

## Derivatives of any order of the confluent hypergeometric function ${}_1F_1(a, b, z)$ with respect to the parameter $a$ or $b$

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The derivatives to any order of the confluent hypergeometric (Kummer) function  $F = {}_1F_1(a, b, z)$  with respect to the parameter  $a$  or  $b$  are investigated and expressed in terms of generalizations of multivariable Kampé de Fériet functions. Various properties (reduction formulas, recurrence relations, particular cases, and series and integral representations) of the defined hypergeometric functions are given. Finally, an application to the two-body Coulomb problem is presented: the derivatives of  $F$  with respect to  $a$  are used to write the scattering wave function as a power series of the Sommerfeld parameter. © 2008 American Institute of Physics.  
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### I. INTRODUCTION

The confluent hypergeometric function  $F = {}_1F_1(a, b; z)$  (or alternatively Whittaker's function) has been studied in great detail from its mathematical point of view.<sup>1-3</sup> The Kummer function, as it is also named, is closely related to a fundamental problem of quantum mechanics: the two-body Coulomb problem. It is well known that the closed form solution of the two-body Coulomb Schrödinger equation both in spherical and parabolic coordinates are written in terms of the Kummer function  $F$ .<sup>4</sup> To perform different types of physical studies (see, e.g., Refs. 5-9) and applications,<sup>10-13</sup> it is necessary to know the mathematical properties of the function. Usually  $F$  is considered as a function of variable  $z$ ; however, in some physical applications, the first ( $a$ ) or second ( $b$ ) parameter may be the physical variable, as, for example, when Coulomb solutions are extended to the complex plane of the energy<sup>5,7</sup> or the angular momentum.<sup>5</sup>

The first and the  $n$ th derivatives with respect to the variable  $z$  is known in a compact form (e.g., Ref. 1). The derivatives with respect to the first or second parameter, on the other hand, have been less studied simply because the mathematical formulation is more difficult (see below). These derivatives, however, are needed in different physical applications, the Coulomb Born series being probably the most well known example. Several forms of the first derivatives have been given in the literature; none of them, however, is compact (except possibly in some special cases). In this contribution we address this issue by providing a compact form not only for the first but also for the  $n$ th derivatives. The usefulness of the investigation is illustrated by considering the two-body Coulomb wave function as a function of the Sommerfeld parameter.

We shall use the following notation for the  $n$ th derivatives:

$$G^{(n)} = G^{(n)}(a, b; z) = \frac{d^n {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| z\right)}{da^n}, \quad (1)$$

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$$H^{(n)} = H^{(n)}(a, b; z) = \frac{d^n {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| z\right)}{db^n}. \quad (2)$$

Let us recall the definition of the confluent hypergeometric function as a power series on the variable  $z$ :

$$F = {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| z\right) = \sum_{n=0}^{\infty} \frac{(a)_n}{n!(b)_n} z^n, \quad (3)$$

where  $(a)_n = \Gamma(a+n)/\Gamma(a)$  is the Pochhammer symbol defined in terms of the gamma function.<sup>1</sup>

A first approach to get the first derivative  $G^{(1)}$ , discussed, for example, in Ref. 1, is based on the use of the derivative of the Pochhammer symbol:

$$\frac{d(a)_n}{da} = (a)_n [\Psi(a+n) - \Psi(a)], \quad (4)$$

and its definition in terms of the digamma function  $\Psi(z)$ .<sup>14</sup> With the previous definition, the first derivatives of  $F$  with respect to  $a$  or  $b$  are

$$G^{(1)} = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} [\Psi(a+n) - \Psi(a)] \frac{z^n}{n!} = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \Psi(a+n) \frac{z^n}{n!} - \Psi(a) {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| z\right), \quad (5a)$$

$$H^{(1)} = - \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} [\Psi(b+n) - \Psi(b)] \frac{z^n}{n!} = - \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \Psi(b+n) \frac{z^n}{n!} + \Psi(b) {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| z\right). \quad (5b)$$

We have therefore an infinite series containing the digamma function.<sup>14</sup> An alternative form is obtained by using the recurrence formula (6.3.6) of Ref. 14:

$$G^{(1)} = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!} \sum_{p=0}^{n-1} \frac{1}{p+a}, \quad (6a)$$

$$H^{(1)} = - \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!} \sum_{p=0}^{n-1} \frac{1}{p+b}. \quad (6b)$$

In one form or the other, the generalization to the  $n$ th derivative is particularly cumbersome.

A second approach makes use of Whittaker functions:

$$M_{\kappa, \mu}(z) = e^{-z/2} z^{1/2+\mu} {}_1F_1\left(\begin{matrix} \frac{1}{2} + \mu - \kappa \\ 1 + 2\mu \end{matrix} \middle| z\right). \quad (7)$$

In the book *The Confluent Hypergeometric Function*,<sup>3</sup> Buchholz studied briefly the first derivative of the Whittaker function with respect to  $\mu$  and gave expression in terms of the digamma function. This author also related the first derivative with respect to  $\kappa$  and  $\mu$  with inhomogeneous differential equations, but no explicit and compact expressions were given for the derivatives  $G^{(1)}$  and  $H^{(1)}$ . Moreover, the generalization to the  $n$ th derivative was not provided.

An algorithm for the computation of  $G^{(n)}$  was given recently by Abad and Sesma.<sup>15</sup> They made use of a convergent expansion of Whittaker's function in series of Bessel functions and of the properties of Buchholz polynomials  $p_j^{(2\mu)}(z)$  ( $j=0, 1, 2, \dots$ ). The main result is

$$M_{\kappa,\mu}^{(n)}(z) = \frac{d^n M_{\kappa,\mu}(z)}{d\kappa^n} = (-1)^n z^{\mu+1/2+n} \sum_{j=0}^{\infty} \frac{p_j^{(2\mu)}(z)}{2^j (2\mu+1)_{j+n}} {}_0F_1 \left( \begin{matrix} \dots \\ 2\mu+1+j+n \end{matrix} \middle| -z\kappa \right). \quad (8)$$

The algorithm is based on this expansion, truncated at a conveniently large value  $j_{\max}$ .

In this paper explicit expressions for the  $n$ th derivatives  $G^{(n)}$  and  $H^{(n)}$  are given in Secs. II and III. The connection with Kampé de Fériét-like multivariable hypergeometric functions is given in Sec. IV, where different properties of these functions are presented. As application of these results, the scattering wave function for the two-body Coulomb problem is expressed as a power series of the Sommerfeld parameter up to order 2 (Sec. V). A summary of the results is given in Sec. VI.

## II. FIRST DERIVATIVE WITH RESPECT TO $a$ OR $b$

With an approach based on the solution of inhomogeneous differential equations related to the confluent hypergeometric function  $F$ , we give here a compact form for the first derivatives  $G^{(1)}$  and  $H^{(1)}$ . The procedure will then be used in the next section to find expressions for the higher derivatives  $G^{(n)}$  and  $H^{(n)}$ .

We start from the differential equation satisfied by the confluent hypergeometric function  $F$ ;

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] F = 0. \quad (9)$$

Since  $F$  is an analytic function of  $z$  and  $a$ ,<sup>1</sup> taking the derivative of Eq. (9) with respect to the first parameter  $a$ , one finds

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] G^{(1)} = F = \sum_{m_1=0}^{\infty} \frac{(a)_{m_1} z^{m_1}}{(b)_{m_1} m_1!} \quad (10)$$

(the use of  $m_1$  as index will become clear in the next section). Similarly, taking the derivative of the differential equation (9) with respect to  $b$  [ $F$  has poles and is not defined for  $b=0, -1, -2, \dots$  (Ref. 1)], we have

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] H^{(1)} = -\frac{dF}{dz} = -\frac{a}{b} {}_1F_1 \left( \begin{matrix} a+1 \\ b+1 \end{matrix} \middle| ; z \right) = -\frac{a}{b} \sum_{m_1=0}^{\infty} \frac{(a+1)_{m_1} z^{m_1}}{(b+1)_{m_1} m_1!}. \quad (11)$$

Now, according to Eq. (4.162) of Ref. 16, the solution of the inhomogeneous differential equation

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] y = z^{m_1} \quad (12)$$

is given by Eq. (4.163):

$$y = \theta_{m_1+1}(a, b; z) = \frac{z^{m_1+1}}{(1+m_1)(b+m_1)} {}_2F_2 \left( \begin{matrix} 1, a+1+m_1 \\ 2+m_1, b+1+m_1 \end{matrix} \middle| ; z \right). \quad (13)$$

Since the differential equation (10) is linear, the solution for  $G^{(1)}$  reads

$$G^{(1)} = \sum_{m_1=0}^{\infty} \frac{(a)_{m_1}}{m_1! (b)_{m_1}} \theta_{m_1+1}(a, b; z), \quad (14)$$

that is to say,

$$G^{(1)} = \frac{z}{(b)_1} \sum_{m_1=0}^{\infty} \frac{(a)_{m_1} (1)_{m_1}}{(b+1)_{m_1} (2)_{m_1} m_1!} {}_2F_2 \left( \begin{matrix} 1, a+1+m_1 \\ 2+m_1, b+1+m_1 \end{matrix} \middle| ; z \right). \quad (15)$$

Similarly, for  $H^{(1)}$  we find

$$H^{(1)} = -\frac{a}{b} \frac{z}{(b)_1} \sum_{m_1=0}^{\infty} \frac{(a+1)_{m_1} (b)_{m_1} (1)_{m_1}}{(b+1)_{m_1} (b+1)_{m_1} (2)_{m_1} m_1!} z^{m_1} {}_2F_2 \left( \begin{matrix} 1, a+1+m_1 \\ 2+m_1, b+1+m_1 \end{matrix} \middle| z \right). \quad (16)$$

These expressions, to the best of our knowledge, have not been given before. Expanding the  ${}_2F_2$  hypergeometric function in series (index  $m_2$ ) and after some algebraic manipulations, one finds

$$G^{(1)} = \frac{z}{(b)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (a)_{m_1} (a+1)_{m_1+m_2}}{(a+1)_{m_1} (2)_{m_1+m_2} (b+1)_{m_1+m_2} m_1! m_2!} z^{m_1+m_2}, \quad (17a)$$

$$H^{(1)} = -\frac{1}{b} \frac{a}{b} z \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (b)_{m_1} (a+1)_{m_1+m_2}}{(b+1)_{m_1} (2)_{m_1+m_2} (b+1)_{m_1+m_2} m_1! m_2!} z^{m_1+m_2}. \quad (17b)$$

These double series could have been obtained also starting directly from expressions (6a) and (6b) using the property

$$\sum_{n=0}^{\infty} \sum_{k=0}^n B(k, n) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} B(k, n+k). \quad (18)$$

However, as mentioned in the Introduction, this technique does not allow for an easy generalization to the  $n$ th derivatives. Moreover, these double series can be related to the following hypergeometric function in two variables:

$$\Theta^{(1)} \left( \begin{matrix} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{matrix} \middle| x_1, x_2 \right) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(a_1)_{m_1} (a_2)_{m_2} (b_1)_{m_1} (b_2)_{m_1+m_2}}{(c_1)_{m_1} (d_1)_{m_1+m_2} (d_2)_{m_1+m_2} m_1! m_2!} x_1^{m_1} x_2^{m_2}, \quad (19)$$

which, as we shall see in Sec. IV, is a Kampé de Fériet-like function. Hence, in terms of  $\Theta^{(1)}$ , the first derivatives  $G^{(1)}$  and  $H^{(1)}$  read

$$G^{(1)} = \frac{z}{(b)_1} \Theta^{(1)} \left( \begin{matrix} 1, 1 | a, a+1 \\ a+1 | 2, b+1 \end{matrix} \middle| z, z \right), \quad (20a)$$

$$H^{(1)} = -\frac{a}{b} \frac{z}{(b)_1} \Theta^{(1)} \left( \begin{matrix} 1, 1 | b, a+1 \\ b+1 | 2, b+1 \end{matrix} \middle| z, z \right). \quad (20b)$$

An alternative formulation of the solution to the inhomogeneous differential equation Eq. (12) is given by a finite sum of powers of  $z$  [see Eq. (4.172) of Ref. 16]:

$$\vartheta_{m_1+1}(a, b; z) = -\frac{1}{a} \frac{m_1! (b)_{m_1}}{(a+1)_{m_1}} \sum_{n=0}^{m_1} \frac{(a)_n z^n}{(b)_n n!} = -\frac{1}{a} \frac{m_1! (b)_{m_1}}{(a+1)_{m_1}} \mathcal{F}^{(m_1)}(a, b, z). \quad (21)$$

As showed notin Ref. 16 [Eq. (4.175)], the functions  $\theta_{m_1+1}(a, b; z)$  and  $\vartheta_{m_1+1}(a, b; z)$  are linked to each other through

$$\vartheta_{m_1+1}(a, b; z) = \theta_{m_1+1}(a, b; z) - \frac{1}{a} \frac{m_1! (b)_{m_1}}{(a+1)_{m_1}} {}_1F_1(a, b; z). \quad (22)$$

The function  $\vartheta_{m_1+1}(a, b; z)$  can be considered as an asymptotic solution of Eq. (12) as it is derived from a series in inverse powers of  $z$ ; note that  $\lim_{m \rightarrow \infty} \mathcal{F}^{(m)}(a, b, z) = {}_1F_1(a, b; z)$ . Both  $\theta_{m_1+1}(a, b; z)$  and  $\vartheta_{m_1+1}(a, b; z)$  are closely related to the inhomogeneous Whittaker functions  $S$  and  $R$  defined by Buchholz.<sup>3</sup> In terms of the finite sum  $\mathcal{F}^{(m_1)}$ , the derivative  $G^{(1)}$  given by Eq. (14) can thus be expressed as

$$G^{(1)} = -\frac{1}{a} \sum_{m_1=0}^{\infty} \frac{(a)_{m_1}}{(a+1)_{m_1}} \mathcal{F}^{(m_1)}(a, b, z). \quad (23)$$

After some algebraic calculations and the application of series rearrangement techniques,<sup>17</sup> the  $G^{(1)}$  function can be reduced to

$$G^{(1)} = -\frac{1}{a} \sum_{m_1=0}^{\infty} \frac{(a)_{m_1}}{(b)_{m_1}} {}_3F_2 \left( \begin{matrix} 1, a, a+m_1 \\ a+1, a+1+m_1 \end{matrix} \middle| 1 \right) \frac{z^{m_1}}{m_1!}. \quad (24)$$

For the particular argument of  $z=1$ , the function the  ${}_3F_2$  simplifies<sup>18</sup> and an expression in terms of digamma functions, leading to Eq. (5a), can be obtained. Following the same procedure, a similar representation for  $H^{(1)}$  can be obtained.

### III. $n$ TH DERIVATIVE WITH RESPECT TO $a$ OR $b$

Without much effort, one may generalize the result to the  $n$ th derivative with respect to  $a$  or  $b$ . Following the same procedure, we define first the inhomogeneous differential equation satisfied by each derivative order.

Consider the second derivative  $G^{(2)}$ . Differentiating with respect to  $a$  Eq. (10) satisfied by  $G^{(1)}$ , we have

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] G^{(2)} = G^{(1)} + \frac{dG^{(0)}}{da} = 2G^{(1)}, \quad (25)$$

where we used  $F=G^{(0)}$ . Taking again the derivative with respect to  $a$ , we obtain for the third derivative

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] G^{(3)} = G^{(2)} + 2 \frac{dG^{(1)}}{da} = 3G^{(2)}, \quad (26)$$

and, following the same procedure, we find that the  $n$ th derivative satisfies the general differential equation

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] G^{(n)} = nG^{(n-1)}. \quad (27)$$

Proceeding as for  $G^{(1)}$ , in Appendix A we give the detailed calculations that lead to the following explicit expressions for  $G^{(2)}$ :

$$G^{(2)} = \frac{z^2}{(b)_2} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (1)_{m_3}}{(3)_{m_1+m_2+m_3} (b+2)_{m_1+m_2+m_3}} \times \frac{(a)_{m_1} (a+1)_{m_1+m_2} (a+2)_{m_1+m_2+m_3}}{(a+1)_{m_1} (a+2)_{m_1+m_2}} \frac{z^{m_1+m_2+m_3}}{m_1! m_2! m_3!}. \quad (28)$$

It can be easily verified by induction that the general expression for  $G^{(n)}$  ( $n \geq 1$ ) reads

$$G^{(n)} = \frac{z^n}{(b)_n} \sum_{m_1=0}^{\infty} \dots \sum_{m_{n+1}=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} \dots (1)_{m_{n+1}}}{(n+1)_{m_1+m_2+\dots+m_{n+1}} (b+n)_{m_1+m_2+\dots+m_{n+1}}} \times \frac{(a)_{m_1} (a+1)_{m_1+m_2} \dots (a+n)_{m_1+m_2+\dots+m_{n+1}}}{(a+1)_{m_1} \dots (a+n)_{m_1+\dots+m_n}} \frac{z^{m_1+m_2+\dots+m_{n+1}}}{m_1! m_2! \dots m_{n+1}!}. \quad (29)$$

Following a similar procedure, one finds the set of equations satisfied by  $H^{(n)}$ :

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] H^{(1)} = - \frac{dF}{dz}, \quad (30a)$$

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] H^{(2)} = - 2 \frac{dH^{(1)}}{dz}, \quad (30b)$$

...

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] H^{(n)} = - n \frac{dH^{(n-1)}}{dz}. \quad (30c)$$

The solution for (30a) was given above by Eq. (20b). The solution for (30b) reads

$$\begin{aligned} H^{(2)} &= (-1)^2 \frac{2}{b^2} \frac{a}{b} z \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (1)_{m_3}}{(2)_{m_1+m_2+m_3} (b+1)_{m_1+m_2+m_3}} \\ &\times \frac{(b)_{m_1} (b)_{m_1+m_2} (a+1)_{m_1+m_2+m_3} z^{m_1+m_2+m_3}}{(b+1)_{m_1} (b+1)_{m_1+m_2} m_1! m_2! m_3!}, \end{aligned} \quad (31)$$

and, by induction, the solution for the  $n$ th derivative  $H^{(n)}$  is

$$\begin{aligned} H^{(n)} &= (-1)^n \frac{n!}{b^n} \frac{a}{b} z \sum_{m_1=0}^{\infty} \cdots \sum_{m_{n+1}=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} \cdots (1)_{m_{n+1}}}{(2)_{m_1+m_2+\cdots+m_{n+1}} (b+1)_{m_1+m_2+\cdots+m_{n+1}}} \\ &\times \frac{(b)_{m_1} (b)_{m_1+m_2} \cdots (b)_{m_1+m_2+\cdots+m_n} (a+1)_{m_1+m_2+\cdots+m_{n+1}} z^{m_1+m_2+\cdots+m_{n+1}}}{(b+1)_{m_1} (b+1)_{m_1+m_2} \cdots (b+1)_{m_1+m_2+\cdots+m_n} m_1! m_2! \cdots m_{n+1}!}. \end{aligned} \quad (32)$$

It is worth mentioning that the system of equations for the  $n$ th derivatives [Eqs. (10) and (25)–(27) for  $G^{(n)}$  and Eqs. (30a)–(30c) for  $H^{(n)}$ ] are all of order 2 and could be numerically solved with well known methods.

#### IV. CONNECTION WITH MULTIVARIABLE HYPERGEOMETRIC FUNCTIONS AND VARIOUS PROPERTIES

It is interesting to notice that the expressions given above for the derivatives of  $F$  with respect to  $a$  and  $b$  can be expressed in terms of generalizations of multivariable Kampé de Fériet hypergeometric functions. In Sec. II we have written the first derivatives  $G^{(1)}$  and  $H^{(1)}$  in terms of the two-variable hypergeometric  $\Theta^{(1)}$ . Similarly, for each  $n$ th derivative ( $n \geq 2$ ), we may associate a different multivariable hypergeometric function which we shall name  $\Theta^{(n)}$ . Several properties of these functions will be presented in this section.

##### A. The definition of $G^{(n)}$ and $H^{(n)}$ in terms of hypergeometric functions

The function  $\Theta^{(1)}$ , defined by Eq. (19), results from the application of the rule used by Appell<sup>19</sup> to the product of the generalized (confluent) hypergeometric functions  ${}_3F_3$  and  ${}_2F_2$ ,

$${}_3F_3 \left( \begin{matrix} a_1, a_2, a_3 \\ c_1, c_2, c_3 \end{matrix} \middle| x_1 \right) {}_2F_2 \left( \begin{matrix} b_1, b_2 \\ d_1, d_2 \end{matrix} \middle| x_2 \right) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{x_1^{m_1} x_2^{m_2}}{m_1! m_2!} \frac{(a_1)_{m_1} (a_2)_{m_1} (a_3)_{m_1} (b_1)_{m_2} (b_2)_{m_2}}{(c_1)_{m_1} (c_2)_{m_1} (c_3)_{m_1} (d_1)_{m_2} (d_2)_{m_2}}.$$

Using the replacements

$$(a_3)_{m_1} (b_1)_{m_2} \rightarrow (a_3)_{m_1+m_2},$$

$$(c_3)_{m_1}(d_2)_{m_2} \rightarrow (c_3)_{m_1+m_2},$$

$$(c_2)_{m_1}(d_1)_{m_2} \rightarrow (c_2)_{m_1+m_2},$$

the following coefficient is generated:

$$\frac{(a_1)_{m_1}(a_2)_{m_1}(a_3)_{m_1}(b_1)_{m_2}(b_2)_{m_2}}{(c_1)_{m_1}(c_2)_{m_1}(c_3)_{m_1}(d_1)_{m_2}(d_2)_{m_2}} \rightarrow \frac{(a_1)_{m_1}(a_2)_{m_1}(b_2)_{m_2}(a_3)_{m_1+m_2}}{(c_1)_{m_1}(c_2)_{m_1+m_2}(c_3)_{m_1+m_2}}.$$

According to the theory presented in Ref. 17, the fact that the functions we started from are confluent hypergeometric functions ensures that the function  $\Theta^{(1)}$  given by Eq. (19) is also a confluent hypergeometric function whose convergency radius is infinity in  $x_1$  and  $x_2$ . The function  $\Theta^{(1)}$  is a Kampé de Fériet function in two variables.

Similarly, for the second order derivatives  $G^{(2)}$  and  $H^{(2)}$ , we may introduce the function

$$\Theta^{(2)}\left( \begin{matrix} a_1, a_2, a_3 | b_1, b_2, b_3 \\ c_1, c_2 | d_1, d_2 \end{matrix} \middle| ; x_1, x_2, x_3 \right) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(a_1)_{m_1}(a_2)_{m_2}(a_3)_{m_3}(b_1)_{m_1}(b_2)_{m_1+m_2}(b_3)_{m_1+m_2+m_3} x_1^{m_1} x_2^{m_2} x_3^{m_3}}{(c_1)_{m_1}(c_2)_{m_1+m_2}(d_1)_{m_1+m_2+m_3}(d_2)_{m_1+m_2+m_3} m_1! m_2! m_3!}, \tag{33}$$

which can be generated using Appell’s technique to the product of generalized (confluent) hypergeometric functions  ${}_4F_4$ ,  ${}_3F_3$ , and  ${}_2F_2$ . Generalizing to the  $n$ th derivative, we introduce the function  $\Theta^{(n)}$  defined by

$$\Theta^{(n)}\left( \begin{matrix} a_1, a_2, \dots, a_{n+1} | b_1, \dots, b_{n+1} \\ c_1, \dots, c_n | d_1, d_2 \end{matrix} \middle| ; x_1, x_2, \dots, x_{n+1} \right) = \sum_{m_1=0}^{\infty} \dots \sum_{m_{n+1}=0}^{\infty} \frac{x_1^{m_1} x_2^{m_2} \dots x_{n+1}^{m_{n+1}}}{m_1! m_2! \dots m_{n+1}!} \times \frac{(a_1)_{m_1}(a_2)_{m_2} \dots (a_{n+1})_{m_{n+1}}(b_1)_{m_1}(b_2)_{m_1+m_2} \dots (b_{n+1})_{m_1+m_2+\dots+m_{n+1}}}{(c_1)_{m_1}(c_2)_{m_1+m_2} \dots (c_n)_{m_1+m_2+\dots+m_n}(d_1)_{m_1+m_2+\dots+m_{n+1}}(d_2)_{m_1+m_2+\dots+m_{n+1}}}, \tag{34}$$

which results from the application of Appell’s technique to the product of  ${}_{n+2}F_{n+2, \dots, 3}F_3$ , and  ${}_2F_2$ . The way in which the coefficients are combined is easily induced from the series given here.

In terms of these (generalized Kampé de Fériet-like) hypergeometric functions, the derivatives  $G^{(n)}$  given in the previous section read

$$G^{(1)}(a, b; z) = \frac{z}{(b)_1} \Theta^{(1)}\left( \begin{matrix} 1, 1 | a, a + 1 \\ a + 1 | 2, b + 1 \end{matrix} \middle| ; z, z \right), \tag{35a}$$

$$G^{(2)}(a, b; z) = \frac{z^2}{(b)_2} \Theta^{(2)}\left( \begin{matrix} 1, 1, 1 | a, a + 1, a + 2 \\ a + 1, a + 2 | 3, b + 2 \end{matrix} \middle| ; z, z, z \right), \tag{35b}$$

$$G^{(n)}(a, b; z) = \frac{z^n}{(b)_n} \Theta^{(n)}\left( \begin{matrix} 1, 1, \dots, 1 | a, a + 1, \dots, a + n \\ a + 1, a + 2, \dots, a + n | n + 1, b + n \end{matrix} \middle| ; z, z, \dots, z \right). \tag{35c}$$

Similar expressions can be obtained for  $H^{(n)}$  following the same procedure:

$$H^{(n)}(a, b; z) = (-1)^n \frac{n! a}{b^n b} z \Theta^{(n)}\left( \begin{matrix} 1, 1, \dots, 1 | b, b, \dots, b, a + 1 \\ b + 1, b + 1, \dots, b + 1 | 2, b + 1 \end{matrix} \middle| ; z, z, \dots, z \right). \tag{36}$$

With these derivatives one may thus provide Taylor expansions for the function  $F$  in power series of  $a$  around  $a_0$  or of  $b$  around  $b_0$ ,

$$F = \sum_{n=0}^{\infty} \frac{(a-a_0)^n}{n!} G^{(n)}(a_0, b; z), \quad (37a)$$

$$F = \sum_{n=0}^{\infty} \frac{(b-b_0)^n}{n!} H^{(n)}(a, b_0; z). \quad (37b)$$

Here we are using the notation

$$G^{(0)}(a_0, b; z) = {}_1F_1\left(\begin{matrix} a_0 \\ b \end{matrix} \middle| ; z\right) \text{ and } H^{(0)}(a, b_0; z) = {}_1F_1\left(\begin{matrix} a \\ b_0 \end{matrix} \middle| ; z\right).$$

In Sec V, we shall use expansion (37a) for  $a_0=0$ .

### B. Particular value: $a=0$

The hypergeometric functions  $\Theta^{(n)}$  defined by Eq. (34) depend on a large number of parameters. However, in the expression of the derivatives  $G^{(n)}$  and  $H^{(n)}$  [Eqs. (35c)–(36)], only the parameters  $a$  and  $b$  of the initial function  $F$  are actually variable. Since in the calculations to be performed in Sec. V we will need the evaluation of  $G^{(n)}(a, b; z)$  (with  $n \geq 1$ ) for  $a=0$ , we now provide explicit formulas for this situation.

The reduction formulas for the  $n$ th derivatives  $G^{(n)}$  in the case  $a=0$  can be related to those, presented in Appendix B, corresponding to the  $\Theta^{(n)}$  functions. The results are

$$G^{(1)}(0, b; z) = \frac{z}{(b)_1} \Theta^{(1)}\left(\begin{matrix} 1, 1|0, 1 \\ 1|2, b+1 \end{matrix} \middle| ; z, z\right) = \frac{z}{(b)_1} {}_2F_2\left(\begin{matrix} 1, 1 \\ 2, b+1 \end{matrix} \middle| ; z\right), \quad (38a)$$

$$G^{(2)}(0, b; z) = \frac{z^2}{(b)_2} \Theta^{(1)}\left(\begin{matrix} 1, 1|1, 2 \\ 2|3, b+2 \end{matrix} \middle| ; z, z\right), \quad (38b)$$

$$G^{(n)}(0, b; z) = \frac{z^n}{(b)_n} \Theta^{(n-1)}\left(\begin{matrix} 1, \dots, 1|1, \dots, n \\ 2, 3, \dots, n|n+1, b+n \end{matrix} \middle| ; z, \dots, z\right). \quad (38c)$$

The  $n$ th derivatives  $G^{(n)}$  ( $n > 1$ ) for  $a=0$ , defined in terms of  $\Theta^{(n)}$ , are thus expressed in terms of a function  $\Theta^{(n-1)}$ .

### C. Recurrence relations for $G^{(n)}$

#### 1. Relations for general $a$ and $b$

Starting from the recurrence relations for the confluent hypergeometric function  $F$ , recurrence relations for the  $\Theta^{(1)}$  function can be easily deduced. For example, consider the contiguous relation (13.4.4) of Ref. 14:

$$b {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| ; z\right) - b {}_1F_1\left(\begin{matrix} a-1 \\ b \end{matrix} \middle| ; z\right) - z {}_1F_1\left(\begin{matrix} a \\ b+1 \end{matrix} \middle| ; z\right) = 0. \quad (39)$$

If we take the derivative with respect to  $a$ , we find

$$bG^{(1)}(a, b; z) - bG^{(1)}(a-1, b; z) - zG^{(1)}(a, b+1; z) = 0, \quad (40)$$

and hence, using Eq. (20a), a relation for  $\Theta^{(1)}$ :



$$\Theta^{(1)}\left(\begin{matrix} 1, 1|a, a+1 \\ a+1|2, b+1 \end{matrix} \middle| z, z\right) - \Theta^{(1)}\left(\begin{matrix} 1, 1|a-1, a \\ a|2, b+1 \end{matrix} \middle| z, z\right) - \frac{z}{b+1}\Theta^{(1)}\left(\begin{matrix} 1, 1|a, a+1 \\ a+1|2, b+2 \end{matrix} \middle| z, z\right) = 0. \quad (41)$$

Similarly using relation (13.4.13) of Ref. 14, one finds a relation providing the derivative of the  $\Theta^{(1)}$  function with respect to  $z$ ,

$$\frac{z}{b} \frac{d}{dz} \Theta^{(1)}\left(\begin{matrix} 1, 1|a, a+1 \\ a+1|2, b+1 \end{matrix} \middle| z, z\right) = \Theta^{(1)}\left(\begin{matrix} 1, 1|a, a+1 \\ a+1|2, b \end{matrix} \middle| z, z\right) - 2\Theta^{(1)}\left(\begin{matrix} 1, 1|a, a+1 \\ a+1|2, b+1 \end{matrix} \middle| z, z\right). \quad (42)$$

Several other relations can be obtained in a similar way and easily generalized to  $\Theta^{(n)}$ .

## 2. Relations for $a=0$

Let us introduce also the following function:

$$G^{(n,m)}(a, b; z) = \frac{z^n}{(b)_n} \Theta^{(n)}\left(\begin{matrix} 1, 1, \dots, 1|a, a+1, \dots, a+n \\ a+1, a+2, \dots, a+n|m+1, b+n \end{matrix} \middle| z, z, \dots, z\right). \quad (43)$$

By inspection of relation (38c), we see that

$$G^{(n,m)}(0, b; z) = \frac{1}{b} z G^{(n-1,m)}(1, b+1; z). \quad (44)$$

As a consequence, we have the following recurrence relation for  $n \geq 2$ :

$$G^{(n)}(0, b; z) = G^{(n,n)}(0, b; z) = \frac{1}{b} z G^{(n-1,n)}(1, b+1; z). \quad (45)$$

## D. Series and integral representations in terms of one-variable hypergeometric functions

In this section we provide series and integral representations for  $\Theta^{(1)}$  in terms of well known one-variable hypergeometric functions (generalization to  $\Theta^{(n)}$  can be easily obtained). Using series rearrangement techniques and different properties for the Pochhammer symbols, it is easy to verify that the following series representations hold for the  $\Theta^{(1)}$  function:

$$\Theta^{(1)}\left(\begin{matrix} a_1, a_2|b_1, b_2 \\ c_1|d_1, d_2 \end{matrix} \middle| x_1, x_2\right) = \sum_{m_1=0}^{\infty} \frac{(a_1)_{m_1} (b_1)_{m_1} (b_2)_{m_1} x_1^{m_1}}{(c_1)_{m_1} (d_1)_{m_1} (d_2)_{m_1} m_1!} {}_2F_2\left(\begin{matrix} a_2, b_2 + m_1 \\ d_1 + m_1, d_2 + m_1 \end{matrix} \middle| x_2\right) \quad (46a)$$

$$= \sum_{m_2=0}^{\infty} \frac{(a_2)_{m_2} (b_2)_{m_2} x_2^{m_2}}{(d_1)_{m_2} (d_2)_{m_2} m_2!} {}_3F_3\left(\begin{matrix} a_1, b_1, b_2 + m_2 \\ c_1, d_1 + m_2, d_2 + m_2 \end{matrix} \middle| x_1\right). \quad (46b)$$

Definitions for  $G^{(1)}$  and  $H^{(1)}$  result immediately from Eqs. (20a) and (20b). Equation (46a) is the formulation encountered in Eqs. (15) and (16). The rate of convergence of these series is faster than the one corresponding to the double series of Eq. (19) as illustrated in Fig. 1, where we plot  $\Theta^{(1)}$  given in Eq. (35a) as a function of  $x_1 = x_2 = ix$  for fixed values of the parameters  $a = i/0.75$  and  $b = 1$  (the value  $b = 1$  and the purely imaginary values of  $a$  and argument correspond to the confluent hypergeometric function appearing in the Coulomb problem, see Sec. V). We used  $m_1 = m_2$  up to 20 to evaluate  $\Theta^{(1)}$  with the double series of Eq. (19) and  $m_1$  up to 20 or 60 with Eq. (46a). As can be noticed from the figure, a much smaller number of terms are needed when the

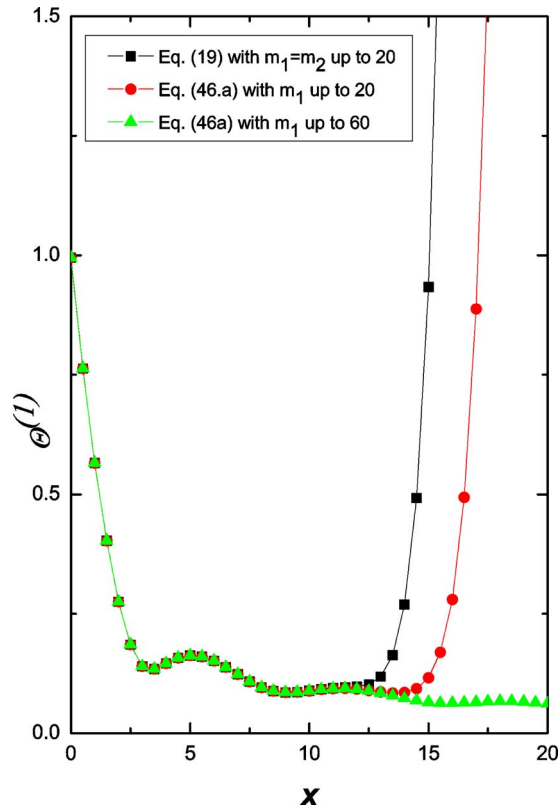


FIG. 1. (Color online) The  $\Theta^{(1)}$  function given in Eq. (35a) is plotted vs the argument  $x_1=x_2=ix$  for fixed values of the parameters  $a=i/0.75$  and  $b=1$ : it is calculated with the double series, Eq. (19) with  $m_1=m_2$  up to 20 (solid line and squares) and the series of Eq. (46a) with  $m_1$  up to 20 (solid lines and circles) or 60 (solid lines and triangles).

single series is used. This is a natural consequence of the fact that the whole series in  $m_2$  has been summed up.

A numerically useful integral representation for  $\Theta^{(1)}$  can be obtained starting from Eq. (46a). Combining the integral representations for the  ${}_2F_2$  (see Ref. 20, p. 854):

$${}_2F_2\left(\begin{matrix} \nu, a \\ \lambda, b \end{matrix} \middle| ; x_2\right) = \frac{\Gamma(\lambda)}{\Gamma(\nu)\Gamma(\lambda-\nu)} \int_0^1 dt(1-t)^{\lambda-\nu-1} t^{\nu-1} {}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| ; x_2 t\right), \quad (47)$$

where  $\Re(\lambda-\nu) > 0$ ,  $\Re \nu > 0$ , and the one corresponding to the  ${}_1F_1$  (Ref. 1):

$${}_1F_1\left(\begin{matrix} a \\ b \end{matrix} \middle| ; z\right) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 du(1-u)^{b-a-1} u^{a-1} e^{zu}, \quad (48)$$

where  $\Re(b-a) > 0$ ,  $\Re a > 0$ , we obtain

$${}_2F_2\left(\begin{matrix} \nu, a \\ \lambda, b \end{matrix} \middle| ; z\right) = \frac{\Gamma(\lambda)\Gamma(b)}{\Gamma(\nu)\Gamma(\lambda-\nu)\Gamma(a)\Gamma(b-a)} \int_0^1 dt(1-t)^{\lambda-\nu-1} t^{\nu-1} \int_0^1 du(1-u)^{b-a-1} u^{a-1} e^{ztu}. \quad (49)$$

The condition over the parameters can be removed by performing the integrations over contours on the complex plane.<sup>1</sup> With this representation, the series of Eq. (46a) becomes

$$\begin{aligned}
& \Theta^{(1)}\left(\begin{array}{c} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{array} \middle| ; x_1, x_2\right) \\
&= \sum_{m_1=0}^{\infty} \frac{(a_1)_{m_1} (b_1)_{m_1} (b_2)_{m_1} x_1^{m_1}}{(c_1)_{m_1} (d_1)_{m_1} (d_2)_{m_1} m_1!} \frac{\Gamma(d_1 + m_1) \Gamma(d_2 + m_1)}{\Gamma(a_2) \Gamma(d_1 + m_1 - a_2) \Gamma(b_2 + m_1) \Gamma(d_2 - b_2)} \\
&\quad \times \int_0^1 dt (1-t)^{d_1+m_1-a_2-1} t^{a_2-1} \int_0^1 du (1-u)^{d_2-b_2-1} u^{b_2+m_1-1} e^{x_2 t u}, \tag{50}
\end{aligned}$$

which after algebraic manipulations converts into

$$\begin{aligned}
& \Theta^{(1)}\left(\begin{array}{c} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{array} \middle| ; x_1, x_2\right) \\
&= \frac{\Gamma(d_1) \Gamma(d_2)}{\Gamma(a_2) \Gamma(d_2 - b_2) \Gamma(b_2) \Gamma(d_1 - a_2)} \int_0^1 dt (1-t)^{d_1-a_2-1} t^{a_2-1} \int_0^1 du (1-u)^{d_2-b_2-1} u^{b_2-1} \\
&\quad \times e^{x_2 t u} {}_2F_2\left(\begin{array}{c} a_1, b_1 \\ c_1, d_1 - a_2 \end{array} \middle| ; x_1 (1-t) u\right). \tag{51}
\end{aligned}$$

This integral representation is particularly useful to numerically evaluate  $\Theta^{(1)}$ , and thus  $G^{(1)}$  and  $H^{(1)}$  through the use of Eqs. (20a) and (20b). Following similar procedures, integral and series representations of this type can be obtained for  $\Theta^{(n)}$ , and hence for  $G^{(n)}$  and  $H^{(n)}$ .

### E. Special cases

When  $b=a$ , the function  $F$  reduces to an exponential  $F=e^z$ , so that there is no parameter dependence and  $G^{(1)}=H^{(1)}=0$ . Although the result is trivial, it should appear also through the  $\Theta^{(1)}$ . Indeed, we have

$$\frac{d}{da} {}_1F_1\left(\begin{array}{c} a \\ a \end{array} \middle| ; z\right) = G^{(1)}(a, a; z) + H^{(1)}(a, a; z), \tag{52}$$

and using Eqs. (20a) and (20b), we immediately find 0.

When  $b=a-1$ , the function  $F$  reduces to

$${}_1F_1\left(\begin{array}{c} a \\ a-1 \end{array} \middle| ; z\right) = e^z {}_1F_1\left(\begin{array}{c} -1 \\ a-1 \end{array} \middle| ; -z\right) = e^z \left(1 + \frac{z}{a-1}\right). \tag{53}$$

The derivative with respect to  $a$  is  $G^{(1)}=-ze^z/(a-1)^2$ , a result which can be easily found by applying, for example, Eq. (20b).

Another interesting situation is when  $b=a+1$  since the  $F$  function is related to the incomplete gamma function

$${}_1F_1\left(\begin{array}{c} a \\ a+1 \end{array} \middle| ; z\right) = a(-z)^{-a} \gamma(a, -z). \tag{54}$$

In this case the derivative of the confluent hypergeometric function with respect to  $a$  reads

$$\frac{d}{da} {}_1F_1\left(\begin{array}{c} a \\ a+1 \end{array} \middle| ; z\right) = G^{(1)}(a, a+1; z) + H^{(1)}(a, a+1; z) = \frac{z}{(a+1)^2} \Theta^{(1)}\left(\begin{array}{c} 1, 1 | a, a+1 \\ a+2 | 2, a+2 \end{array} \middle| ; z, z\right). \tag{55}$$

Hence, the first derivative with respect to  $a$  of the incomplete Gamma function reads

$$\frac{d}{da} \gamma(a, -z) = \gamma(a, -z) \left[ \ln(-z) - \frac{1}{a} \right] + \frac{(-z)^a}{a} \frac{z}{(a+1)^2} \Theta^{(1)} \left( \begin{matrix} 1, 1 | a, a+1 \\ a+2 | 2, a+2 \end{matrix} ; z, z \right)$$

and the  $n$ th derivative can be easily derived with the results given in the previous sections. Other special cases can be considered in a similar manner.

## V. APPLICATION TO THE BORN-LIKE SERIES FOR THE TWO-BODY COULOMB SCATTERING WAVE FUNCTION

As we mentioned in the Introduction, a close connection exists between the Kummer function and the two-body Coulomb problem. Let  $\mathbf{r}$  and  $\mathbf{k}$  respectively represent the relative vector position and momentum between an electron and a heavy nucleus of charge  $Z$  placed at the origin of coordinates. The solution for the scattering problem in parabolic coordinates is given by<sup>4</sup>

$$\Psi^+(\alpha, \mathbf{k}, \mathbf{r}) = N(\alpha) e^{i\mathbf{k}\cdot\mathbf{r}} {}_1F_1 \left( \begin{matrix} \alpha \\ 1 \end{matrix} ; ik\eta \right), \quad (56)$$

where outgoing wave boundary conditions are considered. The parabolic coordinates are  $\xi = r + \hat{\mathbf{k}}\cdot\mathbf{r}$ ,  $\eta = r - \hat{\mathbf{k}}\cdot\mathbf{r}$ , and  $\tan \phi = y/x$ , where the Cartesian coordinates  $x$  and  $y$  correspond to the position of the particle relative to the reference center.<sup>4</sup> Here atomic units ( $\hbar = m_e = e = 1$ ) are used, so that the electron charge is equal to  $-1$ ;  $\alpha = i(Z/k)$  is the Sommerfeld parameter (we have included  $i$  in its definition for convenience). The normalization factor  $N(\alpha)$  is defined in terms of the gamma function as

$$N(\alpha) = e^{-i(\pi/2)\alpha} \Gamma(1 - \alpha). \quad (57)$$

Let us consider the expansion of the scattering wave function  $\Psi^+(\alpha, \mathbf{k}, \mathbf{r})$  in power series of the Sommerfeld parameter  $\alpha$ :

$$\Psi^+(\alpha, \mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \left( \Psi^{(0)+}(\mathbf{k}, \mathbf{r}) + \Psi^{(1)+}(\mathbf{k}, \mathbf{r})\alpha + \Psi^{(2)+}(\mathbf{k}, \mathbf{r})\frac{\alpha^2}{2} + \dots \right), \quad (58)$$

where  $\Psi^{(l)+}(\mathbf{k}, \mathbf{r})$  is given by

$$\Psi^{(l)+}(\mathbf{k}, \mathbf{r}) = \left. \frac{d^l \Psi^+(\alpha, \mathbf{k}, \mathbf{r})}{d\alpha^l} \right|_{\alpha=0}. \quad (59)$$

Such an expansion is interesting as it is related to the Born series for the Coulomb problem. In order to get analytical expressions for the different orders  $\Psi^{(l)+}(\mathbf{k}, \mathbf{r})$  of (58), we shall need the  $n$ th derivatives  $G^{(n)}$  with respect to the first parameter  $\alpha$  of the confluent hypergeometric function  $F$  appearing in (56). Indeed, they appear in the Taylor expansion (37a) of  $F$  around  $a_0=0$ ; we have

$$F = G^{(0)}(0, 1; ik\eta) + G^{(1)}(0, b; ik\eta)\alpha + \frac{\alpha^2}{2} G^{(2)}(0, 1; ik\eta) + \dots, \quad (60)$$

where  $G^{(0)} = {}_1F_1(0, 1; ik\eta) = 1$ . We also need to expand  $N(\alpha)$  in power series of  $\alpha$ :

$$N(\alpha) = N^{(0)} + N^{(1)}\alpha + N^{(2)}\frac{\alpha^2}{2} + \dots, \quad (61)$$

where

$$N^{(0)} = 1, \quad (62a)$$

$$N^{(1)} = \left( \gamma - i\frac{\pi}{2} \right), \quad (62b)$$

$$N^{(2)} = \left( \gamma^2 - i\gamma\pi - \frac{\pi^2}{12} \right), \quad (62c)$$

and  $\gamma$  represents the Euler gamma constant.<sup>14</sup>

Combining the two series expansions (60) and (61) and comparing with (58), the following expressions are readily deduced for the first three terms:

$$\Psi^{(0)+}(\mathbf{k}, \mathbf{r}) = N^{(0)} G^{(0)}(0, 1; ik\eta), \quad (63a)$$

$$\Psi^{(1)+}(\mathbf{k}, \mathbf{r}) = N^{(1)} G^{(0)}(0, 1; ik\eta) + N^{(0)} G^{(1)}(0, 1; ik\eta), \quad (63b)$$

$$\Psi^{(2)+}(\mathbf{k}, \mathbf{r}) = N^{(2)} G^{(0)}(0, 1; ik\eta) + 2N^{(1)} G^{(1)}(0, 1; ik\eta) + N^{(0)} G^{(2)}(0, 1; ik\eta). \quad (63c)$$

Using (62a)–(62c) and the reduction formulas (38a) and (38b) for, respectively,  $G^{(1)}$  and  $G^{(2)}$ , we find

$$\Psi^{(0)+}(\mathbf{k}, \mathbf{r}) = 1, \quad (64a)$$

$$\Psi^{(1)+}(\mathbf{k}, \mathbf{r}) = \left( \gamma - i\frac{\pi}{2} \right) + (ik\eta) {}_2F_2 \left( \begin{matrix} 1, 1 \\ 2, 2 \end{matrix} \middle| ; ik\eta \right), \quad (64b)$$

$$\begin{aligned} \Psi^{(2)+}(\mathbf{k}, \mathbf{r}) = & \left( \gamma^2 - i\gamma\pi - \frac{\pi^2}{12} \right) + 2 \left( \gamma - i\frac{\pi}{2} \right) (ik\eta) {}_2F_2 \left( \begin{matrix} 1, 1 \\ 2, 2 \end{matrix} \middle| ; ik\eta \right) \\ & + \frac{(ik\eta)^2}{2} \Theta^{(1)} \left( \begin{matrix} 1, 1 | 1, 2 \\ 2 | 3, 3 \end{matrix} \middle| ; ik\eta, ik\eta \right). \end{aligned} \quad (64c)$$

The numerical evaluation of  $\Theta^{(1)}$  can be easily performed using one of the representations given in Sec. IV D. The function  ${}_2F_2$  appearing in  $\Psi^{(1)+}$  and  $\Psi^{(2)+}$  can be reduced to simpler functions.<sup>21</sup>

$${}_2F_2 \left( \begin{matrix} 1, 1 \\ 2, 2 \end{matrix} \middle| ; ik\eta \right) = \frac{-\gamma - \log(-ik\eta) - \Gamma(0, -ik\eta)}{ik\eta},$$

where  $\Gamma(a, z)$  represents the incomplete gamma function.<sup>14</sup>

Explicit expressions of  $\Psi^{(n)+}(\mathbf{k}, \mathbf{r})$  have been given here up to order  $n=2$ ; higher orders can be easily obtained in terms of the generalized hypergeometric functions  $\Theta^{(n)}$  [or of  $\Theta^{(n-1)}$  if the reduction formula (45) is used]. In order to reduce the difficulties in their evaluations, further investigation of the properties of the multivariable hypergeometric functions  $\Theta^{(n)}$  defined here is necessary.

## VI. SUMMARY

We have given closed form formulas for the  $n$ th derivatives of the Kummer function with respect to its parameters  $a$  and  $b$ . These derivatives are expressed in terms of multivariable Kampé de Fériet-like hypergeometric functions, named here  $\Theta^{(n)}$ . For  $\Theta^{(1)}$ , which is related to the first derivatives, various types of properties such as recurrence relations and series and integral representations are provided, and some special cases are discussed. The system of ordinary differential equations satisfied for the derivatives of order  $n$  is also given.

The above mathematical study is applied to the physical case of the two-body Coulomb scattering wave function, for which the exact solution in parabolic coordinates is written in terms of the Kummer function. A power series expansion in terms of the Sommerfeld parameter is considered, and analytic (closed form) expressions up to order 2 were given for the terms, which

are functions only of the energy and the (parabolic) coordinate. Further studies of the hypergeometric functions  $\Theta^{(n)}$  here introduced are necessary and this is the subject of our current investigations.

Finally, an investigation of the derivatives of the generalized hypergeometric functions  ${}_pF_q$  with respect to its parameters would also be of interest. In particular, the  ${}_2F_1$  case can be of high interest because of its application to the study of many physical problems.

## ACKNOWLEDGMENTS

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## APPENDIX A: DEMONSTRATION OF FORMULA (28) FOR $G^{(2)}$

To get the explicit formula (28) for  $G^{(2)}$ , we start with the differential equation (25) it satisfies:

$$\left[ z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] G^{(2)} = 2G^{(1)}, \quad (\text{A1})$$

and the expression of  $G^{(1)}$  [Eq. (17a)]:

$$G^{(1)} = \frac{z}{(b)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (a)_{m_1} (a+1)_{m_1+m_2}}{(a+1)_{m_1} (2)_{m_1+m_2} (b+1)_{m_1+m_2} m_1! m_2!} z^{m_1+m_2}. \quad (\text{A2})$$

Using solution (13) of the inhomogeneous Kummer equation (12), we have

$$G^{(2)} = \frac{2}{(b)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (a)_{m_1} (a+1)_{m_1+m_2}}{(a+1)_{m_1} (2)_{m_1+m_2} (b+1)_{m_1+m_2} m_1! m_2!} \theta_{m_1+m_2+1+1}(a, b; z), \quad (\text{A3})$$

which in terms of hypergeometric functions  ${}_2F_2$  becomes

$$G^{(2)} = \frac{2}{(b)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (a)_{m_1} (a+1)_{m_1+m_2}}{(a+1)_{m_1} (2)_{m_1+m_2} (b+1)_{m_1+m_2} m_1! m_2!} z^{m_1+m_2+2} \times \frac{1}{(2+m_1+m_2)(b+1+m_1+m_2)} {}_2F_2 \left( \begin{matrix} 1, m_1+m_2+1+a+1 \\ m_1+m_2+1+2, m_1+m_2+1+b+1 \end{matrix} \middle| ; z \right) \quad (\text{A4})$$

Using the two identities

$$\frac{1}{(n+\lambda)} = \frac{1}{\lambda} \frac{(\lambda)_n}{(\lambda+1)_n},$$

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

and simplifying, we find

$$G^{(2)} = \frac{1}{(b)_1 (b+1)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(1)_{m_1} (1)_{m_2} (a)_{m_1} (a+1)_{m_1+m_2}}{(3)_{m_1+m_2} (a+1)_{m_1} (b+2)_{m_1+m_2}} \times \frac{z^{m_1+m_2+2}}{m_1! m_2!} {}_2F_2 \left( \begin{matrix} 1, a+m_1+m_2+2 \\ m_1+m_2+3, b+m_1+m_2+2 \end{matrix} \middle| ; z \right). \quad (\text{A5})$$

Now, replacing the series expansion (index  $m_3$ ) for the  ${}_2F_2$  function leads to a triple series:

$$G^{(2)} = \frac{1}{(b)_1(b+1)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(1)_{m_1}(1)_{m_2}(a)_{m_1}(a+1)_{m_1+m_2}}{(3)_{m_1+m_2}(a+1)_{m_1}(b+2)_{m_1+m_2}} \\ \times \frac{(1)_{m_3}(a+m_1+m_2+2)_{m_3}}{(m_1+m_2+3)_{m_3}(b+m_1+m_2+2)_{m_3}} \frac{z^{m_1+m_2+m_3+2}}{m_1!m_2!m_3!}, \quad (\text{A6})$$

which, after some algebraic manipulations, finally simplifies into

$$G^{(2)} = \frac{z^2}{(b)_1(b+1)_1} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \frac{(1)_{m_1}(1)_{m_2}(1)_{m_3}}{(3)_{m_1+m_2+m_3}(b+2)_{m_1+m_2+m_3}} \\ \times \frac{(a)_{m_1}(a+1)_{m_1+m_2}(a+2)_{m_1+m_2+m_3}}{(a+1)_{m_1}(a+2)_{m_1+m_2}} \frac{z^{m_1+m_2+m_3}}{m_1!m_2!m_3!}. \quad (\text{A7})$$

Similar calculations can be performed to obtain  $G^{(n)}$  for  $n > 2$ .

## APPENDIX B: REDUCTION FORMULAS FOR $\Theta^{(n)}$

In this appendix, we provide the reduction formulas for the hypergeometric functions  $\Theta^{(n)}$  defined by Eq. (34), in the case where  $b_1$  is set to zero. Starting from the  $n=1$  case, we see that in the double series expansion (19), only the  $m_1=0$  term survives in the summation, so that

$$\Theta^{(1)} \left( \begin{array}{c} a_1, a_2 | 0, b_2 \\ c_1 | d_1, d_2 \end{array} \middle| x_1, x_2 \right) = {}_2F_2 \left( \begin{array}{c} a_2, b_2 \\ d_1, d_2 \end{array} \middle| x_2 \right). \quad (\text{B1})$$

Similarly from Eq. (33) for the  $n=2$  case and from Eq. (34) for the general  $n > 1$  case, one easily finds

$$\Theta^{(2)} \left( \begin{array}{c} a_1, a_2, a_3 | 0, b_2, b_3 \\ c_1, c_2 | d_1, d_2 \end{array} \middle| x_1, x_2, x_3 \right) = \Theta^{(1)} \left( \begin{array}{c} a_2, a_3 | b_2, b_3 \\ c_2 | d_1, d_2 \end{array} \middle| x_2, x_3 \right), \quad (\text{B2})$$

$$\Theta^{(n)} \left( \begin{array}{c} a_1, a_2, \dots, a_{n+1} | 0, b_2, \dots, b_{n+1} \\ c_1, \dots, c_n | d_1, d_2 \end{array} \middle| x_1, x_2, \dots, x_{n+1} \right) \\ = \Theta^{(n-1)} \left( \begin{array}{c} a_2, \dots, a_{n+1} | b_2, \dots, b_{n+1} \\ c_2, \dots, c_n | d_1, d_2 \end{array} \middle| x_2, \dots, x_{n+1} \right). \quad (\text{B3})$$

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