Treatment of the two-body Coulomb problem as a short-range potential

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The scattering wave function and the transition amplitude for the two-body Coulomb problem are written as power series of the Sommerfeld parameter. Making use of a mathematical study of the *n*th derivatives of Kummer function with respect to its first parameter, the series coefficients are expressed analytically in terms of multivariable hypergeometric functions. We establish the connection with the Born series based on the free particle Green's function and show its applicability to long-range potentials. We also relate our analysis to recent works on the distorted-wave theory for the Coulomb problem. For the transition amplitude, the Born series is presented and compared to the series obtained from the exact well-known Rutherford result. Since the two series differ, care must be taken when extracting the relevant information about the scattering. Finally, implications for three-body problems are discussed.

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I. INTRODUCTION

Many important collision processes of interest for the atomic and molecular physics community are ruled by Coulomb long-range forces. The latter imply both mathematical complications and conceptual modifications in the standard scattering theory. To deal with the known difficulties associated to the two-body Coulomb potential, a large variety of strategies have been developed [1]. Among the analytical approaches, the distorted-wave theory [2] allows one to circumvent the difficulties by dressing the initial state through the inclusion of the asymptotic influence of the potential's long-range tail. Other significative advances on the theoretical understanding of this topic have been reported very recently for two- and three-body Coulomb problems [3–8]. On the numerical side, several L^2 conversions of the wave functions have been implemented, in combination with techniques to treat the potential long range [9–14]. In the exterior complex scaling approach for the two-body Coulomb problem, for example, the technique relies on transforming the Schrödinger equation into a nonhomogeneous equation whose nonhomogeneity is the product of the Coulomb potential and a free particle wave function [14]. The problem is solved by rotating the radial coordinate r to the complex plane for values greater than a given r_0. Two additional ingredients appear: (i) the treatment of the source (the nonhomogeneity) and (ii) the enforcement of the boundary condition to the scattering solution [14]. To avoid numerical divergences, the source is set to zero for values of $r \geq r_0$; this corresponds to cutting the Coulomb potential at $r=r_0$. On the other hand, the Coulomb potential appearing on the left side of the equation is not cut. The scattering wave function is set equal zero at a value $r_1 > r_0$: this is *numerically* justified by the fact that the wave function must have, e.g., outgoing behavior and the rotation of the coordinate produces therefore an exponentially decreasing behavior [14]. The solution obtained in this way numerically converges to the exact two-body Coulomb wave function. The same method has been successfully extended and applied for three-body problems [15]. Alternative techniques to deal with the Coulomb potential have been implemented within the framework of other numerical methods such as the convergent close coupling and J matrix (see, e.g., [9,11,13]).

The aim of this paper is to understand the physics behind the traditional Lippmann-Schwinger equation and the Born series for the long-range two-body Coulomb potential. For this purpose, we study the scattering wave function and the transition amplitude, presenting both of them as power series in the Sommerfeld parameter, and establish the connection with the Born series based on the free particle Green's function. We will show that the Born approach is indeed applicable for long-range potentials, but care must be taken when extracting the relevant information about the scattering. The conclusions obtained here would apply equally to three-body problems where Coulomb interactions are used as perturbation potentials; the implications in this case will also be also discussed.

To construct the Born series for the two-body Coulomb potential, we use the closed-form solution of the Schrödinger equation. In parabolic coordinates, it is written in terms of a confluent hypergeometric function ${}_1F_1(a,b;z)$, known also as Kummer function [16–18], where a is related to the Sommerfeld parameter. As we shall see (Sec. II A), the Born series for the scattering wave function can be obtained through the use of the derivatives of the Kummer function with respect to the first parameter a, evaluated at $a=0$. The transition amplitude for the two-body problem will be studied in a similar manner (Sec. III); both these quantities are finally expressed as power series of the Sommerfeld parameter and analytical coefficients are provided in terms of multivariable hypergeometric functions. The investigation will show how the series obtained from the well-known Coulomb scattering amplitude differs from the Born series. The connection with the approach of Kadyrov *et al.* [5] for the wave function will be presented in Sec. II B. We shall also illustrate how the construction of the collision process depends on the chosen decomposition of the Coulomb potential into short- and long-range parts (Sec. II C). A summary of the results as well as implications for three-body problems are presented in Sec. IV.

II. BORN-LIKE SERIES FOR THE SCATTERING WAVE FUNCTION

Consider the two-body Coulomb problem. Let $\mathbf{r}$ and $\mathbf{k}$, respectively, represent the relative vector position and momentum between two charged particles with charges z_1 and z_2, e.g., an electron ($z_1=-e$) and a heavy nucleus of charge $z_2=Ze$. Let $\alpha=\frac{z_1 z_2 \mu}{k}$ be the Sommerfeld parameter, where μ represents the reduced mass of the particles. It is assumed in the following calculations that z_1 is negative and z_2 is positive; atomic units ($\hbar=m_e=e=1$) are used throughout.

The Coulomb solutions for the scattering problem can be expressed in terms of the parabolic coordinates $\xi=r+\hat{\mathbf{k}}\cdot\mathbf{r}$, $\eta=r-\hat{\mathbf{k}}\cdot\mathbf{r}$, and $\tan\phi=\frac{y}{x}$, where the Cartesian coordinates x and y correspond to the position of the particle relative to the reference center [16]. In what follows, we shall analyze explicitly the Coulomb wave function with outgoing boundary conditions

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = N(\alpha) e^{i\mathbf{k}\cdot\mathbf{r}} {}_1F_1\left(\begin{array}{c} -i\alpha \\ 1 \end{array}\middle|\; ;ik\eta\right). \tag{1}$$

The case of the solutions $\Psi^{-}(\alpha,\mathbf{k},\mathbf{r})$ with incoming boundary conditions can be treated similarly. The functions $\Psi^{\pm}(\alpha,\mathbf{k},\mathbf{r})$ are solutions of Schrödinger equation

$$[H_0 + V_c(r) - E]\Psi^{\pm}(\alpha,\mathbf{k},\mathbf{r}) = 0 \tag{2}$$

where $H_0=-\frac{1}{2\mu}\nabla^2$ and $V_c(r)=\frac{z_1 z_2}{r}$ is the Coulomb potential. In Eq. (1), ${}_1F_1(a,b;z)$ is the confluent hypergeometric function [18] and the normalization factor $N(\alpha)$ is defined in terms of the Gamma function $\Gamma(z)$ [18] as

$$N(\alpha) = e^{(-\pi/\alpha 2)}\Gamma(1+i\alpha). \tag{3}$$

The asymptotic form of the Coulomb wave function $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ can be written as [2]

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) \to e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{E}(\alpha,\mathbf{k},\mathbf{r}) + f(\theta)\frac{e^{ikr}}{r}\mathcal{E}_s(\alpha,k,r). \tag{4}$$

Here, $f(\theta)$—the scattering amplitude—represents the probability for the particles coming along the direction $\hat{\mathbf{k}}_i$ to be scattered at an angle θ defined by $\theta=\cos^{-1}(\hat{\mathbf{k}}_i\cdot\hat{\mathbf{k}}_f)$, i.e., leaving the scattering center with momentum k_f in a direction $\hat{\mathbf{k}}_f$ with respect to $\hat{\mathbf{k}}_i$. The quantities $\mathcal{E}(\alpha,\mathbf{k},\mathbf{r})=e^{i\alpha\ln(kr-\mathbf{k}\cdot\mathbf{r})}$ and $\mathcal{E}_s(\alpha,k,r)=e^{-i\alpha\ln(2kr)}$ are the eikonal functions which arise as a consequence of the long-range nature of the Coulomb potential. The "Rutherford" scattering amplitude $f(\theta)$ is explicitly given in Ref. [2]

$$f(\theta) = -\frac{\mu z_1 z_2}{2k^2\sin^2\frac{\theta}{2}}\exp\left[-i\alpha\ln\left(\sin^2\frac{\theta}{2}\right) + 2i\sigma_c\right], \tag{5}$$

where $\sigma_c=\mathrm{Arg}[\Gamma(1+i\alpha)]$. Both terms in Eq. (4) are putting in evidence the "collision" of the incident particles with the scattering center. In a classical sense, see e.g., Ref. [19], the $e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{E}(\alpha,\mathbf{k},\mathbf{r})$ term indicates that the center deviates the incident particle: there appears a *deflection* but not a *scattering* (indeed, the term can be associated with a set of classical particles with trajectories normal to the surface generated by the phase $\mathbf{k}\cdot\mathbf{r}+\alpha\ln(kr-\mathbf{k}\cdot\mathbf{r})$, thus representing the deflection of the particles, but not their scattering). The second term, $f(\theta)\frac{\exp(ikr)}{r}\mathcal{E}_s(\alpha,k,r)$, describes the incident particle being scattered out by the scattering center. This interpretation will be further discussed below.

A. Born series in power of the charge

There are at least two methods that can be applied to obtain a power-series expansion of the wave function $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ in terms of the Sommerfeld parameter α. A first method is based on the Born series for the Coulomb problem [20,21]. It is obtained by solving, with an iterative procedure, the Lippmann-Schwinger equation [22]

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d\mathbf{r}' G_0(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}'), \tag{6}$$

where $G_0(\mathbf{r},\mathbf{r}')$ is the free-particle Green's function [22] and $V(\mathbf{r})$ is the Coulomb potential. The systematic replacement of the left-hand side of Eq. (6) on the right side leads to the following series:

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d\mathbf{r}_1 G_0(\mathbf{r},\mathbf{r}_1)V(\mathbf{r}_1)e^{i\mathbf{k}\cdot\mathbf{r}_1} + \int d\mathbf{r}_2 G_0(\mathbf{r},\mathbf{r}_2)V(\mathbf{r}_2)\int d\mathbf{r}_1 G_0(\mathbf{r}_2,\mathbf{r}_1)V(\mathbf{r}_1)e^{i\mathbf{k}\cdot\mathbf{r}_1} + \cdots. \tag{7}$$

Since the Green's function is inversely proportional to the energy (e.g., its spectral representation), the Born series can thus be considered as a power series of $\frac{z_1 z_2 \mu}{k}$ and an alternative formulation of Eq. (7) is then

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = \Psi_B^{(0)+}(\mathbf{k},\mathbf{r}) + \alpha\Psi_B^{(1)+}(\mathbf{k},\mathbf{r}) + \frac{\alpha^2}{2}\Psi_B^{(2)+}(\mathbf{k},\mathbf{r}) + \cdots, \tag{8}$$

where the first three terms read

$$\Psi_B^{(0)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{9a}$$

$$\Psi_B^{(1)+}(\mathbf{k},\mathbf{r}) = \left(\frac{z_1 z_2 \mu}{k}\right)^{-1}\int d\mathbf{r}_1 G_0(\mathbf{r},\mathbf{r}_1)V(\mathbf{r}_1)e^{i\mathbf{k}\cdot\mathbf{r}_1}, \tag{9b}$$

$$\Psi_B^{(2)+}(\mathbf{k},\mathbf{r}) = 2\left(\frac{z_1 z_2 \mu}{k}\right)^{-2}\int d\mathbf{r}_2 G_0(\mathbf{r},\mathbf{r}_2)V(\mathbf{r}_2) \times \int d\mathbf{r}_1 G_0(\mathbf{r}_2,\mathbf{r}_1)V(\mathbf{r}_1)e^{i\mathbf{k}\cdot\mathbf{r}_1}. \tag{9c}$$

An alternative method is obtained by directly defining $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ as given by the series (8) (where we omit the subscript B). Upon replacement into Schrödinger equation

(2) and grouping according to successive powers of $z_1 z_2$, we find

$$[E-H_0]\Psi^{(0)+}(\mathbf{k},\mathbf{r})=0, \tag{10a}$$

$$[E-H_0]\Psi^{(1)+}(\mathbf{k},\mathbf{r})=\frac{k}{\mu}\frac{1}{r}\Psi^{(0)+}(\mathbf{k},\mathbf{r}), \tag{10b}$$

$$\vdots$$

$$[E-H_0]\Psi^{(n)+}(\mathbf{k},\mathbf{r})=n\,!\,\frac{k}{\mu}\frac{1}{r}\Psi^{(n-1)+}(\mathbf{k},\mathbf{r}). \tag{10c}$$

Each term $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$ $(n>1)$ of the series (8) satisfies a nonhomogeneous Schrödinger equation; using Green's technique, we straightforwardly get the solutions (9a)–(9c).

The standard understanding of the Born series described in the quantum mechanics and collision books [22–24] is as follows. The zeroth order, $\Psi_B^{(0)+}$, represents the asymptotically free incident particles. The first order, $\Psi_B^{(1)+}$, represents only one interaction between the incident particle and the scattering center. The second order, $\Psi_B^{(2)+}$, considers waves which are scattered twice by the potential $V(\mathbf{r})$ and the nth order to n interactions between the incident particles and the dispersion center. The scattering theory also establishes that each term of the series is represented at large distances r by a spherical wave coming from the asymptotic limit of the free particle Green's function $G_0(\mathbf{r},\mathbf{r}_i)$. From these asymptotic limits, the scattering amplitude is obtained to each order [22,24]. This theory also assumes short-range potential as a condition for its validity and the convergency of the series (8), so that distorted-wave approaches are necessary if long-range potentials are involved [5]. This last point is associated to the fact that the plane wave might not be the asymptotic solution of the problem for long-range potentials are involved and divergent phases may appear in the wave functions and transition amplitudes. In the case we are considering here, $V(\mathbf{r})$ is the Coulomb potential $V_c(r)$ which is of long range, so that some doubts appear about the validity of the Born series based on the free-particle Green's function. We shall show below that the Born series (7) converges and builds up the collisional process in a very particular way.

The evaluation of the integrals appearing in Eq. (7) is not an easy task [20] and, to the best of our knowledge, this has not been done before in a general way. Here, we shall show that it is possible to obtain analytically the terms of arbitrary order of the series and shall give the explicit expressions up to order 2. To do this, we use the following approach.

By taking the derivatives of $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ with respect to α, we may write the Taylor series (as done by Botero and Macek [20]) as

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})=\sum_{n=0}^{\infty}\Psi^{(n)+}(\mathbf{k},\mathbf{r})\frac{\alpha^n}{n!}, \tag{11}$$

where

$$\Psi^{(n)+}(\mathbf{k},\mathbf{r})=\left.\frac{d^n\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})}{d\alpha^n}\right|_{\alpha=0}. \tag{12}$$

Such an expansion is interesting as it is related to the previous (Green's) method, since each term $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$ will contain the information about the corresponding order $\Psi_B^{(n)+}(\mathbf{k},\mathbf{r})$ of the Born series (8). Actually, the functions defined by Eq. (12) are the solutions to the nonhomogeneous equations (10a)–(10c).

In order to find the different orders of $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$, we need to combine the expansions in powers of α for both $N(\alpha)$ and the confluent hypergeometric function ${}_1F_1$ appearing in Eq. (1). The series for $N(\alpha)$,

$$N(\alpha)=\sum_{n=0}^{\infty}N^{(n)}\frac{\alpha^n}{n!}, \tag{13}$$

can be easily obtained from Eq. (3) by expanding both the exponential and the Gamma function

$$N(\alpha)=\left[\sum_{k=0}^{\infty}\left(-\frac{\pi}{2}\right)^k\frac{\alpha^k}{k!}\right]\left(\sum_{k=0}^{\infty}\Gamma^{(k)}\frac{\alpha^k}{k!}\right), \tag{14}$$

where $\Gamma^{(k)}$ is the kth derivative of $\Gamma(1+i\alpha)$ evaluated at $\alpha=0$, given analytically in Ref. [18]. Using the property [see Eq. (0.316) of [25]]

$$\sum_{k=0}^{\infty}a_k x^k\sum_{k=0}^{\infty}b_k x^k=\sum_{n=0}^{\infty}\sum_{k=0}^{n}a_k b_{n-k}x^n, \tag{15}$$

we may write

$$N^{(n)}=\sum_{k=0}^{n}\frac{n!}{(n-k)\,!\,k!}\left(-\frac{\pi}{2}\right)^{(n-k)}\Gamma^{(k)}. \tag{16}$$

The first few terms read

$$N^{(0)}=1, \tag{17a}$$

$$N^{(1)}=-\left(i\gamma+\frac{\pi}{2}\right), \tag{17b}$$

$$N^{(2)}=\left(-\gamma^2+i\gamma\pi+\frac{\pi^2}{12}\right), \tag{17c}$$

where γ represents the Euler Gamma constant [18]. As the expansion in powers of α of the confluent hypergeometric (Kummer) function is concerned, we have [26]

$${}_1F_1\left(\begin{array}{c}-i\alpha\\1\end{array}\middle|\,;ik\eta\right)=\sum_{s=0}^{\infty}G^{(s)}(0,1;ik\eta)\frac{\alpha^s}{s!}, \tag{18}$$

where $G^{(0)}(0,1;ik\eta)={}_1F_1(0,1;ik\eta)=1$ and $G^{(s)}(0,1;ik\eta)$ is the sth derivative of ${}_1F_1$ with respect to the parameter α, evaluated at $\alpha=0$; recently [26], we have given explicit expressions for these derivatives and the necessary formulas are recalled in the Appendix. Combining the product of the series given by Eqs. (13) and (18) and reducing it to a single series [again with the property Eq. (15)], we finally find the coefficients of expansion (11),

$$\Psi^{(n)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{s=0}^{n}\frac{n!}{s!\,(n-s)!}N^{(n-s)}G^{(s)}(0,1;ik\eta). \tag{19}$$

Using results (A5) and (A6), the explicit coefficients $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$, up to order 2, read

$$\Psi^{(0)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{20a}$$

$$\Psi^{(1)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\left[-\left(i\gamma+\frac{\pi}{2}\right)-i(ik\eta)\,{}_2F_2\left(\begin{array}{c}1,1\\2,2\end{array}\middle|;ik\eta\right)\right], \tag{20b}$$

$$\Psi^{(2)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\left[\left(-\gamma^2+i\gamma\pi+\frac{\pi^2}{12}\right)+2\left(-\gamma+i\frac{\pi}{2}\right)\times(ik\eta)\,{}_2F_2\left(\begin{array}{c}1,1\\2,2\end{array}\middle|;ik\eta\right)-\frac{(ik\eta)^2}{2}\times\Theta^{(1)}\left(\begin{array}{c}1,1|1,2\\2|3,3\end{array}\middle|;ik\eta,ik\eta\right)\right]. \tag{20c}$$

Higher-order terms $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$ can be easily obtained in terms of the multivariable hypergeometric functions $\Theta^{(n)}$ (see Appendix and [26]). The evaluation of these functions can be performed either by using series representations (see Appendix) or by solving numerically a system of ordinary differential equations that they satisfy (see [26]). Further investigation of the properties of the $\Theta^{(n)}$ functions is nevertheless necessary in order to reduce the difficulties on dealing with their evaluations and applications, and work in this direction is under way.

For $|\alpha|=\frac{|z_1z_2|\mu}{k}\ll 1$, i.e., for large values of the momentum of the particle (or alternatively high energy), a fast convergency of the series (11) is expected. It is important to notice that the Kummer function ${}_1F_1(a,b;z)$ is an entire function of the argument z and also an entire function of a (see, e.g., Ref. [17]); this means that it can be represented as a power series which converges everywhere. Moreover, the Gamma function $\Gamma(z)$ is an analytic function of z whose only finite singularities are $z=0,-1,-2,\ldots$. Thus, since the function $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ of Eq. (1) is a product of two analytic functions, it is itself an analytic function of $\mathbf{r}$ and α. Based on these considerations, the power series in α defined by Eq. (11), and similarly by the Born series (8), *is convergent*. This fact needed to be underlined since the series definition is mathematically correct. There remains the question of how the collision is represented by the traditional Born series.

The results obtained above are illustrated by the following numerical examples. In Fig. 1, we plot $|\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})|^2$ as a function of the parabolic coordinate η for charge values $z_1=-1$ and $z_2=1$, reduced mass $\mu=1$, and relative momentum $k=3$, so that $\alpha=-1/3$. To show the convergence of the Born-like series, also shown are the sums up to order 1 in α, i.e., $|\Psi^{(0)+}+\alpha\Psi^{(1)+}|^2$, and up to order 2, i.e., $|\Psi^{(0)+}+\alpha\Psi^{(1)+}+\frac{\alpha^2}{2}\Psi^{(2)+}|^2$. The zeroth order, $|\Psi^{(0)+}|^2$, is constant and equal to 1 (not shown); the contributions of the first and second orders are clearly noticed. Convergence of the series in α is poorer for larger values of η.

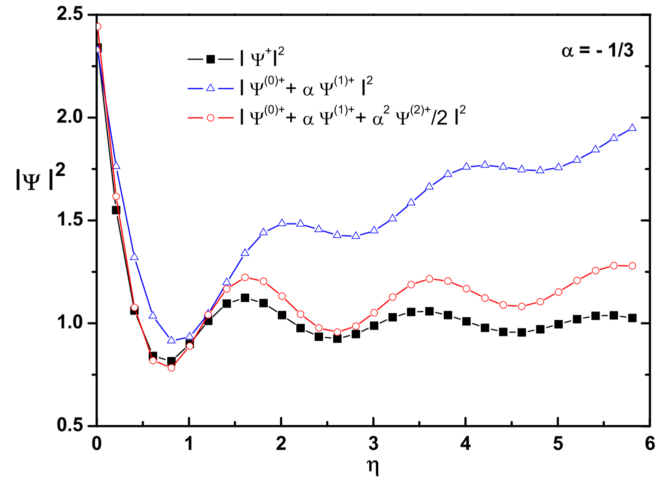

FIG. 1. (Color online) The quantity $|\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})|^2$ is plotted (line with full squares) as a function of the parabolic coordinate η for $\alpha=-1/3$ (charge values $z_1=-1$ and $z_2=1$, reduced mass $\mu=1$, and relative momentum $k=3$). To show the convergence of the Born-like series, the sums up to order 1 in α, i.e., $|\Psi^{(0)+}+\alpha\Psi^{(1)+}|^2$ (line with open triangles), and up to order 2, i.e., $|\Psi^{(0)+}+\alpha\Psi^{(1)+}+\frac{\alpha^2}{2}\Psi^{(2)+}|^2$ (line with open circles), are also shown.

In Fig. 2, the comparison between $|\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})|^2$ and the sum up to second order in α is shown for three values of k and hence three values of α (still with $z_1=-1$, $z_2=1$, and $\mu=1$). For $\alpha=-1$ ($k=1$), the sum up to second order is not sufficient to reproduce the details of the function Ψ^{+}. As k progressively increases to 3 (middle panel) and to 6 (bottom panel), α decreases, a better convergence is observed, and the second-order sum gives a better representation of Ψ^{+}.

As mentioned in Sec. I, we aim to understand the physics behind the Born series (8) for the long-range Coulomb potential and how the scattering process is represented by the series. The zeroth order in the expansion, $\Psi^{(0)+}(\mathbf{k},\mathbf{r})$, is just the plane wave [see Eq. (9a) or (20a)]: it represents the flux of the incident particles and corresponds to no scattering at all. The normalization constant accompanying the plane wave is 1 and corresponds to the zeroth order of the expansion of $N(\alpha)$. This means that no zero-energy resonance is included in the zeroth order at the origin of coordinates, contrary to what happens with the full Coulomb wave function [16].

The first order, $\Psi^{(1)+}(\mathbf{k},\mathbf{r})$, given by Eq. (20b), is a regular function at $\eta=0$ (as can be observed, for example, on Fig. 1). By making the ${}_2F_2$ function explicit, it can also be written in terms of simpler functions

$$\Psi^{(1)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}[i\ln(k\eta)+i\Gamma(0,-ik\eta)], \tag{21}$$

where $\Gamma(a,z)$ is the incomplete Gamma function [27]; note that $\Gamma(0,-iz)$ is related to the exponential integral $\mathrm{Ei}(z)$ [18]. In expression (21), the two functions are individually irregular at $\eta=0$ but their sum is regular. Thus, to first order in α, the Coulomb wave function reads

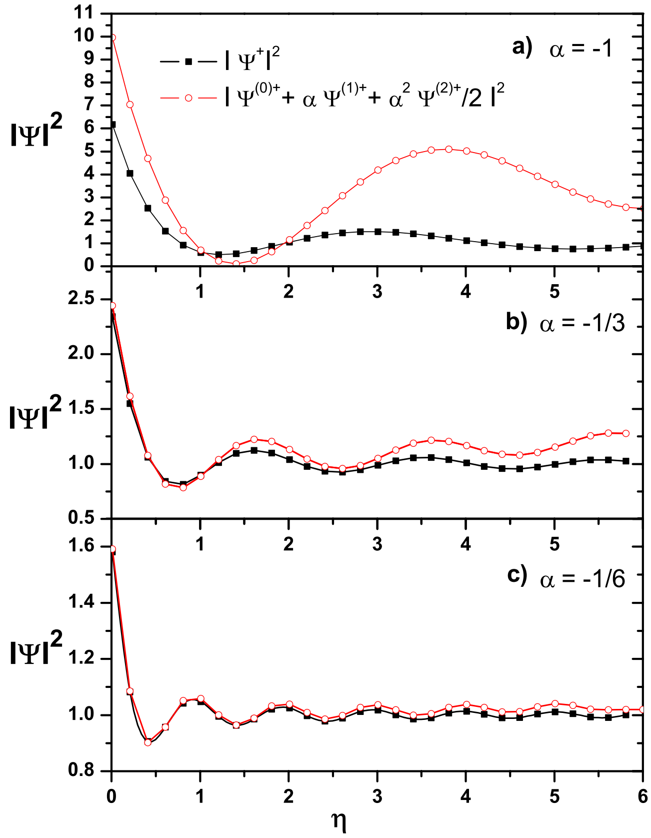

FIG. 2. (Color online) The quantity $|\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})|^2$ is plotted (line with full squares) as a function of the parabolic coordinate η for three values of α as indicated in the panels (charge values $z_1=-1$ and $z_2=1$, reduced mass $\mu=1$). The sums up to order 2, i.e., $|\Psi^{(0)+}+\alpha\Psi^{(1)+}+\frac{\alpha^2}{2}\Psi^{(2)+}|^2$ (line with open circles), are also shown.

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}[1+i\alpha\ln(k\eta)] + i\alpha e^{i\mathbf{k}\cdot\mathbf{r}}\Gamma(0,-ik\eta) + O(\alpha^2). \tag{22}$$

The second-order term $\Psi^{(2)+}(\mathbf{k},\mathbf{r})$ can also be written in terms of simpler functions

$$\Psi^{(2)+}(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\Bigg[\left(-\gamma^2+i\gamma\pi+\frac{\pi^2}{12}\right)-2\left(\gamma-i\frac{\pi}{2}\right)\ln(k\eta) - 2\ln^2(k\eta)-2\Gamma(0,-ik\eta)\ln(k\eta)+J_1+J_2\Bigg], \tag{23}$$

where the two terms

$$J_1 = 2(ik\eta)\int_0^1\int_0^1 dtdu\Gamma[0,-ik\eta(1-t)u]e^{ik\eta tu},$$

$$J_2 = 2(ik\eta)\int_0^1\int_0^1 dtdu\,\ln[(1-t)u]e^{ik\eta tu}$$

result from the use of the integral representation of the hypergeometric $\Theta^{(1)}$, as presented in Ref. [26]. The Coulomb wave function, up to second order in α, reads

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\Bigg[1+i\alpha\ln(k\eta)+(i\alpha)^2\ln^2(k\eta) + \frac{\alpha^2}{2}\left(-\gamma^2+i\gamma\pi+\frac{\pi^2}{12}\right)-\alpha^2\left(\gamma-i\frac{\pi}{2}\right)\ln(k\eta)\Bigg] - i\alpha e^{i\mathbf{k}\cdot\mathbf{r}}\Gamma(0,-ik\eta)[1-i\alpha\ln(k\eta)] + \frac{\alpha^2}{2}e^{i\mathbf{k}\cdot\mathbf{r}}(J_1+J_2)+O(\alpha^3). \tag{24}$$

Let us now analyze the asymptotic behavior, i.e., for large values of η, of each term. We have [27]

$$\Gamma(0,-ik\eta) \approx -\frac{e^{ik\eta}}{ik\eta}{}_2F_0\left(\begin{array}{c}1\,1\\ -\end{array}\middle|;\frac{1}{ik\eta}\right) \approx -\frac{e^{ik\eta}}{ik\eta},$$

where only the first term is retained in the power-series expansion of ${}_2F_0(1,1;\frac{1}{ik\eta})$. Hence, the asymptotic behavior of the first-order term,

$$\Psi^{(1)+}(\mathbf{k},\mathbf{r}) \approx e^{i\mathbf{k}\cdot\mathbf{r}}i\ln(k\eta) - \frac{1}{k(1-\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})}\frac{e^{ikr}}{r}, \tag{25}$$

leads to the following asymptotic form of $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$, up to order 1 in α:

$$\Psi^{+}(\alpha,\mathbf{k},\mathbf{r}) \approx e^{i\mathbf{k}\cdot\mathbf{r}}[1+i\alpha\ln(k\eta)] - \frac{z_1z_2\mu}{k^2(1-\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})}\frac{e^{ikr}}{r}, \tag{26}$$

where α has been explicitly written in the second term.

We observe, from expression (25), that $\Psi^{(1)+}(\mathbf{k},\mathbf{r})$ is not giving a pure spherical wave contribution as would be expected from the scattering theory; a logarithmic term contributes to the plane wave as can be seen from Eq. (22) or its asymptotic form (26). By comparing Eq. (26) to Eq. (4), this contribution can be directly related to the first-order expansion in α of the eikonal function $\mathcal{E}(\alpha,\mathbf{k},\mathbf{r})$. Thus, up to this order, the Born series distinguishes two types of collision: a deflection and a scattering from the dispersion center. Since no spherical wave is involved in the first term of Eq. (22) [or its asymptotic form (26)], it physically represents a deflection of the incident particle. The scattering from the dispersion center, on the other hand, is related to the second term in Eq. (22) [or its asymptotic form (26)] as it involves a spherical wave. Up to the first order in α, the approximation for $f(\theta)$ according to relation (4) is then

$$f^{(0)}(\theta) = -\frac{z_1z_2\mu}{2k^2\sin^2\left(\frac{\theta}{2}\right)}, \tag{27}$$

which is in agreement with the first Born approximation of the transition amplitude [23] (see also Sec. III). In the previous equation, θ is the angle between $\hat{\mathbf{k}}$ and $\hat{\mathbf{r}}$. It is interesting to notice that, to this order in α, there is no trace of the eikonal function $\mathcal{E}_s(\alpha,k,r)$ in the spherical wave of Eq. (26).

We now proceed to the second order in α of $\Psi^{+}(\alpha,\mathbf{k},\mathbf{r})$ given by Eq. (24). The first term (in square brackets) clearly represents a modified plane wave. The first three terms, 1

$+i\alpha\ln(k\eta)+(i\alpha)^2\ln^2(k\eta)$, of the multiplying factor are associated to the power-series expansion of the eikonal function $\mathcal{E}(\alpha,\mathbf{k},\mathbf{r})$; we should point out, however, that it does not correspond exactly to the Taylor expansion since a factor 1/2 is absent. All the other terms build up the eikonal function $\mathcal{E}_s(\alpha,k,r)$. In spite of the presence of individually irregular functions, the function $\Psi^+(\alpha,\mathbf{k},\mathbf{r})$ given by Eq. (24) is regular at the origin. The term involving the incomplete Gamma function $\Gamma(0,-ik\eta)$, multiplied by the factor $[1-i\alpha\ln(k\eta)]$, produces a coupling between angular and radial variables, introducing a modification to the expected spherical eikonal $\mathcal{E}_s(\alpha,k,r)$. The final factorization of the radial and angular parts [see Eq. (4)] appears only when all the terms of the power-series expansion of the logarithmic phase are summed up. This means that the correction due to the long-range potential appearing in $\Psi^{(2)+}$ is not separable. At this stage, it is not possible, thus, to extract $f^{(1)}(\theta)$, the next-order contribution to $f(\theta)$. The terms $e^{i\mathbf{k}\cdot\mathbf{r}}(J_1+J_2)$ are in charge of the regularization of both the plane and the spherical wave contributions, respectively. Similar constructions appear for the higher orders of the series.

As already mentioned in relation with the first order, the collision has to be understood in an extended way: the Born series (7) is not just yielding a spherical wave; because of the long range of the Coulomb potential, it also distorts the plane wave. This part of the collision gives rise to a deflection (but not a scattering) while the terms including asymptotically a spherical wave are representing the particles being really scattered from the dispersion center.

The results described above allow us to conclude that standard Born series can be used with long-range potential. The series obtained for the wave function is convergent and includes the physics of the collision. It is not necessary to introduce distorted-wave functions removing the long-range tail of the potential. However, one must be careful when using the asymptotic limit of the free-particle Green's function and assuming that only spherical waves can appear from each term of the Born series: our analysis shows clearly which important pieces of information can be lost when doing that, the *deflection* and *scattering* contributions being clearly observed in Eq. (24). This separation was introduced by Otranto and Gasaneo [19]—and later on discussed by Otranto and Olson—in the autoionization of helium induced by the collision with heavy-charged ions [28]. The deflected particles give rise to a shift in the position of the autoionization peak, while the scattered particles generate the binary ring as well as the enhancement of the ionization profile known as focusing peak [19,28].

B. Approach of Kadyrov and co-workers

A relation between our results and those presented by Kadyrov and co-workers [5] can be established. In Eq. (4) of [5], the scattering solution of the Schrödinger equation is separated into two terms, named "incident" $\phi_k^+(\mathbf{r})$ and "scattered" $\chi_k^+(\mathbf{r})$,

$$\Psi^+(\alpha,\mathbf{k},\mathbf{r}) = \phi_k^+(\mathbf{r}) + \chi_k^+(\mathbf{r}). \tag{28}$$

Moreover, the authors show that a distorted Born-like series can be defined [Eq. (18) of Ref. [5]] as

$$\Psi^+(\alpha,\mathbf{k},\mathbf{r}) = [\phi_k^{(0)+}(\mathbf{r}) + \chi_k^{(0)+}(\mathbf{r})] + [\phi_k^{(1)+}(\mathbf{r}) + \chi_k^{(1)+}(\mathbf{r})] + \cdots + [\phi_k^{(n)+}(\mathbf{r}) + \chi_k^{(n)+}(\mathbf{r})]. \tag{29}$$

As can be seen from our results for $\Psi^{(n)+}(\mathbf{k},\mathbf{r})$, each term of our expansion has this structure and besides is regular at the origin [this is explicitly shown by Eqs. (21) and (23) for the first and second orders]. According to the Born-like expansion (29), each term contains both incident and scattered contributions. Our zero-order functions, $\phi_k^{(0)+}(\mathbf{r})$ and $\chi_k^{(0)+}(\mathbf{r})$, are the plane wave and zero, respectively. No scattering is observed; this is related to the fact that $\phi_k^{(0)+}(\mathbf{r})$ is the solution of the free-particle Hamiltonian. The sum of all the $\phi_k^{(n)+}(\mathbf{r})$ contributions will give rise to our deflection term, while the sum of the $\chi_k^{(n)+}(\mathbf{r})$ will construct the scattered part responsible for the scattering amplitude. Of course, our $\phi_k^{(0)+}(\mathbf{r})$ and $\phi_k^{(1)+}(\mathbf{r})$, and $\phi_k^{(n)+}(\mathbf{r})$ in general, are different to the corresponding ones presented in [5] because our $\phi_k^{(n)+}(\mathbf{r})$ do not contain the Coulomb logarithmic phase $e^{-i\alpha\ln(k\eta)}$. In addition, the explicit separation of incident and scattered parts will be, in general, quite difficult to perform as detailed above from the analyses of $\Psi^{(1)+}(\mathbf{k},\mathbf{r})$ and $\Psi^{(2)+}(\mathbf{k},\mathbf{r})$.

C. Further comments on successive scattering processes

We now discuss further the expansion of the Coulomb wave function in terms of successive scattering processes. Let us decompose the Coulomb potential $V_c(r)=\frac{z_1z_2}{r}$ as the sum of two terms,

$$V_c(\mathbf{r}) = V_{aux}(\mathbf{r}) + \lambda V_{short}(\mathbf{r}), \tag{30}$$

where the auxiliary potential $V_{aux}(\mathbf{r})$ includes the Coulomb tail and $V_{short}(\mathbf{r})$ is a short-ranged potential with magnitude λ. Proceeding in a similar way as in Sec. II A, but with λ instead of α, we can expand the wave function as

$$\Psi^+(\mathbf{r}) = \sum_n \lambda^n \Psi^{(n)+}(\mathbf{r}), \tag{31}$$

where $\Psi^{(n)+}$ satisfy the following equations:

$$[E-H_a]\Psi^{(0)+}(\mathbf{r}) = 0, \tag{32a}$$

$$[E-H_a]\Psi^{(1)+}(\mathbf{r}) = V_{short}(\mathbf{r})\Psi^{(0)+}(\mathbf{r}), \tag{32b}$$

$$\vdots$$

$$[E-H_a]\Psi^{(n)+}(\mathbf{r}) = V_{short}(\mathbf{r})\Psi^{(n-1)+}(\mathbf{r}), \tag{32c}$$

with $H_a=-\frac{1}{2\mu}\nabla^2+V_{aux}$. As V_{short} is assumed to be of short range, for large values of the coordinate, the right-hand sides of Eqs. (32a)–(32c) vanish. The asymptotic behavior of each term $\Psi^{(n)+}(\mathbf{r})$ will contain a Coulomb phase due to the long range of the potential V_{aux}. Thus, a series solution of the type (31) will construct the collision process in a form which differs from that previously discussed (Sec. II A) since each term will contain the Coulombic tail. The solutions to the nonhomogeneous differential Eqs. (32a)–(32c) can be expressed as integrals

$$\Psi^{(1)+}(\mathbf{r}) = \int G_a(\mathbf{r},\mathbf{r}')V_{short}(\mathbf{r}')\Psi^{(0)+}(\mathbf{r}'), \tag{33a}$$

$$\Psi^{(2)+}(\mathbf{r}) = \int G_a(\mathbf{r},\mathbf{r}')V_{short}(\mathbf{r}')\Psi^{(1)+}(\mathbf{r}'), \tag{33b}$$

$$\vdots$$

$$\Psi^{(n)+}(\mathbf{r}) = \int G_a(\mathbf{r},\mathbf{r}')V_{short}(\mathbf{r}')\Psi^{(n-1)+}(\mathbf{r}'), \tag{33c}$$

with the Green's function defined through

$$(E-H_a)G_a(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{34}$$

The definitions (33a)–(33c) for $\Psi^{(n)+}(\mathbf{r})$ are justified by the fact that no surface integral is expected if V_{short} decreases sufficiently fast, as mentioned in Ref. [5].

An interesting issue arises from the decomposition (30) and is related to the distorted-wave theory: there are infinite ways of defining V_{short} and furthermore there is no unique form to separate the wave function into incident and scattered waves even when there exists a unique solution to the scattering problem. This leads to the same problems encountered with the possible ways to obtain the full Coulomb potential from short-range potentials as discussed in Ref. [29] and also the alternative proposals of Mulherin and Zinnes and van Haeringen [1,30,31]. Different definitions for V_{short} will lead to different constructions of the scattering process and hence of the transition amplitude. We would like to consider now an example of such a separation. It is based on a study of Mulherin and Zinnes [31] which was used by Barrachina and Macek [1], and also by Kadyrov *et al.* [5,8], to define a Lippmann-Schwinger equation for the wave function. According to Refs. [1,5,8], one can choose V_{aux} and V_{short} in the following way:

$$V_{aux}^{\mathrm{MZ}} = \frac{z_1z_2}{r}\left(1-\frac{\alpha}{k\eta}\right), \tag{35}$$

$$V_{short}^{\mathrm{MZ}} = \frac{1}{r\eta}, \tag{36}$$

where $\lambda=\alpha^2/\mu$ defines the magnitude of V_{short} and $\eta=r-\hat{\mathbf{k}}\cdot\mathbf{r}$ is one of the parabolic coordinates. The potential V_{short}^{MZ} is a noncentral potential which diverges at the origin; furthermore, it diverges also along the line defined by $\eta=0$ [32], putting doubts about the validity of the integrals of Eqs. (33a)–(33c). The zeroth order of the wave function, solution of Eq. (32a), is given by [32]

$$\Psi^{(0)\mathrm{MZ}+}(\mathbf{r}) = N^{\mathrm{MZ}}(\alpha)e^{i\mathbf{k}\cdot\mathbf{r}}(ik\eta)^{\lambda}\,{}_1F_1\left(\begin{array}{c}-i\alpha+\lambda\\ 1+2\lambda\end{array}\middle|;ik\eta\right), \tag{37}$$

where

$$N^{\mathrm{MZ}}(\alpha) = (-1)^{-\lambda}\frac{\Gamma(1+\lambda+i\alpha)}{\Gamma(1+2\lambda)}\exp\left(-\frac{\pi}{2}\alpha\right).$$

The asymptotic limit of $\Psi^{(0)\mathrm{MZ}+}(\mathbf{r})$ can be easily derived from that of the Kummer function [18] and leads to the following result:

$$\Psi^{(0)\mathrm{MZ}+}(\mathbf{r}) \to e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{E}(\alpha,\mathbf{k},\mathbf{r}) + f^{\mathrm{MZ}}(\theta)\frac{e^{ikr}}{r}\mathcal{E}_s(\alpha,k,r). \tag{38}$$

The transition amplitude $f^{\mathrm{MZ}}(\theta)$ can be separated in two terms

$$f^{\mathrm{MZ}}(\theta) = f_c^{\mathrm{MZ}}(\theta) + f_{pa}^{\mathrm{MZ}}(\theta),$$

containing, respectively, the scattering by the Coulomb center,

$$f_c^{\mathrm{MZ}}(\theta) = -(-1)^{-\lambda}\frac{z_1z_2\mu}{2k^2\sin^2(\theta/2)}\exp\left[-i\alpha\ln\left(\sin^2\frac{\theta}{2}\right)+i2\tilde{\sigma}_c\right], \tag{39}$$

and that by the parabolic potential V_{short}^{MZ},

$$f_{pa}^{\mathrm{MZ}}(\theta) = -i(-1)^{-\lambda}\frac{\lambda}{2k\sin^2(\theta/2)}\exp\left[-i\alpha\ln\left(\sin^2\frac{\theta}{2}\right)+i2\tilde{\sigma}_c\right], \tag{40}$$

where $\tilde{\sigma}_c=\mathrm{Arg}[\Gamma(1+\lambda+i\alpha)]$. We can clearly see from Eq. (38) that $\Psi^{(0)\mathrm{MZ}+}(\mathbf{r})$ contains both the incident and scattered parts. When compared to the asymptotic form of the Coulomb wave function (4), the incident part has, to order $1/\eta$, an identical behavior; the scattered part, on the other hand, differs not only because of the presence of $f_{pa}^{\mathrm{MZ}}(\theta)$ but also by the presence of $\tilde{\sigma}_c\neq\sigma_c$. A study of the higher orders $\Psi^{(n)\mathrm{MZ}+}(\mathbf{r})$ will show that contributions similar to $f_{pa}^{\mathrm{MZ}}(\theta)$ appear for each order n. Thus, to obtain the transition amplitude (5), through an expansion in powers of $\lambda=\alpha^2/\mu$, it is necessary to decompose the obtained transition amplitudes. The Mulherin-Zinnes (MZ) example illustrates that each potential V_{short} produces a particular construction of the collision process and it may occur that many terms of the expansion are necessary to build the correct result.

III. BORN-LIKE SERIES FOR THE ELASTIC SCATTERING AMPLITUDE

Let us now turn to the scattering amplitude. Consider first the closed form for $f(\theta)$ given by Eq. (5). Expanding it as a power series of α, we have

$$f(\theta) = \sum_{n=0}^{\infty} f^{(n)}\frac{\alpha^n}{n!}, \tag{41}$$

with

$$f^{(0)} = -\frac{\mu z_1z_2}{2k^2\sin^2\frac{\theta}{2}}, \tag{42a}$$

$$f^{(1)} = f^{(0)}\left[-2i\gamma - i\ln\left(\sin^2\frac{\theta}{2}\right)\right], \tag{42b}$$

$$f^{(2)} = -f^{(0)}\left[\ln^2\left(\sin^2\frac{\theta}{2}\right)+4\gamma\ln\left(\sin^2\frac{\theta}{2}\right)+8\gamma^2\right]. \tag{42c}$$

On the other hand, the general definition for the transition amplitude for a particle being scattered from a dispersion center can be found, for example, in Ref. [22]. Applied to the Coulomb problem, it reads

$$f(\theta) = -\frac{\mu}{2\pi}\langle \exp(i\mathbf{k}_f\cdot\mathbf{r})|\frac{z_1z_2}{r}|\Psi_i^+\rangle. \tag{43}$$

Replacing the Born-like series (11) in this definition, we obtain a power series in α for the transition amplitude (labeled B to recall the Born series)

$$f_B(\theta) = \sum_{n=0}^{\infty} f_B^{(n)}\frac{\alpha^n}{n!}, \tag{44}$$

where the coefficient $f_B^{(n)}$ is given by

$$f_B^{(n)} = -\frac{\mu}{2\pi}\langle \exp(i\mathbf{k}_f\cdot\mathbf{r})|\frac{z_1z_2}{r}|\Psi^{(n)+}(\mathbf{k}_i,\mathbf{r})\rangle. \tag{45}$$

Let $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$ be the momentum transfer defined in terms of initial and final momenta of the particles. Upon substitution of $\Psi^{(n)+}(\mathbf{k}_i,\mathbf{r})$ by the sum (19) and through the introduction of an integration factor $e^{-\epsilon r}$, with $\epsilon\to 0$ and $\epsilon>0$, we may perform analytically the integration term by term. Using the techniques discussed in Refs. [33–35] and defining

$$U = -2\frac{\mathbf{k}_i\cdot\mathbf{q}+i\epsilon k_i}{q^2+\epsilon^2}, \tag{46}$$

one finds

$$\int d\mathbf{r}G^{(s)}(0,1;ik_i\eta)\frac{e^{i\mathbf{q}\cdot\mathbf{r}-\epsilon r}}{r} = \frac{4\pi}{q^2+\epsilon^2}i^sU^sI^{(s)}(U), \tag{47}$$

and hence the following expression for the transition amplitude $f_B^{(n)}(\theta)$:

$$f_B^{(n)}(\theta) = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}\sum_{s=0}^{n}\frac{i^sn!}{s!\,(n-s)!}N^{(n-s)}U^sI^{(s)}(U). \tag{48}$$

In Eqs. (47) and (48),

$$I^{(s)}(U) = \Lambda^{(s)}\left(\begin{array}{c} 1,1,\ldots,1|1,2,\ldots,s \\ 2,3,\ldots,s|s+1\end{array}\middle|;-U,-U,\ldots,-U\right), \tag{49}$$

where $\Lambda^{(s)}$ is the multivariable generalized hypergeometric function defined by

$$\Lambda^{(s)}\left(\begin{array}{c} a_1,a_2,\ldots,a_s|b_1,\ldots,b_s \\ d_1,\ldots,d_s|f_1\end{array}\middle|;x_1,x_2,\ldots,x_s\right) = \sum_{m_1=0}^{\infty}\cdots\sum_{m_s=0}^{\infty}\frac{x_1^{m_1}x_2^{m_2}\cdots x_s^{m_s}}{m_1!\,m_2!\cdots m_s!}\frac{(a_1)_{m_1}(a_2)_{m_2}\cdots(a_s)_{m_s}}{(f_1)_{m_1+m_2+\cdots+m_s}} \times\frac{(b_1)_{m_1}(b_2)_{m_1+m_2}\cdots(b_s)_{m_1+m_2+\cdots+m_s}}{(d_1)_{m_1}(d_2)_{m_1+m_2}\cdots(d_s)_{m_1+m_2+\cdots+m_{s-1}}}. \tag{50}$$

For $s=0$, 1, and 2, we get, respectively,

$$I^{(0)}(U) = 1, \tag{51a}$$

$$I^{(1)}(U) = {}_2F_1\left(\begin{array}{c}1,1\\2\end{array}\middle|;-U\right) = \ln(1+U), \tag{51b}$$

$$I^{(2)}(U) = \Lambda^{(2)}\left(\begin{array}{c}1,1|1,2\\2|3\end{array}\middle|;-U,-U\right) = \frac{1}{1+U}F_3\left(1,1,1,1,3;-U;\frac{U}{1+U}\right), \tag{51c}$$

where $F_3(a,a',b,b',c;x,y)$ is one of the Appell functions [36].

The convergence arguments used before for the wave function can be equally applied to ensure convergency of the series (44), as a function of α, for $f_B(\theta)$. Since $\Psi^+(\alpha,\mathbf{k},\mathbf{r})$ is an analytic function of α and $\mathbf{r}$, the integration on the coordinate appearing in Eq. (43) can be exchanged with the series symbol without affecting the convergency of the series in α; this can be stated because the functions appearing in the integral defining $f_B^{(n)}$, Eq. (45), do not depend on α. Thus, we conclude that the series in α for the transition amplitude converges everywhere.

The zeroth order in α is given by

$$f_B^{(0)} = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}I^{(0)}(U) = -2\frac{z_1z_2\mu}{q^2+\epsilon^2}. \tag{52}$$

The first order in α reads

$$f_B^{(1)} = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}[N^{(1)}I^{(0)}(U)+N^{(0)}iUI^{(1)}(U)] \tag{53}$$

and using the result (51b) for $I^{(1)}(U)$, we find

$$f_B^{(1)} = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}\left[-\left(i\gamma+\frac{\pi}{2}\right)+i\ln(1+U)\right]. \tag{54}$$

The second-order contribution is given by

$$f_B^{(2)} = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}[N^{(2)}I^{(0)}(U)+2iN^{(1)}UI^{(1)}(U) - N^{(0)}U^2I^{(2)}(U)] \tag{55}$$

and using the simplifications (51b) and (51c) and collecting, we find

$$f_B^{(2)} = -2\mu\frac{z_1z_2}{q^2+\epsilon^2}\left[\left(-\gamma^2+i\gamma\pi+\frac{\pi^2}{12}\right) - 2i\left(i\gamma+\frac{\pi}{2}\right)U\ln(1+U) - \frac{U^2}{1+U}F_3\left(1,1,1,1,3;-U;\frac{U}{1+U}\right)\right]. \tag{56}$$

When considering on-shell calculations, i.e., energy conservation $k_i=k_f=k$, the momentum transfer becomes $q=2k\sin(\frac{\theta}{2})$. In the limit of $\epsilon\to 0$, the result (52) is in agreement with relation (27) or (42a), i.e., the first Born approximation for the Coulomb potential (see also [23]).

The next order in α, $f_B^{(1)}$, given by Eq. (54), should be compared to $f^{(1)}$ given by Eq. (42b). According to the discussion of the previous section, the sum of the constant and the logarithmic terms in Eq. (54) includes contributions of the deflection (associated to the plane wave) and the dispersion (related to the spherical waves) [see $\Psi^{(1)+}$, Eq. (26)]. No trace of the plane wave contribution is included in Eq. (42b), thus Eqs. (54) and (42b) must give different results. While it was relatively easy to separate out the plane and spherical wave parts to the multiple collision orders for the wave function, the same is not true for the transition amplitude. In fact, the integration of the separated parts of $\Psi^{(1)+}$, given by Eq. (21), leads to singular integrals. However, this is not the case when the integration is performed to obtain Eq. (54) because regular functions are integrated. We may try to identify the different contributions of the final expression (54). From $\ln(1+U)$, it is easy to separate the term $\ln(q^2+\epsilon^2)$ which, in the limit of $\epsilon \to 0$ and energy conservation, coincides with the $\ln(\sin^2\frac{\theta}{2})$ appearing in Eq. (42b). However, it is not possible to replace $\epsilon=0$ to evaluate Eq. (54), since the limit process must be conserved to avoid the appearance of unwanted divergencies. For this reason, extra terms arise, so that Eqs. (54) and (42b) differ, putting in evidence the presence of the abovementioned plane wave contribution. These results are in agreement with those presented in Ref. [21].

It is not easy to disentangle the contributions already for the first order and the situation is even more complicated for higher orders as can be seen from the inspection of $f_B^{(2)}$ of Eq. (56). Term by term, the contributions of the series (44) do not correspond to the correct ones given by Eqs. (42a)–(42c). However, since the series expansion for the Coulomb wave function converges, the final result obtained by summing all the terms is correct and mathematically well-founded. Similarly to what happened for the wave function (Sec. II A), the Born series terms construct the Rutherford scattering amplitude (5) because they include not only the dispersion, but also the deflection associated to the plane wave, produced by the long range of the Coulomb potential. The identification of the difference between the series expansion in the two approaches was one of the goals of this paper. The implications for the three-body problem will be carefully discussed in the next section.

It has been stated in Refs. [1,5] that the definition (43) for the scattering amplitude is not correct for long-ranged potentials. Instead, the authors introduced the following definition, in post form:

$$f(\theta) = \frac{-\mu}{2\pi}\langle \exp[i\mathbf{k}_f\cdot\mathbf{r} - i\alpha\ln(kr+\mathbf{k}\cdot\mathbf{r})]|\frac{\alpha^2}{r\xi}|\Psi_i^+\rangle. \quad (57)$$

The explicit calculation [1] of this amplitude yields exactly the Rutherford scattering amplitude given by Eq. (5). This result was confirmed in Ref. [5].

We could proceed as done above with Eq. (43) by replacing the Born-like expansion (11) in the definition (57). We do not give here the details of the resulting Born series terms since they would not allow for a separation of deflected and scattered contributions coming from each term $\Psi^{(n)+}$ of the wave function. Thus, even when the correct transition amplitude definition is used, the series obtained will not agree with the expansions (42a)–(42c) and superior orders. The correct result, however, will be found only when all the terms of the series are included. To obtain an order-to-order correspondence in the series, a different expansion of Ψ_i^+ should be considered. We should also mention that, from the discussion presented at the end of Sect. II, some doubts about the validity of the formulation (57) arise. These are supported by the fact that there exist infinite forms to build the collision process based on the distorted-wave theory. As shown above, the transition amplitude will contain information about the collision produced by the auxiliary potential, which may be of long range and thus affect the particles' movement up to infinite distances.

IV. SUMMARY AND DISCUSSION

We have studied expansions of the two-body Coulomb scattering problem in terms of the Sommerfeld parameter. Using closed-form expressions for the *n*th derivatives of the Kummer function with respect to its first parameter, the scattering wave function is written as power series in the Sommerfeld parameter. The coefficients for any order, which are functions of the energy and the (parabolic) coordinate, are expressed analytically in terms of multivariable hypergeometric functions, named here as $\Theta^{(n)}$. A relatively fast convergence is observed for small values of the Sommerfeld parameter. The first- and second-order contributions are studied in detail and compared to those issued from the closed-form wave function. Their asymptotic behavior shows the presence of unexpected contributions which construct the deflection of the particles related to the well-known eikonal factors.

The expansion for the scattering wave function is then used to evaluate the transition amplitude for the collision process between two charged particles. To each coefficient of the wave function corresponds a coefficient for the transition amplitude and analytic expressions are given for any order in terms of another set of multivariable hypergeometric functions, named here as $\Lambda^{(n)}$.

The connection between the above power series and the Born series, based on the free particle Green's function, is established both for the Coulomb wave function and the scattering amplitude. The series derived from the well-known Rutherford scattering amplitude is shown to differ from that obtained when using the Born series.

A discussion about distorted-wave Born series for the wave function is also presented. The decomposition of the Coulomb potential as a sum of one short- (V_{short}) and a long-ranged potential allows one to define a distorted Hamiltonian whose solutions include, in principle, the appropriated Coulomb phase. Each term of the series will contain both the incident and scattered waves as presented by Kadyrov and *et al.* [5,8]. However, the scattering process construction obtained from the distorted-wave Born series depends on the choice of potential V_{short}; besides, the transition amplitude will not coincide with the correct one deduced from the asymptotic limit of the Coulomb wave function. We have also discussed the alternative definition of transition amplitude proposed by Barrachina and Macek [1] and Kadyrov and co-workers [5,8], which results from a particular choice of the distortion potential (proposal of Mulherin and Zinnes).

The solutions to the distorted potential effectively include the Coulomb phase; this can be seen already from the zeroth order. We have also shown that the Born series will need many terms to build the appropriated transition matrix.

The analysis presented here for the two-body problem can be extended directly to three-body problems. Our results were derived from a Lippmann-Schwinger equation where the Coulomb potential is used as a perturbation; the unperturbed initial state, the plane wave in our case, has no trace of the long-range tail. Lippmann-Schwinger equations of this type are often used in the study of three-body problems. As in Eq. (6), the three-body wave functions are generally constructed as the sum of two terms: one being the initial unperturbed state and the second, the scattering state itself, contains all the information about the collision. In most of the theoretical and numerical approaches to the full three-body solution, the unperturbed initial state does not include one or more of the long-range asymptotic Coulomb tails. This means that the latter must be constructed when solving the Schrödinger equation as explicitly shown in the two-body problem case (Sec. II). The asymptotic influence of the Coulomb potentials, associated to the initial state, should appear entangled with the scattering part of the wave function: the disentanglement is a very difficult, if not impossible, task. This clearly means that the use of initial states not including the appropriated asymptotic form leads to fake transition amplitudes since they include, simultaneously, the deflection together with the true result. However, as discussed in Sec. III, if the wave function used to evaluate the transition amplitude is the exact solution of the problem, the final result is the correct one. This is what happens, for example, with the convergent close-coupling [10] and the exterior complex scaling [15] approaches as can be clearly seen from the results presented in the literature (fake results may appear, however, if convergency is not reached within numerical calculations). Even when numerically exact solutions are built, the obtained transition amplitudes intrinsically contain information about the deflection terms which correspond to one of the Coulomb interactions not included in the unperturbed state, e.g., the electron-electron interaction in the case of electron-atom collisions. However, the correct transition amplitude will emerge from the numerical calculations if convergency toward the exact wave function is reached. The same difficulty appears in those calculations based on the Born series, either for the wave function or the transition amplitude. It is not clear to us, however, what could be the effect on calculated cross sections of the abovementioned entanglement. It is worth reminding that the Born series approach has been, and is currently being used, for describing different collision processes (see, for example, the double-ionization study of neutral atoms by electron impact [37]). More studies are necessary to clarify all these issues associated to the three-body problems. Important steps toward that directions were presented in a series of papers [4,5,7,8] where new definitions for the zeroth-order wave function and transition amplitude were given. These proposals seem to be the appropriated starting points for perturbative calculations; however, they require to be further investigated to see if the difficulties, observed in the two-body Born-like series discussed here, appear or not.

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APPENDIX: THE $G^{(n)}$ FUNCTION

The confluent hypergeometric function (Kummer function) can be defined as a power series on the variable z [17]

$$F = {}_1F_1\left(\begin{array}{c} a \\ b \end{array} \middle| ;z \right) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!}, \tag{A1}$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is the Pochhammer symbol defined in terms of the Gamma function [18]. In [26], we have studied the derivatives of order n of $F = {}_1F_1(a,b;z)$ with respect to its first parameter a,

$$G^{(n)} = G^{(n)}(a,b;z) = \frac{d^n {}_1F_1\left(\begin{array}{c} a \\ b \end{array} \middle| ;z \right)}{da^n}. \tag{A2}$$

Starting from the differential equation satisfied by F and using results of [38], we have found that the derivatives $G^{(n)}$ can be written as

$$G^{(n)}(a,b,z) = \frac{z^n}{(b)_n} \Theta^{(n)}\left(\begin{array}{c} 1,1,\ldots,1 | a,a+1,\ldots,a+n \\ a+1,a+2,\ldots,a+n | n+1,b+n \end{array} \middle| ;z,z,\ldots,z \right), \tag{A3}$$

where we introduced the multivariable hypergeometric function [26]

$$\Theta^{(n)}\left(\begin{array}{c} a_1,a_2,\ldots,a_{n+1}|b_1,\ldots,b_{n+1} \\ c_1,\ldots,c_n|d_1,d_2 \end{array}\middle|;x_1,x_2,\ldots,x_{n+1}\right)$$
$$=\sum_{m_1=0}^{\infty}\cdots\sum_{m_{n+1}=0}^{\infty}\frac{x_1^{m_1}x_2^{m_2}\cdots x_{n+1}^{m_{n+1}}}{m_1!\,m_2!\cdots m_{n+1}!}\frac{(a_1)_{m_1}(a_2)_{m_2}\cdots(a_{n+1})_{m_{n+1}}(b_1)_{m_1}(b_2)_{m_1+m_2}\cdots(b_{n+1})_{m_1+m_2+\cdots+m_{n+1}}}{(c_1)_{m_1}(c_2)_{m_1+m_2}\cdots(c_n)_{m_1+m_2+\cdots+m_n}(d_1)_{m_1+m_2+\cdots+m_{n+1}}(d_2)_{m_1+m_2+\cdots+m_{n+1}}}, \quad (A4)$$

which is a Kampé de Fériet–like function.

For the first derivative, $n=1$, $\Theta^{(1)}$ is a two-variable hypergeometric function. For $a=0$, $\Theta^{(1)}$ can be expressed in terms of the well-known ${}_2F_2$ hypergeometric function [25] leading to the following result:

$$G^{(1)}(0,b,z)=\frac{z}{(b)_1}\,{}_2F_2\left(\begin{array}{c} 1,1 \\ 2,b+1 \end{array}\middle|;z\right). \quad (A5)$$

The second derivative $G^{(2)}$ is expressed in terms of the two-variable hypergeometric function $\Theta^{(1)}$ [26]

$$G^{(2)}(0,b,z)=\frac{z^2}{(b)_2}\Theta^{(1)}\left(\begin{array}{c} 1,1|1,2 \\ 2|3,b+2 \end{array}\middle|;z,z\right). \quad (A6)$$

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