameters since they allow us, for example, to write a Taylor expansion around given values a_0, b_0 or c_0.

While the nth derivative with respect to the variable z has been expressed in a compact form [1, 3], the same cannot be stated for the derivatives with respect to the parameters a, b or c. Expressions for the first derivative with respect to a parameter have been presented but only for some special values of the parameters (see Brychkov's very recent handbook [8] and references therein). The formulations are relatively complicated and cannot be easily generalized to derivatives of higher order. The main aim of this paper is to obtain compact forms for the derivatives with respect to the parameters for the Gaussian hypergeometric function ${}_2F_1\,(a, b, c; z)$ with any a, b, c, not only for the first but also for the nth derivative. The method employed uses the second-order linear differential equation satisfied by the hypergeometric function, and is similar to that presented in a recent publication [9] in which the derivatives with respect to the parameters a and b of the confluent hypergeometric function ${}_1F_1\,(a, b; z)$ were investigated.

To illustrate the usefulness of the mathematical formulation in a physical situation, we have considered the two-body Coulomb scattering wavefunction in spherical coordinates. A charge Sturmian L^2 representation leads to a family of Pollaczek-*like* orthogonal polynomials directly related to Gaussian hypergeometric functions [10–12]. For this application, the physical variable is the charge and appears in the first parameter of ${}_2F_1$. The explicit expression of these polynomials, as well as many of their properties, require the derivatives of a ${}_2F_1$ function with respect to the first parameter.

2. nth derivatives of the ${}_2F_1$ hypergeometric functions with respect to the parameters

Consider the Gaussian hypergeometric function

$$F = {}_2F_1\,(a, b, c; z) = \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n}\frac{z^n}{n!}, \tag{1}$$

where the Pochhammer symbol $(\gamma)_n = \Gamma(\gamma+n)/\Gamma(\gamma)$ is defined in terms of the Gamma function [1]. In what follows, we shall use the following notation for the nth derivatives with respect to the parameters a, b or c:

$$G_a^{(n)} = \frac{\mathrm{d}^n F}{\mathrm{d}a^n}, \qquad G_b^{(n)} = \frac{\mathrm{d}^n F}{\mathrm{d}b^n}, \tag{2a}$$

$$H_c^{(n)} = \frac{\mathrm{d}^n F}{\mathrm{d}c^n}. \tag{2b}$$

As a and b play a similar role, we shall study only the nth derivatives with respect to a and c (those with respect to b may then be obtained by interchanging a and b).

Let us start with the first derivatives. Using the derivative of the Pochhammer symbol [3], $\frac{\mathrm{d}(\gamma)_n}{\mathrm{d}\gamma} = (\gamma)_n[\Psi(\gamma+n) - \Psi(\gamma)]$, we find for $G_a^{(1)}$

$$G_a^{(1)} = \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n}[\Psi(a+n) - \Psi(a)]\frac{z^n}{n!}. \tag{3}$$

We have therefore an infinite series containing the Digamma function $\Psi\,(z)$ [3]. An alternative formulation is obtained by using the recurrence formula (6.3.6) of [3]

$$G_a^{(1)} = \sum_{n=0}^{\infty} \frac{(a)_{n+1}\,(b)_{n+1}}{(c)_{n+1}}\frac{z^{n+1}}{(n+1)!}\sum_{s=0}^{n}\frac{1}{s+a}. \tag{4}$$

Similar equations can be derived for $H_c^{(1)}$.

It is clear that the generalization to the nth derivative, in either formulation, is particularly cumbersome. To circumvent this difficulty we may consider the approach followed in [9], which uses

$$\frac{1}{(s+a_i)} = \frac{1}{a_i}\frac{(a_i)_s}{(a_i+1)_s}, \tag{5}$$

and the rearrangement series technique (see, for example, chapter 2 of [13])

$$\sum_{n=0}^{\infty}\sum_{k=0}^{n} B(k,n) = \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} B(k,n+k). \tag{6}$$

With simple algebraic manipulations one finds, for example in the case of $G_a^{(1)}$,

$$G_a^{(1)} = \frac{z}{a}\frac{ab}{c}\sum_{n=0}^{\infty}\sum_{s=0}^{\infty}\frac{(1)_n(1)_s\,(a)_s}{(2)_{n+s}\,(a+1)_s}\frac{(a+1)_{n+s}\,(b+1)_{n+s}}{(c+1)_{n+s}}\frac{z^{n+s}}{s!n!}. \tag{7}$$

This double series can be related to the following hypergeometric function in two variables:

$$\begin{aligned}&{}_2\Theta_1^{(1)}\left(\begin{matrix}a_1,a_2|\,b_1,b_2,b_3\\ c_1|\,d_1,d_2\end{matrix}\right|;x_1,x_2\Bigg)\\ &\quad=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\frac{(a_1)_{m_1}\,(a_2)_{m_2}\,(b_1)_{m_1}}{(c_1)_{m_1}}\frac{(b_2)_{m_1+m_2}\,(b_3)_{m_1+m_2}}{(d_1)_{m_1+m_2}\,(d_2)_{m_1+m_2}}\frac{x_1^{m_1}x_2^{m_2}}{m_1!m_2!},\end{aligned} \tag{8}$$

which, as we shall see, is a Kampé de Fériet-like function [14]. In terms of ${}_2\Theta_1^{(1)}$, the first derivatives read

$$G_a^{(1)} = \frac{d_2F_1}{da} = \frac{z}{a}\frac{ab}{c}\,{}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,a,a+1,b+1\\ a+1|\,2,c+1\end{matrix}\right|;z,z\Bigg) \tag{9a}$$

$$H_c^{(1)} = \frac{d_2F_1}{dc} = -\frac{z}{c}\frac{ab}{c}\,{}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,c,a+1,b+1\\ c+1|\,2,c+1\end{matrix}\right|;z,z\Bigg). \tag{9b}$$

The expression for $G_b^{(1)}$ is obtained directly by interchanging a with b in (9a).

The generalization to the nth derivatives can be obtained in a similar way, but we found that it is more convenient, as shown below, to use the second-order linear differential equation satisfied by the hypergeometric function, i.e.,

$$\left[z(1-z)\frac{\mathrm{d}^2}{\mathrm{d}z^2} + (c-(a+b+1)z)\frac{\mathrm{d}}{\mathrm{d}z} - ab\right]F = 0, \tag{10}$$

where $F = {}_2F_1(a,b,c;z)$ is an analytical function of $z \in \mathbb{C} - \{0,1,\infty\}$, and a, b, c can be real or complex parameters. Since F is an analytical function of the variable z and of the parameters a, b, c, we may take the derivative of (10) with respect to the parameters

$$\left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2} + (c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z} - ab\right]G_a^{(1)} = z\frac{\mathrm{d}F}{\mathrm{d}z} + bF \tag{11a}$$

$$\left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2} + (c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z} - ab\right]H_c^{(1)} = -\frac{\mathrm{d}F}{\mathrm{d}z}. \tag{11b}$$

Using the derivative with respect to z, $\frac{\mathrm{d}F}{\mathrm{d}z} = \frac{ab}{c}\,{}_2F_1(a+1,b+1,c+1;z)$, and several contiguous relations for F, it can be easily shown that

$$z\frac{\mathrm{d}F}{\mathrm{d}z} + bF = b\;{}_2F_1(a,b+1,c;z)$$

so that the right-hand sides of the differential equations (11*a*) and (11*b*) are power series of z. We may therefore use the solution of the following non-homogeneous differential equation (equation (6.184) of Babister [15])

$$\left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z}-ab\right]y=z^{m_1} \tag{12}$$

given by equation (6.185) [15]

$$\begin{aligned} y=\theta_{m_1+1}&=\frac{z^{m_1+1}}{(m_1+1)\,(m_1+c)}\;{}_3F_2\,(1,m_1+a+1,m_1+b+1;m_1+2,m_1+c+1;z)\\ &=\frac{(1)_{m_1}}{(2)_{m_1}}\frac{(c)_{m_1}}{(c+1)_{m_1}\,(c)_1}z^{m_1+1}\;{}_3F_2\,(1,m_1+a+1,m_1+b+1;m_1+2,m_1+c+1;z)\,, \end{aligned} \tag{13}$$

where the series converges for $|z|<1$, and for $|z|=1$ as long as $\mathrm{Re}(c-a-b)>0$. Since the differential equations (11*a*) and (11*b*) are linear, the solutions for $G_a^{(1)}$ and $H_c^{(1)}$ can be easily found. For example, for $G_a^{(1)}$, we have

$$\begin{aligned} G_a^{(1)}&=b\sum_{m_1=0}^{\infty}\frac{(a)_{m_1}\,(b+1)_{m_1}}{(c)_{m_1}}\frac{\theta_{m_1+1}}{m_1!}\\ &=\frac{b}{c}z\sum_{m_1=0}^{\infty}\frac{(a)_{m_1}\,(b+1)_{m_1}}{(c+1)_{m_1}}\frac{(1)_{m_1}}{(2)_{m_1}}\frac{z^{m_1}}{m_1!}\\ &\quad\times\,{}_3F_2\,(1,m_1+a+1,m_1+b+1;m_1+2,m_1+c+1;z)\,. \end{aligned} \tag{14}$$

Replacing ${}_3F_2$ by its power series definition we find

$$\begin{aligned} G_a^{(1)}&=\frac{b}{c}z\sum_{m_1=0}^{\infty}\frac{(a)_{m_1}\,(b+1)_{m_1}}{(c+1)_{m_1}}\frac{(1)_{m_1}}{(2)_{m_1}}\frac{z^{m_1}}{m_1!}\\ &\quad\times\sum_{m_2=0}^{\infty}\frac{(1)_{m_2}\,(a+1+m_1)_{m_2}\,(b+1+m_1)_{m_2}}{(2+m_1)_{m_2}\,(c+1+m_1)_{m_2}}\frac{z^{m_2}}{m_2!}. \end{aligned} \tag{15}$$

Using the identity $(\gamma)_{m+n}=(\gamma)_m\,(\gamma+m)_n$ and simplifying, we find for $G_a^{(1)}$ the result given by equation (7). The procedure is similar for $H_c^{(1)}$, resulting finally in the compact form given by (9*b*).

Let us now turn to the derivatives of order n, starting from the second derivative. Differentiating equations (11*a*) and (11*b*) with respect to a or c, respectively, we find the following differential equations for $G_a^{(2)}$ and $H_c^{(2)}$:

$$\begin{aligned} \left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z}-ab\right]G_a^{(2)}&=2\left(z\frac{\mathrm{d}G_a^{(1)}}{\mathrm{d}z}+bG_a^{(1)}\right)\\ &=2bG_a^{(1)}(a,b+1,c;z), \end{aligned} \tag{16a}$$

$$\left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z}-ab\right]H_c^{(2)}=-2\frac{\mathrm{d}H_c^{(1)}}{\mathrm{d}z}. \tag{16b}$$

The generalization to order n is straightforward

$$\begin{aligned} \left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z}-ab\right]G_a^{(n)}&=n\left(z\frac{\mathrm{d}G_a^{(n-1)}}{\mathrm{d}z}+bG_a^{(n-1)}\right)\\ &=nbG_a^{(n-1)}(a,b+1,c;z), \end{aligned} \tag{17a}$$

$$\left[z\,(1-z)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2}+(c-(a+b+1)\,z)\,\frac{\mathrm{d}}{\mathrm{d}z}-ab\right]H_c^{(n)}=-n\frac{\mathrm{d}H_c^{(n-1)}}{\mathrm{d}z}. \qquad (17b)$$

Since the right-hand sides of these differential equations are again power series in z, we may proceed as done for the first derivatives. For example, for $G_a^{(2)}$ we find

$$G_a^{(2)}=\frac{(b)_2}{(c)_2}z^2\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\sum_{m_3=0}^{\infty}(1)_{m_1}\,(1)_{m_2}\,(1)_{m_3}\,\frac{(a)_{m_1}\,(a+1)_{m_1+m_2}\,(a+2)_{m_1+m_2+m_3}}{(a+1)_{m_1}}$$
$$\times\frac{(b+2)_{m_1+m_2+m_3}}{(a+2)_{m_1+m_2}\,(3)_{m_1+m_2+m_3}\,(c+2)_{m_1+m_2+m_3}}\,\frac{z^{m_1+m_2+m_3}}{m_1!m_2!m_3!}. \qquad (18)$$

Similarly to the case of the first derivatives, it is convenient to introduce a hypergeometric in $n+1$ variables

$$_2\Theta_1^{(n)}\left(\begin{matrix}a_1,a_2,\ldots,a_{n+1}\,|\,b_1,b_2,\ldots,b_{n+2}\\ c_1,\ldots,c_n\,|\,d_1,d_2\end{matrix}\;\middle|\;;x_1,\ldots,x_{n+1}\right)$$
$$=\sum_{m_1=0}^{\infty}\cdots\sum_{m_{n+1}=0}^{\infty}(a_1)_{m_1}\,(a_2)_{m_2}\cdots(a_{n+1})_{m_{n+1}}\,\frac{(b_1)_{m_1}\,(b_2)_{m_1+m_2}\ldots(b_{n+1})_{m_1+m_2+\cdots+m_{n+1}}}{(c_1)_{m_1}\,(c_2)_{m_1+m_2}\cdots(c_n)_{m_1+m_2+\cdots+m_n}}$$
$$\times\frac{(b_{n+2})_{m_1+m_2+\cdots+m_{n+1}}}{(d_1)_{m_1+m_2+\cdots+m_{n+1}}\,(d_2)_{m_1+m_2+\cdots+m_{n+1}}}\,\frac{x_1^{m_1}x_2^{m_2}\cdots x_{n+1}^{m_{n+1}}}{m_1!m_2!\cdots m_{n+1}!}. \qquad (19)$$

In terms of these new functions the nth derivatives read

$$G_a^{(n)}=\frac{(b)_n}{(c)_n}z^n\;{}_2\Theta_1^{(n)}\left(\begin{matrix}1,1,\ldots,1\,|\,a,a+1,\ldots,a+n,b+n\\ a+1,\ldots,a+n\,|\,n+1,c+n\end{matrix}\;\middle|\;;z,\ldots,z\right) \qquad (20a)$$

$$H_c^{(n)}=(-1)^n\,\frac{n!}{c^n}\frac{ab}{c}z{}_2\Theta_1^{(n)}\left(\begin{matrix}1,1,\ldots,1\,|\,c,c,\ldots,c,a+1,b+1\\ c+1,\ldots,c+1\,|\,2,c+1\end{matrix}\;\middle|\;;z,\ldots,z\right). \qquad (20b)$$

3. Properties of the function ${}_2\Theta_1^{(1)}$

3.1. Connection with multivariable hypergeometric functions

The function ${}_2\Theta_1^{(1)}$, defined by equation (19), results from the application of the rule used by Appell and Kampé de Fériet [14] to the product of the generalized confluent hypergeometric functions ${}_4F_3$ and ${}_3F_2$

$${}_4F_3\left(\begin{matrix}a_1,a_2,a_3,a_4\\ c_1,c_2,c_3\end{matrix}\;\middle|\;;x_1\right)\times\,{}_3F_2\left(\begin{matrix}b_1,b_2,b_3\\ d_1,d_2\end{matrix}\;\middle|\;;x_2\right)$$
$$=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\frac{(a_1)_{m_1}\,(a_2)_{m_1}\,(a_3)_{m_1}\,(a_4)_{m_1}}{(c_1)_{m_1}\,(c_2)_{m_1}\,(c_3)_{m_1}}\,\frac{(b_1)_{m_2}\,(b_2)_{m_2}\,(b_3)_{m_2}}{(d_1)_{m_2}\,(d_2)_{m_2}}\,\frac{x_1^{m_1}}{m_1!}\,\frac{x_2^{m_2}}{m_2!}.$$

Indeed, replacing the pairs of products as

$$(a_3)_{m_1}\,(b_2)_{m_2}\rightarrow(b_2)_{m_1+m_2}$$
$$(a_4)_{m_1}\,(b_3)_{m_2}\rightarrow(b_3)_{m_1+m_2}$$
$$(c_2)_{m_1}\,(d_1)_{m_2}\rightarrow(d_1)_{m_1+m_2}$$
$$(c_3)_{m_1}\,(d_2)_{m_2}\rightarrow(d_2)_{m_1+m_2}$$

we obtain the expression

$$\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}(a_1)_{m_1}(b_1)_{m_2}\frac{(a_2)_{m_1}}{(c_1)_{m_1}}\frac{(b_2)_{m_1+m_2}}{(d_1)_{m_1+m_2}}\frac{(b_3)_{m_1+m_2}}{(d_2)_{m_1+m_2}}\frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}.$$

The fact that ${}_2\Theta_1^{(1)}$ is generated by the product of two hypergeometric ${}_pF_q$ functions with $p = q + 1$ [13] which converge absolutely in the unit disc, ensures that the ${}_2\Theta_1^{(1)}$ function converges in the same region. Similarly, we may apply Appell's method to ${}_2\Theta_1^{(2)}$, through the product of ${}_5F_4$, ${}_4F_3$ and ${}_3F_2$. Generalizing this procedure by using the product ${}_{n+3}F_{n+2}, {}_{n+2}F_{n+1}, \ldots, {}_4F_3$ and ${}_3F_2$ we get the expression for ${}_2\Theta_1^{(n)}$ given by (19), which are Kampé de Fériet functions in $n + 1$ variables.

3.2. Recurrence relations

Starting from the recurrence relations for the confluent hypergeometric function F, recurrence relations for the ${}_2\Theta_1^{(1)}$ function can be easily deduced. For example, consider the contiguous relation (15.2.20) of [3]

$$c\,(1-z)\;{}_2F_1(a,b,c;z) - c\;{}_2F_1(a-1,b,c;z) + (c-b)z\;{}_2F_1(a,b,c+1;z) = 0.$$

Derivating n times with respect to a, we get the following relation:

$$c\,(1-z)\,G_a^{(n)}(a,b,c;z) - cG_a^{(n)}(a-1,b,c;z) + (c-b)zG_a^{(n)}(a,b,c+1;z) = 0.$$

The replacement of $G_a^{(n)}$ by ${}_2\Theta_1^{(n)}$ through equation (20a), provides a recurrence relation between ${}_2\Theta_1^{(n)}$ functions. In the $n = 1$ case, for example,

$$(1-z)\;{}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,a,a+1,b+1\\ a+1|\,2,c+1\end{matrix}\;\middle|\;;z,z\right) - {}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,a-1,a,b+1\\ a|\,2,c+1\end{matrix}\;\middle|\;;z,z\right)$$
$$+z\frac{c-b}{c+1}\;{}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,a,a+1,b+1\\ a+1|\,2,c+2\end{matrix}\;\middle|\;;z,z\right) = 0. \qquad (21)$$

3.3. Special values $a = 0$ or $b = 0$

It is easy to see, from the series definition (19), that for the special values $a = 0$ (and similarly for $b = 0$), the ${}_2\Theta_1^{(n)}$ function which appears for the nth derivative $G_a^{(n)}$ (equation (20a)) reduces to a ${}_2\Theta_1^{(n-1)}$ function.

Another special case arises when either a or b is a negative integer $-p$, since the Gaussian function reduces then to a polynomial of degree p. As a consequence, in the nth derivatives, one of the $n+1$ infinite series terminates. An important case corresponds to Jacobi polynomials [16].

3.4. Series representation in terms of one variable hypergeometric functions

From definition (8) of the ${}_2\Theta_1^{(1)}$ function, we provide the following series representations:

$${}_2\Theta_1^{(1)}\left(\begin{matrix}a_1,a_2|\,b_1,b_2,b_3\\ c_1|\,d_1,d_2\end{matrix}\;\middle|\;;x_1,x_2\right) = \sum_{m_1=0}^{\infty}\frac{(a_1)_{m_1}(b_1)_{m_1}(b_2)_{m_1}(b_3)_{m_1}}{(c_1)_{m_1}(d_1)_{m_1}(d_2)_{m_1}}\frac{x_1^{m_1}}{m_1!}$$
$$\times\;{}_3F_2\,(a_2, b_2+m_1, b_3+m_1; d_1+m_1, d_2+m_1; x_2) \qquad (22)$$
$$= \sum_{m_2=0}^{\infty}\frac{(a_2)_{m_2}(b_2)_{m_2}(b_3)_{m_2}}{(d_1)_{m_2}(d_2)_{m_2}}\frac{x_2^{m_2}}{m_2!}\;{}_4F_3\,(a_1, b_1, b_2+m_2, b_3+m_3; c_1, d_1+m_2, d_2+m_2; x_1)\,. \qquad (23)$$

Similar representations can be easily written for the more general ${}_2\Theta_1^{(n)}$ hypergeometric functions.

4. Application: Pollaczek-*like* polynomials

The two-body Coulomb problem is of fundamental importance in atomic physics, not only because it is one of the few problems that can be solved in closed form, but also for its application to the many-body problems. Very important methods to deal with collisional reactions use L^2 representations of the continuum Coulomb wavefunction. An example of that is the *J*-matrix method where a Sturmian representation of the Coulomb function is used [10]. In this section, we establish the connection between this representation and the derivatives of the Gaussian function studied in the previous sections.

Consider the two-body Coulomb problem, corresponding to a potential Z/r, a reduced mass μ and an energy $E = k^2/(2\mu)$. In spherical coordinates (r, θ, ϕ), the solution reads [17]

$$\Psi(\mathbf{r}) = R_{l,k}(r)\, Y_l^m(\theta, \phi),$$

where $R_{l,k}(r)$ and $Y_l^m(\theta, \phi)$ represent, respectively, the radial and angular parts of the wavefunction. The angular part is represented by the spherical harmonics $Y_l^m(\theta, \phi)$ and depend on the angular quantum numbers l and m. Defining the Sommerfeld parameter $\alpha = \frac{Z\mu}{\sqrt{2E}}$, the radial part is given in terms of the Kummer hypergeometric function

$$R_{l,k}(r) = N_{l,k}\,(2kr)^l\, \mathrm{e}^{\mathrm{i}kr}\, {}_1F_1(l + 1 - \mathrm{i}\alpha, 2l + 2, -2\mathrm{i}kr), \tag{24}$$

with the normalization constant

$$N_{l,k} = \left(\frac{2}{\pi k}\right)^{1/2} \frac{|\Gamma(l + 1 - \mathrm{i}\alpha)|}{\Gamma(2l + 2)} \mathrm{e}^{\pi\alpha/2}. \tag{25}$$

The L^2 representation used by the *J*-matrix method is obtained by projecting the functions $R_{l,k}(r)$ in terms of *Laguerre-type* Coulomb–Sturmian functions

$$\phi_{l,n}(r) = (\lambda r)^l\, \mathrm{e}^{-\lambda r/2} L_n^{2l+1}(\lambda r), \tag{26}$$

which depend on a parameter λ that can be either real or complex. In the following expansion [11, 18],

$$R_{l,k} = N_{l,k} \sum_{n=0}^{\infty} \frac{n!}{\Gamma(n + 2l + 2)} p_n^{l+1}(x, \alpha)\phi_{l,n}(r) \tag{27}$$

the coefficients $p_n^{l+1}(x, \alpha)$ can be expressed in terms of Gaussian hypergeometric functions for any real or complex value of the energy E. In particular, for positive energies E, they read

$$p_n^{l+1}(x, \alpha) = \frac{\Gamma(n + 2l + 2)}{n!\,\Gamma(2l + 2)} \mathrm{e}^{\mathrm{i}n\theta}\, {}_2F_1(l + 1 - \mathrm{i}\alpha, -n, 2l + 2; z), \tag{28}$$

where $x = \cos\theta = \frac{E-\lambda^2/2\mu}{E+\lambda^2/2\mu}$ and $z = 1 - \mathrm{e}^{-2\mathrm{i}\theta}$. As can be seen from this expression, the energy E appears in the exponential prefactor, and twice in the Gaussian function (through the argument z and in the first parameter, through α). The charge Z, on the other hand, is only present in the first parameter of the Gaussian function, through α. The coefficients $p_n^{l+1}(x, \alpha)$ possess very interesting properties from the physical point of view. When using expansion (27), all physical properties of the Coulomb wavefunction are transferred to $p_n^{l+1}(x, \alpha)$, since the functions $\phi_{l,n}(r)$ do not depend on either the charge Z or the energy E. For example, in the complex plane of the energy E, the position of the bound states and the poles of the scattering matrix can be related to each coefficient $p_n^{l+1}(x, \alpha)$, as illustrated for example in [19]. The functions $p_n^{l+1}(x,\alpha)$ are also very interesting from the mathematical point of view. Indeed, the expansion of $p_n^{l+1}(x,\alpha)$ in powers (i) of the energy yields coefficients which are Pollaczek polynomials of degree n [18] and (ii) of the charge gives also polynomials, which are different from those defined by Pollaczek, but may be named Pollaczek-*like* [11, 12]. Both sets of polynomials have different generating functions, orthogonal and completeness relations, etc. A study of all these properties is object of our current investigations.

No analytic expression has been given for any of the mentioned polynomials in terms of either energy or charge. This is probably due to the presence of these variables also in the parameters of the Gaussian function. In what follows, we shall give a general and analytic expression for the coefficients considering the charge as variable. The polynomials in terms of the energy can be obtained following a similar procedure.

As explained above, the Z dependence in $p_n^{l+1}(x,\alpha)$ appears, through α, only in the first parameter of the Gaussian function. A power series in α (and consequently in Z) can be derived through the Taylor series

$$ {}_2F_1(a,-n,2l+2;z) = \sum_{m=0}^{\infty} \frac{(-\mathrm{i}\alpha)^m}{m!} \left. \frac{\mathrm{d}^m {}_2F_1(a,-n,2l+2;z)}{\mathrm{d}a^m} \right|_{a=l+1} \tag{29} $$

where $a = l+1-\mathrm{i}\alpha$. We therefore need expressions for $G_a^{(n)}$, evaluated at $a = l+1$, which can be easily obtained form the expressions given in section 2. The first three functions read

$$ G_a^{(0)}\big|_{a=l+1} = {}_2F_1(l+1,-n,2l+2;z), \tag{30a} $$

$$ G_a^{(1)}\big|_{a=l+1} = \frac{(-n)_1}{(2l+2)_1} z\, {}_2\Theta_1^{(1)} \left(\begin{matrix} 1, 1 |\, l+1, l+2, 1-n \\ l+2 |\, 2, 2l+3 \end{matrix} \middle|\, ; z, z \right), \tag{30b} $$

$$ G_a^{(2)}\big|_{a=l+1} = \frac{(-n)_2}{(2l+2)_2} z^2\, {}_2\Theta_1^{(2)} \left(\begin{matrix} 1, 1, 1 |\, l+1, l+2, l+3, 2-n \\ l+2, l+3 |\, 3, 2l+4 \end{matrix} \middle|\, ; z, z, z \right), \tag{30c} $$

and the mth coefficient

$$ G_a^{(m)}|_{a=l+1} = \frac{(-n)_m}{(2l+2)_m} z^m \times {}_2\Theta_1^{(m)} \left(\begin{matrix} 1, 1, \ldots, 1 |\, l+1, l+2, \ldots, l+1+m, m-n \\ l+2, \ldots, l+1+m |\, m+1, 2l+2+m \end{matrix} \middle|\, ; z, \ldots, z \right). \tag{31} $$

The factor $(-n)_m$ appearing in this expression indicates that the series (29) terminates after n terms. The polynomials $p_n^{l+1}(x,\alpha)$ given by (28) may thus be written as

$$ p_n^{l+1}(x,\alpha) = \frac{(2l+2)_n}{n!} (1-z)^{-\frac{n}{2}} \sum_{m=0}^{n} \frac{(-\mathrm{i}\alpha)^m}{m!} G_a^{(m)}\big|_{a=l+1}, \tag{32} $$

where the relation $\mathrm{e}^{\mathrm{i}\theta} = \frac{1}{\sqrt{1-z}}$ was used. Besides, as discussed in section 3.3, the functions ${}_2\Theta_1^{(m)}$ reduce to polynomials because one of the parameters is a negative integer. The first three $p_n^{l+1}(x,\alpha)$ are

$$ \begin{aligned} p_0^{l+1}(x,\alpha) &= 1, \\ p_1^{l+1}(x,\alpha) &= (2l+2)(1-z)^{-\frac{1}{2}} \left[1 - \frac{z}{2} - (-\mathrm{i}\alpha) \frac{z}{2l+2} \right] \\ p_2^{l+1}(x,\alpha) &= \frac{(2l+2)_2}{2!} (1-z)^{-1} \left\{ \left[1 - z + \frac{(l+2)z^2}{2(2l+3)} \right] \right. \\ &\quad \left. - (-\mathrm{i}\alpha) \left[\frac{1}{l+1} z \left(1 - \frac{z}{2} \right) \right] + \frac{(-\mathrm{i}\alpha)^2}{2!} \left[\frac{2}{(2l+2)_2} z^2 \right] \right\}. \end{aligned} $$

These simple expressions were derived from the reductions to polynomials of ${}_2F_1$ with a negative integer as parameter, and from the result

$${}_2\Theta_1^{(1)}\left(\begin{matrix}1,1|\,l+1,l+2,-1\\ l+2|\,2,2l+3\end{matrix}\middle|;z,z\right)=1-\frac{z}{2}$$

which can be deduced from its definition or with the help of the series (22). Following similar procedures expression for further $p_n^{l+1}(x,\alpha)$ can be derived.

From the two expansions (27) and (32), the Coulomb wavefunction can be written as the following double series:

$$R_{l,k}=N_{l,k}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{Z^m}{m!}g_{l,m,n}(z)\,\phi_{l,n}(r)\,, \tag{33}$$

where

$$g_{l,m,n}(z)=\frac{(-\mathrm{i})^m}{\Gamma(2l+2)}\left(\frac{\mu}{\sqrt{2E}}\right)^m(1-z)^{-\frac{n}{2}}\,G_a^{(m)}\big|_{a=l+1}. \tag{34}$$

Except for the normalization factor $N_{l,k}$, in this formulation the dependence on the charge, the energy and the radial coordinate are fully separated. Using relation (6), we may transform the sum over m into an infinite sum, to finally get

$$R_{l,k}=N_{l,k}\sum_{m=0}^{\infty}\frac{Z^m}{m!}\left[\sum_{n=0}^{\infty}\widetilde{g}_{l,m,n}(z)\,\phi_{l,n+m}(r)\right], \tag{35}$$

where

$$\widetilde{g}_{l,m,n}(z)=\frac{(-\mathrm{i})^m}{\Gamma(2l+2)}\left(\frac{\mu}{\sqrt{2E}\sqrt{1-z}}\right)^m(1-z)^{-\frac{n}{2}}\,G_a^{(m)}\big|_{a=l+1}\,. \tag{36}$$

In this formulation, the sum over m corresponds to the power series expansion of the charge Z of the Kummer function of equation (24); the result is equivalent to that presented in our previous paper [9] but expressed here in spherical coordinates. Combining this power series expansion with that of the normalization constant $N_{l,k}$, the Born series for the radial Coulomb wavefunction can be easily derived [9]. With the result (35), we are not only giving all orders of the power series of the Kummer function but also its L^2 representation in terms of Sturmian functions.

5. Conclusions

We have studied the derivatives to any order of the Gaussian hypergeometric function ${}_2F_1(a,b,c;z)$ with respect to the parameters a,b and c. We have shown that they can be expressed in terms of generalizations of multivariable Kampé de Fériet functions, noted ${}_2\Theta_1^{(n)}$, for which several properties were established.

The usefulness of these derivatives has been illustrated through a physical application: the two-body Coulomb scattering problem. In a L^2 representation of the Coulomb wavefunction using Sturmian functions, we have been able to express explicitly the charge dependence of the corresponding charge polynomials. Besides this application, the mathematical results presented here might be useful in a wide range of physical and mathematical problems since the Gaussian function is the one-variable hypergeometric function which appears most frequently.

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