

Derivatives of any order of the hypergeometric function  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$  with respect to the parameters  $a_j$  and  $b_j$

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys. A: Math. Theor. 43 085210

(<http://iopscience.iop.org/1751-8121/43/8/085210>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.158

The article was downloaded on 03/06/2010 at 08:57

Please note that [terms and conditions apply](#).

# Derivatives of any order of the hypergeometric function ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$ with respect to the parameters $a_i$ and $b_i$

L U Ancarani<sup>1</sup> and G Gasaneo<sup>2</sup>

<sup>1</sup> Laboratoire de Physique Moléculaire et des Collisions, Université Paul Verlaine-Metz, 57078 Metz, France

<sup>2</sup> Departamento de Física, Universidad Nacional del Sur and Consejo Nacional de Investigaciones Científicas y Técnicas, 8000 Bahía Blanca, Buenos Aires, Argentina

Received 12 October 2009, in final form 7 January 2010

Published 8 February 2010

Online at [stacks.iop.org/JPhysA/43/085210](http://stacks.iop.org/JPhysA/43/085210)

## Abstract

The derivatives of any order of the general hypergeometric function  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$  with respect to the parameters  $a_i$  or  $b_i$  are expressed, in compact form, in terms of generalizations of multivariable Kampé de Fériet functions. To achieve this, use is made of Babister's solution to non-homogeneous differential equations for  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$ . An application to Hahn polynomials, which are  ${}_3F_2$  functions, is given as an illustration.

PACS numbers: 02.30.Gp, 02.30.Hq

## 1. Introduction

Generalized hypergeometric functions  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$  have been studied extensively from their mathematical point of view [1, 2]. They occur in a wide variety of problems in theoretical physics, applied mathematics, statistics and engineering sciences. Just to mention a few examples in the field of quantum mechanics: (i) the confluent hypergeometric Kummer function  ${}_1F_1$  is closely related to the two-body Coulomb problem [3] (see also the recent study in [4]); (ii) the Gauss hypergeometric function  ${}_2F_1$  is the solution of Schrödinger's equation when solving the Pöschl–Teller, Wood–Saxon or Hulthén potentials [5]. Another very important case is related to the angular momentum theory (see [6] and references therein); the functions  ${}_3F_2$  and  ${}_4F_3$  are related to the Clebsch–Gordan and Racah coefficients, respectively [7]. Besides, there is a large set of hypergeometric-type polynomials whose variable is located in one or more of the parameters of the corresponding functions  ${}_pF_q$ . Some examples are the Wilson polynomial, the continuous dual Hahn polynomial, the continuous Hahn polynomial, the Charlier polynomial and the Pollaczek-like polynomial [6], among many others [8, 9]. These polynomials are of great importance in mathematics as well as in many areas

of physics. A few examples of their applications are discussed by Nikiforov, Suslov and Uvarov [10]. Of particular interest for the authors is the example discussed in connection with the transformation of the Coulomb radial eigenfunctions to parabolic coordinates, the transformation coefficients being expressed in terms of Hahn polynomials.

In some cases, one or several parameters—rather than the variable itself—play an important role. It is thus essential to be able to study the functions  ${}_pF_q$  as a function of  $a_i$  or  $b_i$ , rather than  $z$ . One important tool is then provided by the derivatives of the  ${}_pF_q$  function with respect to these parameters since they allow us, for example, to write a Taylor expansion around some given values  $\tilde{a}_i$  or  $\tilde{b}_i$ . While the  $n$ th derivative, with respect to the variable  $z$ , has been expressed in a compact form [1, 2], the same cannot be stated for the derivatives with respect to the parameters. Expressions for the first derivative with respect to a parameter have been presented but only for a few special values of the parameters (see Brychkov’s very recent handbook [11] and references therein). Some examples of specific results which can be found in the literature are the derivative of Bessel functions (which are related to  ${}_1F_1$  functions) with respect to the order [12]; the derivatives of associated Legendre functions with respect to the order and degree [13, 14], and of Jacobi polynomials with respect of the parameters [15] (these are related to  ${}_2F_1$  functions). The formulations are relatively complicated, and cannot be easily generalized to the derivatives of higher order. In the case of the confluent  ${}_1F_1$  and Gauss  ${}_2F_1$  hypergeometric functions, it has been recently [4, 6] shown that the  $n$ th derivatives can be systematically expressed in terms of generalizations of multivariable Kampé de Fériet functions. This was achieved using the second-order linear differential equations satisfied by the hypergeometric functions. Following a similar path, in this paper, we shall show how this can be extended systematically to generalized hypergeometric functions  ${}_pF_q$ , using the linear differential equation they satisfy. While this generalization may appear relatively trivial, the demonstration is not.

We start, in section 2, with the first derivative, and illustrate how the use of the derivative of Pochhammer symbols is particularly cumbersome. To easily generalize the  $n$ th derivative, the use of differential equations is seen (section 3) to be systematic and allows us to reach general compact forms. An application involving Hahn polynomials is given in section 4.

## 2. First derivative of the generalized hypergeometric functions ${}_pF_q$ with respect to the parameters

Consider the generalized hypergeometric function

$${}_pF_q = {}_pF_q \left( \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| z \right) = \sum_{n=0}^{\infty} A_n \frac{z^n}{n!} = \sum_{n=0}^{\infty} \frac{(a_1)_n \dots (a_p)_n z^n}{(b_1)_n \dots (b_q)_n n!}, \quad (1)$$

where the Pochhammer symbol  $(\lambda)_n = \Gamma(\lambda + n)/\Gamma(\lambda)$  is defined in terms of the Gamma function [1]. Since all  $a_i$  (respectively  $b_i$ ) play an equivalent role, for notation simplicity we shall consider hereafter only the derivative with respect to  $a_1$  (respectively  $b_1$ ). In what follows, we shall use the following notation for the  $n$ th derivatives with respect to the parameters  $a_1$  or  $b_1$ :

$$G_{a_1}^{(n)} = \frac{d^n {}_pF_q}{da_1^n}, \quad (2a)$$

$$H_{b_1}^{(n)} = \frac{d^n {}_pF_q}{db_1^n}. \quad (2b)$$

Let us start with the first derivatives. Using the derivative of the Pochhammer symbol given by [16]

$$\frac{d(\lambda)_n}{d\lambda} = (\lambda)_n [\Psi(\lambda + n) - \Psi(\lambda)], \tag{3}$$

we find

$$G_{a_1}^{(1)} = \sum_{n=0}^{\infty} A_n [\Psi(a_1 + n) - \Psi(a_1)] \frac{z^n}{n!} = \sum_{n=0}^{\infty} A_{n+1} [\Psi(a_1 + n + 1) - \Psi(a_1)] \frac{z^{n+1}}{(n+1)!} \tag{4a}$$

$$H_{b_1}^{(1)} = - \sum_{n=0}^{\infty} A_n [\Psi(b_1 + n) - \Psi(b_1)] \frac{z^n}{n!} = - \sum_{n=0}^{\infty} A_{n+1} [\Psi(b_1 + n + 1) - \Psi(b_1)] \frac{z^{n+1}}{(n+1)!} \tag{4b}$$

We therefore have an infinite series containing the Digamma function  $\Psi(z) = d[\ln\Gamma(z)]/dz$  [16]. Using the recurrence formula (equation (6.3.6) of [16])

$$\Psi(n+z) = \Psi(z) + \sum_{s=0}^{n-1} \frac{1}{s+z},$$

we can derive the alternative formulation

$$G_{a_1}^{(1)} = \sum_{n=0}^{\infty} A_{n+1} \frac{z^{n+1}}{(n+1)!} \sum_{s=0}^n \frac{1}{s+a_1}, \tag{5a}$$

$$H_{b_1}^{(1)} = - \sum_{n=0}^{\infty} A_{n+1} \frac{z^{n+1}}{(n+1)!} \sum_{s=0}^n \frac{1}{s+b_1}. \tag{5b}$$

It is clear that the generalization to the  $n$ th derivative, in either formulation, is particularly cumbersome.

To circumvent this difficulty we may consider the following approach. Using

$$\frac{1}{(s+a_1)} = \frac{1}{a_1} \frac{(a_1)_s}{(a_1+1)_s}, \tag{6}$$

and the rearrangement series technique (see, for example, chapter 2 of [17])

$$\sum_{n=0}^{\infty} \sum_{k=0}^n B(k, n) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} B(k, n+k), \tag{7}$$

we find, in the case of  $G_{a_1}^{(1)}$ ,

$$G_{a_1}^{(1)} = \sum_{n=0}^{\infty} A_{n+1} \frac{z^{n+1}}{(n+1)!} \sum_{s=0}^n \frac{1}{a_1} \frac{(a_1)_s}{(a_1+1)_s} = \frac{z}{a_1} \sum_{n=0}^{\infty} \sum_{s=0}^{\infty} A_{n+1+s} \frac{z^{n+s}}{(n+1+s)!} \frac{(a_1)_s}{(a_1+1)_s}. \tag{8}$$

Now using the property  $(\lambda)_{n+1+s} = (\lambda+1)_{n+s}(\lambda)$ , we have

$$A_{n+1+s} = \frac{(a_1+1)_{n+s} \cdots (a_p+1)_{n+s}}{(b_1+1)_{n+s} \cdots (b_q+1)_{n+s}} A_1. \tag{9}$$

Noting that  $(n+1+s)! = (2)_{n+s}$ , and collecting, we find

$$G_{a_1}^{(1)} = \frac{z}{a_1} A_1 \sum_{n=0}^{\infty} \sum_{s=0}^{\infty} \frac{(1)_n (1)_s (a_1)_s}{(2)_{n+s} (a_1+1)_s} \frac{(a_1+1)_{n+s} \cdots (a_p+1)_{n+s}}{(b_1+1)_{n+s} \cdots (b_q+1)_{n+s}} \frac{z^{n+s}}{s! n!}. \tag{10}$$

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

$$\begin{aligned}
 & {}_p\Theta_q^{(1)} \left( \alpha_1, \alpha_2 \mid \beta_1, \beta_2, \dots, \beta_{p+1} \mid \gamma_1 \mid \delta_1, \delta_2, \dots, \delta_{q+1} \mid ; x_1, x_2 \right) \\
 &= \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(\alpha_1)_{m_1} (\alpha_2)_{m_2} (\beta_1)_{m_1}}{(\gamma_1)_{m_1}} \frac{(\beta_2)_{m_1+m_2} \cdots (\beta_{p+1})_{m_1+m_2}}{(\delta_1)_{m_1+m_2} (\delta_2)_{m_1+m_2} \cdots (\delta_{q+1})_{m_1+m_2}} \frac{x_1^{m_1} x_2^{m_2}}{m_1! m_2!}, \quad (11)
 \end{aligned}$$

which, as can be seen following procedures similar to those explained in [4, 6], is a Kampé de Fériet-like function [18]. The convergence conditions discussed in [17] apply to this two-variable function. In terms of  ${}_p\Theta_q^{(1)}$ , we have

$$G_{a_1}^{(1)} = \frac{z}{a_1} A_{1p} \Theta_q^{(1)} \left( 1, 1 \mid a_1, a_1 + 1, \dots, a_p + 1 \mid a_1 + 1 \mid 2, b_1 + 1, \dots, b_q + 1 \mid ; z, z \right) \quad (12)$$

and similarly

$$H_{b_1}^{(1)} = -\frac{z}{b_1} A_{1p} \Theta_q^{(1)} \left( 1, 1 \mid b_1, a_1 + 1, \dots, a_p + 1 \mid b_1 + 1 \mid 2, b_1 + 1, \dots, b_q + 1 \mid ; z, z \right) \quad (13)$$

The generalization to the  $n$ th derivatives can be obtained in a similar way, but we found that it is more convenient and systematic, as shown in the next section, to use the differential equation satisfied by the hypergeometric function  ${}_pF_q$ .

### 3. $n$ th derivatives of the ${}_pF_q$ hypergeometric functions with respect to the parameters

Defining the differential operator

$$\begin{aligned}
 \hat{D} = & \frac{d}{dz} \left( z \frac{d}{dz} + b_1 - 1 \right) \left( z \frac{d}{dz} + b_2 - 1 \right) \cdots \left( z \frac{d}{dz} + b_q - 1 \right) \\
 & - \left( z \frac{d}{dz} + a_1 \right) \left( z \frac{d}{dz} + a_2 \right) \cdots \left( z \frac{d}{dz} + a_p \right), \quad (14)
 \end{aligned}$$

the linear differential equation satisfied by  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$  reads (for example, equation (8.6) of [19])

$$\hat{D} {}_pF_q = 0, \quad (15)$$

where  ${}_pF_q$  is an analytical function of  $z \in \mathbb{C} - \{0, 1, \infty\}$ , and  $a_i, b_i$  can be real or complex parameters. Since  ${}_pF_q$  is an analytical function of the variable  $z$ , and of the parameters  $a_i$  and  $b_i$ , we may take the derivative of (15) with respect to the parameters. Upon differentiation of (15) with respect to  $a_1$ , respectively  $b_1$ , we have that the derivatives  $G_{a_1}^{(1)}$  and  $H_{b_1}^{(1)}$  satisfy the following non-homogeneous linear differential equations:

$$\hat{D} G_{a_1}^{(1)} = \left[ \left( z \frac{d}{dz} + a_2 \right) \cdots \left( z \frac{d}{dz} + a_p \right) \right] {}_pF_q = X_{a_1}^{(1)} \quad (16a)$$

$$\hat{D} H_{b_1}^{(1)} = - \left[ \frac{d}{dz} \left( z \frac{d}{dz} + b_2 - 1 \right) \cdots \left( z \frac{d}{dz} + b_q - 1 \right) \right] {}_pF_q = Y_{b_1}^{(1)}. \quad (16b)$$

In our previous investigations, we have noticed that—for the cases  $(p = 1, q = 1)$  [4] and  $(p = 2, q = 1)$  [6]—the right-hand sides (rhs) of (16a) and (16b) could be expressed with a single hypergeometric function  ${}_pF_q$  but with modified parameters  $a_i$  and/or  $b_i$ ; these rhs are thus known power series of  $z$ . Equations (16a) and (16b) are therefore related to

the non-homogeneous differential equations with a generic positive power of  $z$  on the rhs ( $z^{\sigma-1}$ ,  $\sigma \geq 1$ ),

$$\hat{D}y = z^{\sigma-1} \tag{17}$$

which have been studied in detail, for example, in Babister’s book [19]; the solutions  $y$  (see equation (8.60) of [19]) read

$$y = {}_p f_{q,\sigma}(z) = \frac{z^\sigma}{\sigma(\sigma + b_1 - 1) \cdots (\sigma + b_q - 1)} {}_{p+1}F_{q+1} \left( \begin{matrix} 1, \sigma + a_1, \dots, \sigma + a_p \\ \sigma + 1, \sigma + b_1, \dots, \sigma + b_q \end{matrix} \middle| z \right) \tag{18}$$

where the series converges for all  $z$  if  $p \leq q$ , and for  $|z| < 1$ , if  $p = q + 1$ . In [4, 6] we made use of this result, for the ( $p = 1, q = 1$ ) and ( $p = 2, q = 1$ ) cases (the detailed solutions are given by equations (4.162) and (6.184) of [19], respectively) to write explicitly the derivatives  $G_{a_i}^{(1)}$  and  $H_{b_i}^{(1)}$  in terms of double infinite series.

Since the solution (18) is provided for any  $p$  and  $q$ , we may proceed—in a similar manner—with the generalization. First of all, we have to identify the reduction of the rhs of (16a) and (16b) as  ${}_p F_q$  functions, for any  $p$  and  $q$ . Using the explicit series expansion of  ${}_p F_q$  and property (6), it is relatively easy to verify that

$$\left( z \frac{d}{dz} + a_i \right) {}_p F_q = a_i {}_p F_q \left( \begin{matrix} a_1, \dots, a_{i-1}, a_i + 1, a_{i+1}, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| z \right), \tag{19a}$$

$$\left( z \frac{d}{dz} + b_i - 1 \right) {}_p F_q = (b_i - 1) {}_p F_q \left( \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_{i-1}, b_i - 1, b_{i+1}, \dots, b_q \end{matrix} \middle| z \right). \tag{19b}$$

Hence, by successive applications of the differential operators on the rhs of (16a) and (16b), we obtain

$$X_{a_1}^{(1)} = \frac{1}{a_1} \left( \prod_{j=1}^p a_j \right) {}_p F_q \left( \begin{matrix} a_1, a_2 + 1, \dots, a_p + 1 \\ b_1, \dots, b_q \end{matrix} \middle| z \right), \tag{20a}$$

$$Y_{b_1}^{(1)} = -\frac{1}{b_1} \left( \prod_{j=1}^p a_j \right) {}_p F_q \left( \begin{matrix} a_1 + 1, \dots, a_p + 1 \\ b_1 + 1, b_2, \dots, b_q \end{matrix} \middle| z \right). \tag{20b}$$

Though seemingly simple, this result plays a key role in the rest of this work. Using the fact that the differential equations (16a) and (16b) are linear and that the rhs of (20a) and (20b) are linear combinations of powers of  $z$ , we may use the general solution (18) to find the solutions for  $G_{a_1}^{(1)}$  and  $H_{b_1}^{(1)}$ . For example, for  $G_{a_1}^{(1)}$ , we have

$$\begin{aligned} G_{a_1}^{(1)} &= \frac{1}{a_1} \left( \prod_{j=1}^p a_j \right) \sum_{m_1=0}^{\infty} \frac{(a_1)_{m_1} (a_2 + 1)_{m_1} \cdots (a_p + 1)_{m_1}}{(b_1)_{m_1} \cdots (b_q)_{m_1}} \frac{1}{m_1!} {}_p f_{q,m_1+1}(z) \\ &= z \frac{A_1}{a_1} \sum_{m_1=0}^{\infty} \frac{(1)_{m_1}}{(2)_{m_1}} \frac{(a_1)_{m_1} (a_2 + 1)_{m_1} \cdots (a_p + 1)_{m_1}}{(b_1 + 1)_{m_1} \cdots (b_q + 1)_{m_1}} \frac{z^{m_1}}{m_1!} \\ &\quad \times {}_{p+1}F_{q+1} \left( \begin{matrix} 1, a_1 + 1 + m_1, \dots, a_p + 1 + m_1 \\ 2 + m_1, b_1 + 1 + m_1, \dots, b_q + 1 + m_1 \end{matrix} \middle| z \right) \end{aligned} \tag{21}$$

where relation (6) was used again for the second equality. Replacing the  ${}_{p+1}F_{q+1}$  function by its power series definition, we obtain the double series

$$G_{a_1}^{(1)} = z \frac{A_1}{a_1} \sum_{m_1=0}^{\infty} \frac{(1)_{m_1} (a_1)_{m_1} (a_2 + 1)_{m_1} \cdots (a_p + 1)_{m_1}}{(2)_{m_1} (b_1 + 1)_{m_1} \cdots (b_q + 1)_{m_1}} \frac{z^{m_1}}{m_1!} \\ \times \sum_{m_2=0}^{\infty} \frac{(1)_{m_2} (a_1 + 1 + m_1)_{m_2} \cdots (a_p + 1 + m_1)_{m_2}}{(2 + m_1)_{m_2} (b_1 + 1 + m_1)_{m_2} \cdots (b_q + 1 + m_1)_{m_2}} \frac{z^{m_2}}{m_2!}. \quad (22)$$

Using the identity

$$(\lambda)_{m+n} = (\lambda)_m (\lambda + m)_n,$$

and simplifying, we finally find the result already given by equation (10). The procedure is similar for  $H_{b_1}^{(1)}$ , and the result is given, in compact form, by (13).

Let us now turn to the derivatives of order  $n$ , starting from the second derivative. Differentiating equations (16a) and (20a) with respect to  $a_1$ , we find the following non-homogenous differential equation for  $G_{a_1}^{(2)}$ :

$$\hat{D}G_{a_1}^{(2)} = 2 \left[ \left( z \frac{d}{dz} + a_2 \right) \cdots \left( z \frac{d}{dz} + a_p \right) \right] G_{a_1}^{(1)} \\ = 2 \frac{1}{a_1} \left( \prod_{j=1}^p a_j \right) G_{a_1}^{(1)}(a_1, a_2 + 1, \dots, a_p + 1; b_1, \dots, b_q; z). \quad (23)$$

Similarly, differentiating equation (16b) with respect to  $b_1$ , we find

$$\hat{D}H_{b_1}^{(2)} = -2 \left[ \frac{d}{dz} \left( z \frac{d}{dz} + b_2 - 1 \right) \cdots \left( z \frac{d}{dz} + b_q - 1 \right) \right] H_{b_1}^{(1)} \\ = -2 \frac{1}{b_1} \left( \prod_{j=1}^q b_j \right) \frac{d}{dz} H_{b_1}^{(1)}(a_1, \dots, a_p; b_1, b_2 - 1, \dots, b_q - 1; z). \quad (24)$$

The second equality results from the successive application for  $i \neq 1$  of the property:

$$\left( z \frac{d}{dz} + b_i - 1 \right) H_{b_1}^{(1)}(a_1, \dots, a_p; b_1, \dots, b_q; z) \\ = b_i H_{b_1}^{(1)}(a_1, \dots, a_p; b_1, \dots, b_{i-1}, b_i - 1, b_{i+1}, \dots, b_q; z) \quad (25)$$

which can be shown using the explicit form (13) for  $H_{b_1}^{(1)}$ .

The generalization to order  $n > 2$  is straightforward:

$$\hat{D}G_{a_1}^{(n)} = n \frac{1}{a_1} \left( \prod_{j=1}^p a_j \right) G_{a_1}^{(n-1)}(a_1, a_2 + 1, \dots, a_p + 1; b_1, \dots, b_q; z) \quad (26a)$$

$$\hat{D}H_{a_1}^{(n)} = -n \frac{1}{b_1} \left( \prod_{j=1}^q b_j \right) \frac{d}{dz} H_{b_1}^{(n-1)}(a_1, \dots, a_p; b_1, b_2 - 1, \dots, b_q - 1; z). \quad (26b)$$

Since the rhs of these differential equations are again power series in  $z$ , we may proceed as done for the first derivatives. For example, for  $G_{a_1}^{(2)}$  we find

$$G_{a_1}^{(2)} = \frac{A_2}{(a_1)_2} z^2 \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (1)_{m_3}}{(a_1 + 1)_{m_1} (a_1 + 2)_{m_1+m_2} (3)_{m_1+m_2+m_3}} \frac{1}{(a_1 + 1)_{m_1} (a_1 + 2)_{m_1+m_2}} \\ \times \frac{(a_1 + 2)_{m_1+m_2+m_3} (a_2 + 2)_{m_1+m_2+m_3} \cdots (a_p + 2)_{m_1+m_2+m_3}}{(b_1 + 2)_{m_1+m_2+m_3} (b_2 + 2)_{m_1+m_2+m_3} \cdots (b_q + 2)_{m_1+m_2+m_3}} \frac{z^{m_1+m_2+m_3}}{m_1! m_2! m_3!}. \quad (27)$$

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

$$\begin{aligned}
 & {}_p\Theta_q^{(n)} \left( \begin{matrix} \alpha_1, \alpha_2, \dots, \alpha_{n+1} | \beta_1, \beta_2, \dots, \beta_{n+p} \\ \gamma_1, \dots, \gamma_n | \delta_1, \dots, \delta_{q+1} \end{matrix} ; x_1, \dots, x_{n+1} \right) \\
 &= \sum_{m_1=0}^{\infty} \cdots \sum_{m_{n+1}=0}^{\infty} (\alpha_1)_{m_1} (\alpha_2)_{m_2} \cdots (\alpha_{n+1})_{m_{n+1}} \frac{(\beta_1)_{m_1} (\beta_2)_{m_1+m_2} \cdots (\beta_n)_{m_1+m_2+\dots+m_n}}{(\gamma_1)_{m_1} (\gamma_2)_{m_1+m_2} \cdots (\gamma_n)_{m_1+m_2+\dots+m_n}} \\
 &\quad \times \frac{(\beta_{n+1})_{m_1+m_2+\dots+m_{n+1}} \cdots (\beta_{n+p})_{m_1+m_2+\dots+m_{n+1}} x_1^{m_1} x_2^{m_2} \cdots x_{n+1}^{m_{n+1}}}{(\delta_1)_{m_1+m_2+\dots+m_{n+1}} \cdots (\delta_{q+1})_{m_1+m_2+\dots+m_{n+1}} m_1! m_2! \cdots m_{n+1}!}. \tag{28}
 \end{aligned}$$

In terms of these hypergeometric functions, the second derivatives  $G_{a_1}^{(2)}$  and  $H_{b_1}^{(2)}$  are related to  ${}_p\Theta_q^{(2)}$  functions:

$$G_{a_1}^{(2)} = \frac{A_2}{(a_1)_2} z^2 {}_p\Theta_q^{(2)} \left( \begin{matrix} 1, 1, 1 | a_1, a_1 + 1, a_1 + 2, \dots, a_p + 2 \\ a_1 + 1, a_1 + 2 | 3, b_1 + 2, \dots, b_q + 2 \end{matrix} ; z, z, z \right) \tag{29a}$$

$$H_{b_1}^{(2)} = 2!(-1)^2 \frac{A_1}{b_1^2} z {}_p\Theta_q^{(2)} \left( \begin{matrix} 1, 1, 1 | b_1, b_1, a_1 + 1, \dots, a_p + 1 \\ b_1 + 1, b_1 + 1 | 2, b_1 + 1, \dots, b_q + 1 \end{matrix} ; z, z, z \right). \tag{29b}$$

By induction one may demonstrate that the  $n$ th derivatives read

$$G_{a_1}^{(n)} = \frac{A_n}{(a_1)_n} z^n {}_p\Theta_q^{(n)} \left( \begin{matrix} 1, 1, \dots, 1 | a_1, a_1 + 1, \dots, a_1 + n, a_2 + n, \dots, a_p + n \\ a_1 + 1, \dots, a_1 + n | n + 1, b_1 + n, \dots, b_q + n \end{matrix} ; z, \dots, z \right) \tag{30a}$$

$$H_{b_1}^{(n)} = n! (-1)^n \frac{A_1}{b_1^n} z {}_p\Theta_q^{(n)} \left( \begin{matrix} 1, 1, \dots, 1 | b_1, b_1, \dots, b_1, a_1 + 1, \dots, a_p + 1 \\ b_1 + 1, \dots, b_1 + 1 | 2, b_1 + 1, \dots, b_q + 1 \end{matrix} ; z, \dots, z \right) \tag{30b}$$

These two formulas are the main results of this paper. For the cases  $(p = 1, q = 1)$  [4] and  $(p = 2, q = 1)$  [6], they reduce to those previously published. The function  ${}_p\Theta_q^{(n)}$  given by (28) are Kampé de Fériet functions in  $n + 1$  variables. This can be seen by applying the rule, for a particular set  $(p, q)$ , used by Appell and Kampé de Fériet [18] to the product of the generalized confluent hypergeometric functions (see [4, 6] for the particular cases  $(p = 1, q = 1)$  and  $(p = 2, q = 1)$ ).

Various properties for  ${}_p\Theta_q^{(n)}$  can be established. For example, starting from recurrence relations for the hypergeometric function  ${}_pF_q$ , recurrence relations for the  ${}_p\Theta_q^{(n)}$  function can be easily deduced. For illustration, consider the recurrence relation [20]

$$\begin{aligned}
 & \left( \prod_{j=1}^q b_j \right) \left( {}_pF_q \left( \begin{matrix} a_1, a_2, \dots, a_p \\ b_1, \dots, b_q \end{matrix} ; z \right) - {}_pF_q \left( \begin{matrix} a_1 + 1, a_2, \dots, a_p \\ b_1, \dots, b_q \end{matrix} ; z \right) \right) \\
 & \quad + z \left( \prod_{j=2}^p a_j \right) {}_pF_q \left( \begin{matrix} a_1 + 1, a_2 + 1, \dots, a_p + 1 \\ b_1 + 1, \dots, b_q + 1 \end{matrix} ; z \right) = 0. \tag{31}
 \end{aligned}$$



Derivating  $n$  times with respect to  $a_1$ , we obtain

$$\left(\prod_{j=1}^q b_j\right) \left(G_{a_1}^{(n)}(a_1, a_2, \dots, a_p, b_1, \dots, b_q; z) - G_{a_1}^{(n)}(a_1 + 1, a_2, \dots, a_p, b_1, \dots, b_q; z)\right) + z \left(\prod_{j=2}^p a_j\right) G_{a_1}^{(n)}(a_1 + 1, a_2 + 1, \dots, a_p + 1, b_1 + 1, \dots, b_q + 1; z) = 0. \quad (32)$$

Replacing then each  $G_{a_1}^{(n)}$  function by its expression (30a), a three-term recurrence relation for the hypergeometric function  ${}_p\Theta_q^{(n)}$  is obtained. Similarly to the ( $p = 1, q = 1$ ) [4] and ( $p = 2, q = 1$ ) [6] cases, different types of integral representations can be established for the  ${}_p\Theta_q^{(n)}$  functions; however, the convergence regions and restrictions of applications will depend on the values of  $p$  and  $q$ .

Special values of the parameters can lead to simplifications. If one of the  $a_i = 0$ , one of the sums reduces to a single term, and the function  ${}_p\Theta_q^{(n)}$  will contain only  $n$  variables instead of  $n + 1$ . This has been discussed, for the case ( $p = 1, q = 1$ ), in connection with the Taylor expansion of the Coulomb wavefunction in [4]; for that case, the  ${}_1\Theta_1^{(n)}$  functions are related to  ${}_1\Theta_1^{(n-1)}$  functions. Another interesting example results when one of the parameters  $a_i$  is a negative integer; in this case one of the  $n + 1$  infinite sums appearing in  ${}_p\Theta_q^{(n)}$  will be truncated.

#### 4. Application

Among the many possible applications of the results presented above we would like to briefly discuss the one related to recent developments in collisional problems [21–24] and closely connected to the theory of Hahn polynomials [9].

Two alternative methods have been recently introduced to deal with fragmentation or break-up problems, in which a particle collides with, e.g. a two-body bound subsystem (collisional three-body problems), and after the collision the three particles are separated. To describe this type of processes Aquilanti and co-workers [21–23] introduced the hyperquantization method. This consists in a discretized version of the hyperspherical adiabatic method in which the three-body wavefunction is written as the sum of products of angular and radial functions. The angular functions are obtained as the solution of the hyperspherical adiabatic equation [21]. The free-particle adiabatic equation can be solved in closed form and leads to products of spherical harmonic times Jacobi polynomials. These functions have been used as a basis set to solve different types of structure and collisional problems [21]. The hyperquantization approach is based on the discretization of Jacobi polynomials on a regular lattice. This is done thanks to the properties of Hahn polynomials and their relation with Jacobi polynomials. Within the second method, Gasaneo and co-workers [24] introduced a Sturmian hyperspherical approach for breakup problems based on the discretization of the Sturmian equations on a regular lattice. Instead of adiabatic basis, use is made of Sturmian basis which are more efficient to deal with collisional problems [25]. With this approach, both the hyper-radial and the hyper-angle equations are discretized on a regular lattice. Generalized polynomials, including Jacobi's, are derived from the resulting difference equations. The angular functions appearing in the hyperquantization are particular cases of the proposal of Gasaneo and co-workers. When free-particle angular Sturmians are defined, the theory presented in [10] can be used to establish the connection between the discretized Sturmians and the Hahn polynomials.

To clarify and illustrate the previous discussion, we consider hereafter the limit representation of Jacobi polynomials  $P_n^{(\alpha,\beta)}(\cos \theta)$  used in [21]:

$$\lim_{X \rightarrow \infty} \left( \frac{X+1}{2} \right)^{\frac{1}{2}} Q_{n,\xi}^{\alpha,\beta,X} = N_{n,\alpha,\beta} \cos^\beta \frac{\theta}{2} \sin^\alpha \frac{\theta}{2} P_n^{(\alpha,\beta)}(\cos \theta), \tag{33}$$

where  $N_{n,\alpha,\beta}$  represents a normalization constant and the angular variable  $\theta$  is transformed into  $\xi$  through

$$\cos \theta = \frac{X - 2\xi}{X + 1}. \tag{34}$$

The functions  $Q_{n,\xi}^{\alpha,\beta,X}$  may be expressed as follows:

$$Q_{n,\xi}^{\alpha,\beta,X} = (w(\xi) \pi_n)^{\frac{1}{2}} Q_n(\xi, \alpha, \beta, X), \tag{35}$$

where the Hahn polynomials  $Q_n(\xi, \alpha, \beta, X)$  (with norm  $\pi_n$ ) are orthogonal with respect to  $w(\xi)$  (see [21] and references therein).

These mathematical formulas can be used to represent Jacobi polynomials on a grid of points. Here  $\xi$  is the discrete variable, and  $n$  is the degree of the polynomial; both vary in the range  $0 < n, \xi \leq X$ , where  $X$  represents the number of points on the lattice. On the other hand, the Hahn polynomials can be expressed in closed form in terms of  ${}_3F_2$  generalized hypergeometric functions of argument one [17]:

$$Q_n(\xi, \alpha, \beta, X) = {}_3F_2 \left( \begin{matrix} -n, -\xi, n + \alpha + \beta + 1 \\ \alpha + 1, -X \end{matrix} \middle| 1 \right), \tag{36}$$

where the variable  $\xi$  appears in the second parameter. To the best of our knowledge, no analytic expressions have been published for these polynomials as a function of the variable  $\xi$ . Here we do not want to perform explicitly the calculations, but to show how this can be achieved. Using the Taylor series expansion

$${}_3F_2 \left( \begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix} \middle| z \right) = \sum_{n=0}^{\infty} \frac{(a_2)^n}{n!} G_{a_2}^{(n)} \Big|_{a_2=0}, \tag{37}$$

the different orders  $G_{a_2}^{(n)} \Big|_{a_2=0}$  can be expressed in terms of multivariable hypergeometric functions  ${}_3\Theta_2^{(n)}$  as shown in section 3. In this way, explicit closed forms can be provided for the discrete representation of the Hahn polynomials, which in turn can be further used to obtain expressions for the fragmentation transition amplitude derived in [24].

### 5. Conclusions

We have studied the derivatives to any order of the generalized hypergeometric function  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$  with respect to the parameters  $a_i$  and  $b_i$ . Using Babister’s solution to non-homogeneous differential equations for  ${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z)$ , we have shown that they can be expressed in terms of generalizations of multivariable Kampé de Fériet functions, noted  ${}_p\Theta_q^{(n)}$ , in  $n + 1$  variables  $z$ .

As illustrated for example in the application (see equation (37)), the derivatives with respect to the parameters can be used, for example, to write Taylor expansions of  ${}_pF_q$  around some given values  $\tilde{a}_1$  (or  $\tilde{b}_1$ ) appearing in the numerator (or denominator) as

$${}_pF_q = \sum_{n=0}^{\infty} \frac{(a_1 - \tilde{a}_1)^n}{n!} G_{a_1}^{(n)} \Big|_{a_1=\tilde{a}_1} \tag{38a}$$

$${}_pF_q = \sum_{n=0}^{\infty} \frac{(b_1 - \tilde{b}_1)^n}{n!} H_{b_1}^{(n)} \Big|_{b_1=\tilde{b}_1}, \quad (38b)$$

where  $G_{a_1}^{(0)} \Big|_{a_1=\tilde{a}_1}$  and  $H_{b_1}^{(0)} \Big|_{b_1=\tilde{b}_1}$  are the values of the function  ${}_pF_q$  calculated at  $a_1 = \tilde{a}_1$  and  $b_1 = \tilde{b}_1$ , respectively.

The mathematical results presented in this paper might be useful in a wide range of physical and mathematical problems in which a hypergeometric function  ${}_pF_q$  appears. One of such problems is the one discussed in section 4. Fragmentation problems are of fundamental importance in atomic and chemical physics. In many cases, optimization of the existing methods developed to deal with fragmentation problems lead to discrete hypergeometric-type polynomials (see, e.g., [26]) whose variables appear as one of the parameters of the hypergeometric function. In view of these applications, the study of these polynomials and their properties is paramount. As shown for example in section 4, such polynomials are connected to multivariable hypergeometric functions  ${}_p\Theta_q^{(n)}$ , and this connection might be of some help for further comprehension of these polynomials. As mentioned in the introduction, many important polynomials are defined in terms of the generalized  ${}_pF_q$  functions, the polynomial variable being located in one or more of the parameters of a  ${}_pF_q$  [6, 8, 9]. The present results, combined with the method described in section 4 of [6] for the  ${}_2F_1$  case in connection with Pollaczek-like polynomials, could be applied to obtain interesting closed form expressions for other hypergeometric-type polynomials.

## Acknowledgments

This work has been partially supported by grant PGI 24/F038 of Universidad Nacional del Sur. The support provided by the Lorraine region for the visit of the Dr Gasaneo to the Laboratoire de Physique Moléculaire et des Collisions, Université Paul Verlaine-Metz is also gratefully acknowledged.

## References

- [1] Erdelyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol I, II and III (New York: McGraw-Hill)
- [2] Exton H 1976 *Multiple Hypergeometric Functions and Applications* (New York: Wiley)
- [3] Landau L D and Lifshitz E M 1965 *Quantum Mechanics: Non-Relativistic Theory* (Oxford: Pergamon)
- [4] Ancarani L U and Gasaneo G 2008 *J. Math. Phys.* **49** 063508
- [5] Flüge S 1971 *Practical Quantum Mechanics I* (Berlin: Springer)
- [6] Ancarani L U and Gasaneo G 2009 *J. Phys. A: Math. Theor.* **42** 395208
- [7] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 *Quantum Theory of Angular Momentum* (Singapore: World Scientific)
- [8] Koekoek R and Swarttouw R 1998 *Report no. 98-17*, Delft University of Technology
- [9] Andrews G E, Askey R and Roy R 2000 *Special Functions* (Cambridge: Cambridge University Press)
- [10] Nikiforov A F, Suslov S K and Uvarov V B 1991 *Classical Orthogonal Polynomials of a Discrete Variable* (Berlin: Springer)
- [11] Brychkov Yu A 2008 *Handbook of Special Functions: Derivatives, Integrals, Series and Other Formulas* (London: Chapman and Hall)
- [12] Brychkov Yu A and Geddes K O 2005 *Integr. Transform Spec. Funct.* **16** 187
- [13] Brychkov Yu A 2009 *Integr. Transform Spec. Funct.* DOI: [10.1080/10652460903069660](https://doi.org/10.1080/10652460903069660)
- [14] Szmytkowski R 2009 *J. Math. Chem.* **46** 231
- [15] Froehlich J 1994 *Integr. Transform Spec. Funct.* **2** 253
- [16] Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (New York: Dover)
- [17] Srivastava H M and Manocha H L 1978 *A Treatise on Generating Functions* (Chichester: Ellis Horwood)

- 
- [18] Appell P and Kampé de Fériet J 1926 *Fonctions Hypergéométriques et Hypersphériques; Polynomes d'Hermite* (Paris: Gauthier-Villars)
- [19] Babister A W 1967 *Transcendental Functions Satisfying Nonhomogeneous Linear Differential Equations* (New York: Macmillan)
- [20] <http://functions.wolfram.com/07.31.17.0007.01>
- [21] Aquilanti V, Cavalli S and De Fazio D 1998 *J. Chem. Phys.* **109** 3792
- [22] Aquilanti V, Cavalli S, De Fazio D, Volpi A, Aguilar A, Gimenez X and Lucas JM 1998 *J. Chem. Phys.* **109** 3805
- [23] Anderson R W and Aquilanti V 2006 *J. Chem. Phys.* **124** 214104
- [24] Gasaneo G, Mitnik D M, Frapiccini A L, Colavecchia F D and Randazzo JM 2009 *J. Phys. Chem. A* **113** 14573
- [25] Macek J H and Ovchinnikov S Yu 1996 *Phys. Rev. A* **54** 544
- [26] Lo J Q W and Shizgal B D 2008 *J. Phys. B: At. Mol. Opt. Phys.* **41** 185103