Two-body Coulomb scattering and complex scaling

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The two-body Coulomb scattering problem is solved using the standard complex-scaling method. The explicit enforcement of the scattering boundary condition is avoided. Splitting of the scattering wave function based on the Coulomb modified plane wave is considered. This decomposition leads to a three-dimensional Schrödinger equation with a source term. Partial-wave expansion is carried out and the asymptotic form of the solution is determined. This splitting does not lead to simplification of the scattering boundary condition if complex scaling is invoked. An alternative splitting carried out only on the partial-wave level is introduced and this method is proven to be very useful. The scattered part of the wave function tends to zero at large interparticle distances. This property permits easy numerical solution: the scattered part of the wave function can be expanded on a bound-state-type basis. The method can be applied not only for a pure Coulomb potential but also in the presence of a short-range interaction.

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I. INTRODUCTION

For many years, the method of complex scaling (CS) has been an excellent tool to calculate half-life times of resonance states. CS has been successfully applied in many areas of quantum physics [1,2] and was extended to collision processes very early on [3,4]. However, a drawback of standard CS (or uniform CS) emerged immediately after the introduction of the method. For scattering problems, the CS procedure can be applied only for short-range potentials [3,5]. This is indeed serious since the long-range Coulomb interaction cannot be neglected in the majority of the problems of atomic and nuclear physics. Several modifications have been suggested [6–8], but none of them has gained widespread acceptance. After these initial applications, the scattering aspects of CS have been neglected.

The turning point was the work in Ref. [9], where it was shown that scattering calculations with exterior CS can be successfully performed for long-range interactions. After this pioneering work, the exterior CS method has been applied for a variety of three-body Coulomb problems, even above the three-body breakup threshold, with great success [10–13]. A comprehensive description of the exterior CS method and benchmark calculations for the electron-hydrogen scattering are given in [14]. The exterior CS method has proven to be one of the most successful numerical methods to deal with collision processes. However, recently, the exterior CS method has been under scrutiny since in the method an artificial cutoff in some of the interaction is used. To solve this problem, a modification of the original exterior CS method has been suggested and checked in two-body calculations [15,16]. An extension to the three-body problem has also been sketched [17].

Recently, it was shown [18] that standard CS can be applied for scattering problems when a short-range potential is added to the pure Coulomb interaction. The method is based on two potential formalisms. A similar approach has been suggested also in [19]. In the present paper, we rigorously develop a method which is equally good for a pure Coulomb interaction and for the general case too (i.e., a short-range potential is added to the Coulomb interaction). This approach does not rely on the two potential formalisms and a dangerous cutoff will not be introduced.

In the case of a two-body problem, the wave function depends on the interparticle coordinate $\mathbf{r}$. The scattering solution of the Schrödinger equation with momentum $\mathbf{k}$ is denoted by $\psi^+(\mathbf{k},\mathbf{r})$. This wave function will be called the three-dimensional (3D) wave function. It is assumed that the wave function satisfies appropriate scattering boundary conditions. The aim of the application of any CS method is to introduce an alternative equation instead of the Schrödinger equation with simplified boundary conditions. The expectation is that the solution of this alternative equation is square integrable, and therefore it can be approximated by bound-state-type basis functions. In this way, the explicit use of the complicated scattering asymptotic form of the wave function can be avoided and the numerical calculation can be simplified.

In contrast to the resonance-state calculation in the scattering problem, CS is not applied directly to the full wave function. First, a splitting of the total-wave function is carried out. The full scattering solution is searched for in the form

$$\psi^+(\mathbf{k},\mathbf{r}) = \phi_0(\mathbf{k},\mathbf{r}) + \psi^{sc+}(\mathbf{k},\mathbf{r}), \tag{1}$$

where $\phi_0(\mathbf{k},\mathbf{r})$ is a known function. From the Schrödinger equation for the scattered part of the wave function, the so-called driven Schrödinger equation (or Schrödinger equation with a source term)

$$(E - \hat{H})\psi^{sc+}(\mathbf{k},\mathbf{r}) = S(\mathbf{k},\mathbf{r}) \tag{2}$$

can be derived. The source term is given by $S(\mathbf{k},\mathbf{r}) = (\hat{H} - E)\phi_0(\mathbf{k},\mathbf{r})$. The Hamiltonian and energy are denoted by $\hat{H}$ and E, respectively.

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We mention that the two-body Coulomb problem with a source term has been recently thoroughly investigated in [20]. Complicated but exact solutions have been given for very general sources. Basis functions with a proper two-body scattering asymptotic have been generated from the exact solutions and used in the J-matrix method [21]. The driven Schrödinger equation has been applied for realistic three-body scattering problems too [22,23]. However, in these works, CS was not applied and the complicated scattering boundary conditions were implemented using either the finite-element method or Sturmian expansion.

The use of CS in scattering calculations means that the coordinate $\mathbf{r}$ in Eq. (2) is replaced by $\mathbf{r}e^{i\theta}$, where $0 < \theta < \pi/2$. The boundary condition is simplified if after complex scaling the scattered part of the wave function goes to zero when the interparticle distance tends to infinity. It is easy to see that this property is fulfilled if $\psi^{sc+}(\mathbf{k},\mathbf{r})$ contains only an outgoing spherical wave. In the paper, this property will be investigated for different splittings of the full wave function.

The organization of the paper is the following. In Sec. II, the known expressions of the two-body Coulomb scattering are reviewed. The driven Schrödinger equation is introduced in Sec. III. The splitting of the total-wave function in Eq. (1) is carried out on a 3D level; however, the splitting can be carried out only on a partial-wave (pw) level. Different 3D and pw splittings will be considered and it will be shown that there are cases when the 3D and pw splittings are not equivalent. The Coulomb modified plane wave (CMPW) plays a basic role in the recent surface integral formalism of the scattering theory [24,25]. The properties of the 3D splitting based on the CMPW will be investigated in Sec. IV. A useful pw splitting from the point of view of CS will be introduced in Sec. V. Finally, numerical examples will be presented both for the pure Coulomb case and for a potential having short- and long-range parts. The conclusions will be given in Sec. VII.

II. EXACT SOLUTIONS OF THE TWO-BODY COULOMB PROBLEM

First, we collect a few known expressions [26] for the two-body Coulomb scattering in order to fix the notations. As usual, we take $\hbar = m = e = 1$ (where m is the reduced mass); the energy is $E = k^2/2 > 0$ and the Coulomb potential reads $\gamma k/r$, where γ is the Sommerfeld parameter. We consider the Schrödinger equation with a pure two-body Coulomb interaction,

$$\left(-\frac{1}{2}\Delta_{\mathbf{r}} + \frac{\gamma k}{r} - \frac{k^2}{2}\right)\psi(\mathbf{k},\mathbf{r}) = 0, \tag{3}$$

where $\Delta_{\mathbf{r}}$ is the Laplace operator. The Coulomb scattering state

$$\psi_c^+(\mathbf{k},\mathbf{r}) = e^{-\pi\gamma/2}\Gamma(1+i\gamma)e^{i\mathbf{kr}}M(-i\gamma,1,ikr - i\mathbf{kr}) \tag{4}$$

is a solution of (3). Here, $M(a,b,z)$ is the regular confluent hypergeometric function [27]. The partial-wave expansion is given by the well-known form

$$\psi_c^+(\mathbf{k},\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)\psi_l^+(k,r)P_l(\cos\vartheta), \tag{5}$$

where $P_l(z)$ is the Legendre polynomial and ϑ is the angle between the vectors $\mathbf{k}$ and $\mathbf{r}$. The full radial part $\psi_l^+(k,r)$ is expressed with the help of the regular Coulomb function $F_l(k,r)$ as

$$\psi_l^+(k,r) = \frac{1}{kr}i^l\exp(i\sigma_l)F_l(k,r). \tag{6}$$

The explicit formula reads

$$\psi_l^+(k,r) = \frac{\Gamma(l+1+i\gamma)}{\Gamma(2l+2)}e^{-\gamma\pi/2}e^{-ikr}(2ikr)^l \times M(l+1-i\gamma,2l+2,2ikr), \tag{7}$$

and the Coulomb phase shift is defined by $e^{2i\sigma_l} = \Gamma(l+1+i\gamma)/\Gamma(l+1-i\gamma)$. The pw components $\psi_l^+(k,r)$ satisfy the radial Schrödinger equation

$$\left[-\frac{1}{2r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{2r^2} + \frac{\gamma k}{r} - \frac{k^2}{2}\right]\psi_l(k,r) = 0. \tag{8}$$

The Coulomb scattering function can be split into so-called incoming and scattered waves [28]. Using the identity 7.2.2.9 in [29], we can write

$$\psi_c^+(\mathbf{k},\mathbf{r}) = \psi_i(\mathbf{k},\mathbf{r}) + \psi_s(\mathbf{k},\mathbf{r}), \tag{9}$$

where

$$\psi_i(\mathbf{k},\mathbf{r}) = e^{\pi\gamma/2}e^{i\mathbf{kr}}U(-i\gamma,1,ikr - i\mathbf{kr}), \tag{10}$$

and

$$\psi_s(\mathbf{k},\mathbf{r}) = e^{\pi\gamma/2}\frac{\Gamma(1+i\gamma)}{\Gamma(-i\gamma)}e^{ikr}U(1+i\gamma,1,i\mathbf{kr} - ikr). \tag{11}$$

The notation $U(a,b,z)$ stands for the irregular confluent hypergeometric function [27]. Interestingly, not only $\psi_c^+(\mathbf{k},\mathbf{r})$ but the functions $\psi_i(\mathbf{k},\mathbf{r})$ and $\psi_s(\mathbf{k},\mathbf{r})$ satisfy the 3D Schrödinger equation (3).

The partial-wave expansions of the incoming and scattered parts are given in [28]. Later we will use them, so we quote the main result of paper [28]. We use a very similar notation as in [28], however, we have rewritten the Whittaker function W in terms of U.

The pw expansions of $\psi_i(\mathbf{k},\mathbf{r})$ and $\psi_s(\mathbf{k},\mathbf{r})$ are given in the same form as (5), but the pw components now read

$$\psi_{i,l}(k,r) = \omega_{i,l}(k,r) + \chi_l(k,r) \tag{12}$$

and

$$\psi_{s,l}(k,r) = \omega_{s,l}(k,r) - \chi_l(k,r). \tag{13}$$

We note that our definitions of $\omega_{i,l}$, $\omega_{s,l}$, and χ_l are constant times of the original ones [28]. The explicit expressions are the following:

$$\omega_{i,l}(k,r) = e^{-ikr}e^{\gamma\pi/2}(-1)^{l+1}(2ikr)^l \times U(l+1-i\gamma,2l+2,2ikr), \tag{14}$$

$$\omega_{s,l}(k,r) = e^{ikr}e^{2i\sigma_l+\gamma\pi/2}(-1)^{l+1}(2ikr)^l \times U(l+1+i\gamma,2l+2,-2ikr), \tag{15}$$

and

$$\chi_l(k,r) = \frac{e^{ikr+\gamma\pi/2}}{2ikr}\frac{(-1)^l}{(2ikr)^l}\frac{\Gamma(2l+1)}{\Gamma(l+1-i\gamma)} \times \sum_{n=0}^{l}\frac{(-1)^n(i\gamma-l)_n}{(-2l)_n n!}(2ikr)^n. \quad (16)$$

The equation

$$\psi_l^+(k,r) = \omega_{i,l}(k,r) + \omega_{s,l}(k,r) \quad (17)$$

is also proven in [28]. We mention that the splitting (17) simply follows from (7) if the function $M(l+1-i\gamma,2l+2,2ikr)$ is rewritten in terms of the irregular confluent hypergeometric functions U using equation 7.2.2.9 of [29].

Although the functions $\psi_i(\mathbf{k},\mathbf{r})$ and $\psi_s(\mathbf{k},\mathbf{r})$ are solutions of the 3D Schrödinger equation (3), surprisingly the partial-wave components $\psi_{i,l}(k,r)$ and $\psi_{s,l}(k,r)$ do not satisfy the radial Schrödinger equation (8) (for details see [28]). This property will be proven to be very important for our method.

By using the asymptotic expansion 13.5.2 of [27], we get the asymptotic form of the Coulomb scattering wave function in the well-known form

$$\psi_c^+(\mathbf{k},\mathbf{r}) = e^{i\mathbf{kr}}(kr-\mathbf{kr})^{i\gamma}\left[1+O\left(\frac{1}{kr}\right)\right] + f_c(\cos(\vartheta))\frac{e^{ikr-i\gamma\ln(2kr)}}{r}\left[1+O\left(\frac{1}{kr}\right)\right], \quad (18)$$

where $f_c(\cos(\vartheta))$ is the Coulomb scattering amplitude. The function $e^{i\mathbf{kr}}(kr-\mathbf{kr})^{i\gamma}$ is called the CMPW.

III. DRIVEN SCHRÖDINGER EQUATION

The scattering solution of the Schrödinger equation is searched for in the form (1). From the Schrödinger equation (3) with a simple rearrangement, the driven Schrödinger equation (or Schrödinger equation with a source term)

$$\left(\frac{p^2}{2}+\frac{1}{2}\Delta_{\mathbf{r}}-\frac{\gamma k}{r}\right)\psi^{sc+}(\mathbf{k},\mathbf{r}) = S(\mathbf{k},\mathbf{r}) \quad (19)$$

can be derived for $\psi_c^{sc+}(\mathbf{k},\mathbf{r})$. The source term is given by

$$S(\mathbf{k},\mathbf{r}) = \left(-\frac{1}{2}\Delta_{\mathbf{r}}+\frac{\gamma k}{r}-\frac{k^2}{2}\right)\phi_0(\mathbf{k},\mathbf{r}). \quad (20)$$

We mention that the driven Schrödinger equation (19) has been studied in [20]. For quite general sources, very complicated analytic solutions can be found [20]. The aim of our paper is to derive an easy numerical method to solve (19) and, from the scattered part of the wave function, deduce the scattering amplitude.

The asymptotic form (18) inspires the following choice for $\phi_0(\mathbf{k},\mathbf{r})$:

$$\phi_0(\mathbf{k},\mathbf{r}) = e^{i\mathbf{kr}}(kr-\mathbf{kr})^{i\gamma}. \quad (21)$$

This splitting is based on the CMPW and it has been used in [24,25] in order to derive the surface integral formalism of the scattering theory. By using Descartes coordinates, it is easy to derive a simple form for the source term,

$$S(\mathbf{k},\mathbf{r}) = \frac{\gamma^2 k}{r(kr-\mathbf{kr})}e^{i\mathbf{kr}}(kr-\mathbf{kr})^{i\gamma}. \quad (22)$$

We may try to use the splitting based in the incoming Coulomb wave function, i.e., we make the choice

$$\phi_0(\mathbf{k},\mathbf{r}) = \psi_i(\mathbf{k},\mathbf{r}), \quad (23)$$

instead of (21). In this case, we get $S(\mathbf{k},\mathbf{r})=0$. This follows from the fact that the function $\psi_i(\mathbf{k},\mathbf{r})$ satisfies (3). Here we do not get a driven Schrödinger equation; $\psi^{sc+}(\mathbf{k},\mathbf{r})$ satisfies the original homogeneous equation (3) and $\psi^{sc+}(\mathbf{k},\mathbf{r}) = \psi_s(\mathbf{k},\mathbf{r})$.

If we want to derive the pw form of the driven Schrödinger equation (19), we have to have the pw expansions of the source term,

$$S(\mathbf{k},\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)S_l(k,r)P_l(\cos(\vartheta)), \quad (24)$$

and of $\phi_0(\mathbf{k},\mathbf{r})$,

$$\phi_0(\mathbf{k},\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)\phi_{0,l}(k,r)P_l(\cos(\vartheta)). \quad (25)$$

By using the operator identity [30]

$$\Delta_{\mathbf{r}} = \frac{1}{r}\frac{d^2}{dr^2}r - \frac{\hat{L}^2}{r^2}, \quad (26)$$

where $\hat{L}^2$ is the square of the orbital angular momentum operator, we can derive the partial-wave form of the driven Schrödinger equation (19) as

$$\left[\frac{k^2}{2}+\frac{1}{2r}\frac{d^2}{dr^2}r-\frac{l(l+1)}{2r^2}-\frac{\gamma k}{r}\right]\psi_l^{sc+}(k,r) = S_l(k,r), \quad (27)$$

where

$$\psi^{sc+}(\mathbf{k},\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)\psi_l^{sc+}(k,r)P_l(\cos(\vartheta)). \quad (28)$$

Later, it will prove to be very useful if we make the splitting of the scattering wave function not in the 3D form (1), but on the pw level. We take the pw component of the scattering wave function in the form

$$\psi_l^+(k,r) = \tilde{\phi}_{0,l}(k,r) + \tilde{\psi}_l^{sc+}(k,r), \quad (29)$$

where $\tilde{\phi}_{0,l}(k,r)$ is a fixed known function and $\tilde{\psi}_l^{sc+}(k,r)$ is considered as an unknown function. From the partial-wave Schrödinger equation, we get the nonhomogeneous differential equation

$$\left[\frac{k^2}{2}+\frac{1}{2r}\frac{d^2}{dr^2}r-\frac{l(l+1)}{2r^2}-\frac{\gamma k}{r}\right]\tilde{\psi}_l^{sc+}(k,r) = \tilde{S}_l(k,r), \quad (30)$$

where

$$\tilde{S}_l(k,r) = \left[-\frac{1}{2r}\frac{d^2}{dr^2}r+\frac{l(l+1)}{2r^2}+\frac{\gamma k}{r}-\frac{k^2}{2}\right]\tilde{\phi}_{0,l}(k,r). \quad (31)$$

If we take $\tilde{\phi}_{0,l}(k,r)$ identical to the partial-wave component of $\phi_0(\mathbf{k},\mathbf{r})$, i.e., $\tilde{\phi}_{0,l}(k,r) = \phi_{0,l}(k,r)$, then the source terms $S_l(k,r)$ and $\tilde{S}_l(k,r)$ are identical if in Eq. (20) the action of the Laplace operator can be given in the form (26). This replacement, however, is valid only for those functions which are finite at $r = 0$ (see [30], p. 496).

In the case of splitting based on (23), the function $\psi_i(\mathbf{k},\mathbf{r})$ is not finite at $r = 0$. In this circumstance, the 3D splitting and the pw level splitting are different. We have already seen that the 3D splitting based on (23) does not lead to a driven Schrödinger equation. However, if we make the pw splitting

$$\psi_l^+(k,r) = \psi_{i,l}(k,r) + \tilde{\psi}_l^{sc+}(k,r), \tag{32}$$

i.e., we take $\tilde{\phi}_{0,l}(k,r) = \psi_{i,l}(k,r)$, then we get a driven radial Schrödinger equation. The direct calculation of (31) gives the following source term:

$$\tilde{S}_l(k,r) = \frac{e^{ikr+\gamma\pi/2}}{2r^2\Gamma(-i\gamma)}. \tag{33}$$

Interestingly, the source term is independent from l. The derivation of (33) is given in Appendix A.

IV. PARTIAL-WAVE EXPANSION AND ASYMPTOTIC FORMS

The pw expansion of $\psi_i(\mathbf{k},\mathbf{r})$ is given in [28] and we have reviewed it earlier. We now determine the corresponding expansion of the CMPW. The pw expansion of the CMPW is written in the standard form

$$e^{i\mathbf{kr}}(kr - \mathbf{kr})^{i\gamma} = \sum_{l=0}^{\infty}(2l+1)\tau_l(k,r)P_l(\cos(\vartheta)), \tag{34}$$

and the radial functions are given by the integral

$$\tau_l(k,r) = \frac{1}{2}(kr)^{i\gamma}\int_{-1}^{1} e^{ikrx}(1-x)^{i\gamma}P_l(x)dx. \tag{35}$$

A compact expression for the pw component of the CMPW can be given for arbitrary l. Using (35) and the integral 2.17.5.6 in [29], we get

$$\tau_l(k,r) = \frac{(-i\gamma)_l}{(1+i\gamma)_{l+1}}(2kr)^{i\gamma}e^{ikr}\,{}_2F_2(1+i\gamma, 1+i\gamma; l+2+i\gamma, 1+i\gamma-l; -2ikr), \tag{36}$$

where $(a)_n$ is the Pochhammer symbol.

For the application of complex scaling, we have to know the asymptotic behavior of the scattered part of the wave function, $\psi_l^{sc+}(k,r)$. Here we derive formulas valid at large r values. With the help of the expression 13.5.2 from [27], we get the following asymptotic expansions valid at $r \to \infty$:

$$\omega_{i,l}(k,r) \sim \frac{e^{-ikr}(2kr)^{i\gamma}}{2ikr}(-1)^{l+1}\sum_{n=0}^{\infty}a_{i,n}^l\frac{1}{(2ikr)^n} \tag{37}$$

and

$$\omega_{s,l}(k,r) \sim \frac{e^{ikr}(2kr)^{-i\gamma}}{2ikr}e^{2i\sigma_l}\sum_{n=0}^{\infty}a_{s,n}^l\frac{1}{(2ikr)^n}. \tag{38}$$

The expansion coefficients are given by $a_{i,n}^l = (-1)^n(l+1-i\gamma)_n(-l-i\gamma)_n/n!$ and $a_{s,n}^l = (l+1+i\gamma)_n(-l+i\gamma)_n/n!$. These asymptotic forms show that with the help of the splitting (17), the incoming and outgoing spherical waves are clearly separated in the pw Coulomb scattering wave function.

In order to derive an asymptotic expansion of $\tau_l(k,r)$, we express (36) in terms of Meijer's G function. By using 5.11.1(2) from [31], we get

$$\tau_l(k,r) = e^{ikr}(2kr)^{i\gamma}(-1)^l \times G_{2,3}^{1,2}\left(2ikr\,\middle|\begin{matrix}-i\gamma, & -i\gamma \\ 0, & -1-i\gamma-l,\ l-i\gamma\end{matrix}\right). \tag{39}$$

We are interested in the asymptotic behavior after CS is carried out, i.e., r is replaced by $re^{i\theta}$ and $0 < \theta < \pi$. We give the asymptotic expansion valid in this case. By considering the expression 6.5.32 from [27], we can derive

$$\tau_l(k,re^{i\theta}) \sim \frac{e^{-ikre^{i\theta}}}{2ikre^{i\theta}}(2kre^{i\theta})^{i\gamma}(-1)^{l+1}\sum_{n=0}^{\infty}\frac{d_n^l(-2)^n}{(2ikre^{i\theta})^n}, \tag{40}$$

where the expansion coefficients satisfy the recursion

$$4(n+1)d_{n+1}^l = 2[2n^2 - n(2i\gamma-1) - l^2 - l - i\gamma]d_n^l - n(n-l-i\gamma-1)(n+l-i\gamma)d_{n-1}^l, \tag{41}$$

and $d_0^l = 1$.

Since the pw components are related to each other by the simple relation

$$\psi_l^+(k,r) = \tau_l(k,r) + \psi_l^{sc+}(k,r), \tag{42}$$

and we have the splitting (17), we can write

$$\psi_l^{sc+}(k,r) = [\omega_{i,l}(k,r) - \tau_l(k,r)] + \omega_{s,l}(k,r). \tag{43}$$

We notice that the last term in (43), $\omega_{s,l}(k,r)$, asymptotically contains only an outgoing spherical wave [see Eq. (38)], so the applicability of CS is determined by the behavior of $\omega_{i,l}(k,re^{i\theta}) - \tau_l(k,re^{i\theta})$ at $r \to \infty$. Fortunately, the asymptotic expansions of the functions $\omega_{i,l}(k,r)$ and $\tau_l(k,r)$ are carried out using the same asymptotic sequence of functions $\{e^{-ikr}(2kr)^{i\gamma}(-1)^{l+1}/(2ikr)^n,\ n = 0,1,2,\ldots\}$, so we can simply add and subtract the asymptotic expansions as required [32]. Using (37) and (40), we can write the following asymptotic expansion:

$$[\omega_{i,l}(k,re^{i\theta}) - \tau_l(k,re^{i\theta})] \sim \frac{e^{-ikre^{i\theta}}}{2ikre^{i\theta}}(2kre^{i\theta})^{i\gamma}(-1)^{l+1} \times \sum_{n=0}^{\infty}\frac{a_{i,n}^l - d_n^l(-2)^n}{(2ikre^{i\theta})^n}. \tag{44}$$

Let us now investigate (44). We realize that $a_{i,0}^l - d_0^l = 0$. This means that in leading order, $\psi_l^{sc+}(k,re^{i\theta})$ does not contain a complex-scaled incoming spherical wave. However, in higher orders, $\psi_l^{sc+}(k,re^{i\theta})$ does contain a complex-scaled "generalized" incoming spherical wave $(e^{-ikr}/r^n, n > 1)$. This means that the complex-scaled scattered part of the wave function $\psi_l^{sc+}(k,re^{i\theta})$ does not tend to zero as $r \to \infty$.

This finding is demonstrated in Fig. 1. Both the left-hand side and the right-hand side of (44) are displayed. From the asymptotic expansion only, the next-to-leading order term is considered (the leading-order term is zero). The real part of the

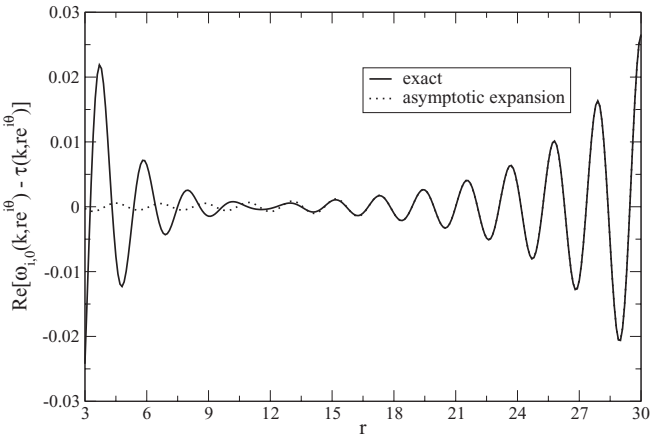

FIG. 1. The function $\omega_{i,0}(k,r) - \tau_0(k,r)$ and the next-to-leading order term of its asymptotic expansion (44) are complex scaled using $\theta = 0.1$. Only the real parts are displayed. The momentum is $k = 3$, the Sommerfeld parameter is $\gamma = 1/3$, and $l = 0$. The solid line denotes the exact values and the dashed line corresponds to the asymptotic expansion (44).

function $\omega_{i,0}(k,re^{i\theta}) - \tau_0(k,re^{i\theta})$ first starts to oscillate with decreasing order of amplitude; however, at larger r values, the presence of the terms of the form $e^{-ikre^{i\theta}}/(re^{i\theta})^n$ dominates and the amplitude of the oscillation becomes larger and larger.

We have a very unfortunate result: if we use the 3D splitting based on the CMPW, then the scattered part of the wave function asymptotically contains both incoming and outgoing spherical waves. This fact prevents the application of complex scaling.

V. COMPLEX SCALING AND SCATTERING STATES

In the previous section, we have established that the splitting of the wave function based on the CMPW, i.e., choice (21), is useless from the point of view of CS. Now we turn to the splitting (32), which is carried out on the pw level. The scattered part of the wave function is given by

$$\tilde{\psi}_l^{sc+}(k,r) = \omega_{s,l}(k,r) - \chi_l(k,r). \tag{45}$$

This equation follows from (12), (17), and (32). The asymptotic form (38) and the expression (16) for $\chi_l(k,r)$ show that the scattered part of the wave function now contains only an outgoing spherical wave and so complex scaling can be safely applied. From (16) and (38), we get, in leading order,

$$\tilde{\psi}_l^{sc+}(k,r) = e^{2i\sigma_l}\frac{e^{ikr}(2kr)^{-i\gamma}}{2ikr}\left[1 + O\left(\frac{1}{|2ikr|}\right)\right] - \frac{e^{ikr+\gamma\pi/2}}{2ikr}\frac{(-1)^l\Gamma(2l+1)}{\Gamma(l+1-i\gamma)} \times \left[\frac{(i\gamma-l)_l}{\Gamma(2l+1)} + O\left(\frac{1}{|2ikr|}\right)\right]. \tag{46}$$

Let us make a variable transformation and replace r with $re^{i\theta}$ in the partial-wave driven Schrödinger equation (27), and furthermore introduce a new function with the definition

$$\tilde{\psi}_{l,\theta}^{sc+}(k,r) = e^{i3\theta/2}\tilde{\psi}_l^{sc+}(k,re^{i\theta}), \tag{47}$$

where θ is an arbitrary fixed real number. A simple calculation gives the equation

$$\left[\frac{k^2}{2} + e^{-2i\theta}\frac{1}{2r}\frac{d^2}{dr^2}r - e^{-2i\theta}\frac{l(l+1)}{2r^2} - e^{-i\theta}\frac{\gamma k}{r}\right]\tilde{\psi}_{l,\theta}^{sc+}(k,r) = \tilde{S}_{l,\theta}(k,r), \tag{48}$$

where the complex-scaled source term is defined by

$$\tilde{S}_{l,\theta}(k,r) = e^{i3\theta/2}\tilde{S}_l(k,re^{i\theta}). \tag{49}$$

The advantage of the complex-scaled driven Schrödinger equation (48) is that its solution behaves very simply asymptotically. If the scaling angle satisfies the condition $0 < \theta < \pi$, then from (46) it follows that

$$\lim_{r\to\infty}\tilde{\psi}_{l,\theta}^{sc+}(k,r) = 0. \tag{50}$$

From the asymptotic form (46), we can establish the following local representation of the partial-wave Coulomb S matrix:

$$e^{2i\sigma_l} \approx (2kre^{i\theta})^{i\gamma}\left[e^{-ikre^{i\theta}}2ikre^{-i\theta/2}\tilde{\psi}_{l,\theta}^{sc+}(k,r) + \frac{e^{\gamma\pi/2}(-1)^l(i\gamma-l)_l}{\Gamma(l+1-i\gamma)}\right], \quad r\to\infty. \tag{51}$$

The local representation of the phase shift given in [15] is different from (51) since the splittings of the scattering wave function are distinct.

The function $\tilde{\psi}_l^{sc+}(k,r)$ is not regular at $r = 0$. However, the validity of the limit

$$\lim_{r\to 0} r^{l+1}\tilde{\psi}_l^{sc+}(k,r) = 0 \tag{52}$$

can be easily demonstrated. Details are given in Appendix B. In order to give a simple boundary condition at $r = 0$, we make the transformation $h_{l,\theta}^{sc+}(k,r) = r^{l+1}\tilde{\psi}_{l,\theta}^{sc+}(k,r)$. This transformation leads to a regular function at $r = 0$. For the new function, we get the differential equation

$$\left(\frac{k^2}{2} + e^{-2i\theta}\frac{1}{2}\frac{d^2}{dr^2} - e^{-2i\theta}\frac{l}{r}\frac{d}{dr} - e^{-i\theta}\frac{\gamma k}{r}\right)h_{l,\theta}^{sc+}(k,r) = r^{l+1}\tilde{S}_{l,\theta}(k,r). \tag{53}$$

The price we pay for the simplification at $r = 0$ is the appearance of a first-order derivative in the equation.

From the earlier considerations presented, it is obvious that the method based on the splitting (32) can be extended to the case when a short-range interaction $V_s(r)$ is added to the pure Coulomb interaction. In this case, the inhomogeneous differential equation (53) is replaced by

$$\left[\frac{k^2}{2} + e^{-2i\theta}\frac{1}{2}\frac{d^2}{dr^2} - e^{-2i\theta}\frac{l}{r}\frac{d}{dr} - e^{-i\theta}\frac{\gamma k}{r} - V_s(re^{i\theta})\right] \times h_{l,\theta}^{sc+}(k,r) = r^{l+1}S_{l,\theta}^{tot}(k,r), \tag{54}$$

where the new source term reads

$$S_{l,\theta}^{tot}(k,r) = \tilde{S}_{l,\theta}(k,r) + e^{i3\theta/2}\psi_{i,l}(k,re^{i\theta})V_s(re^{i\theta}). \tag{55}$$

VI. NUMERICAL RESULTS

The differential equations (53) or (54) have to be solved with the boundary conditions

$$h^{sc+}_{l,\theta}(k,0) = 0 \tag{56}$$

and

$$\lim_{r\to\infty} h^{sc+}_{l,\theta}(k,r) = 0. \tag{57}$$

In numerical calculations instead of (57), the boundary condition

$$h^{sc+}_{l,\theta}(k,R) = 0 \tag{58}$$

can be used. Here, R is a positive and otherwise arbitrary large number. The boundary condition (58) is, of course, an approximation, and how the result depends on R has to be investigated. The value of R should be in the asymptotic region where (46) is satisfied.

The finite-element method is chosen as a numerical technique for the solution of Eqs. (53) or (54). The method and the basis functions used in any elements are described in [33]. The same method was used also in [15]. For the presented calculations, equally spaced finite elements of length 1 are taken. The degree of the Lobatto shape functions [33] is denoted by N, and the same N value is used at each element. The θ parameter of the CS was chosen to 0.1 radian.

First, the pure Coulomb case is considered, i.e., the potential is given by $1/r$. In this case, the numerical result can be compared to the known analytical solution. The momentum is $k = 3$ and the considered orbital angular momentum is $l = 0$. The phase shift is calculated with the help of the local representation (51). In this equation, for $\tilde{\psi}^{sc+}_{l,\theta}(k,r)$, either the exact solution or the approximate one determined by the finite-element method can be used. In the second example, the potential $7.5r^2\exp(-r)$ is added to the previous pure Coulomb term. The very same two cases were studied in [15], where a different splitting of the wave function and the exterior complex-scaling method were used.

The upper panel of Fig. 2 shows the results of the calculations carried out using a pure Coulomb potential. In this case, the exact solution (dashed black line) can be compared to the numerical ones. In the finite-element method, the boundary condition (58) is imposed at two different R values ($R = 250$ and 1000). We note that for $r > R$, the finite-element solution is not defined. The boundary condition should be set at infinity [see (57)], but a finite R value is taken, so it can be expected that the numerical solution is not accurate enough around the point where the boundary condition is set up. This can be clearly seen in Fig. 2. If we choose $R = 250$, then there is an oscillation with a large amplitude around $r = 250$. If the boundary condition is set up at a larger R value, then the oscillatory region is pushed out around this value. In Fig. 2, the oscillatory region moved from $r = 250$ to $r = 1000$ simply by changing the value of the parameter R from $R = 250$ to $R = 1000$. The effect of the boundary condition is noticeable. However, if this edge effect is not considered, then the local representation of the phase shift is practically constant on a huge region. This is a useful feature since it helps to determine a unique value of the phase shift of the numerical calculation. In contrast, the local approximation of the phase shift in [15] tends to the exact value by a persistent oscillation with decreasing order of amplitude.

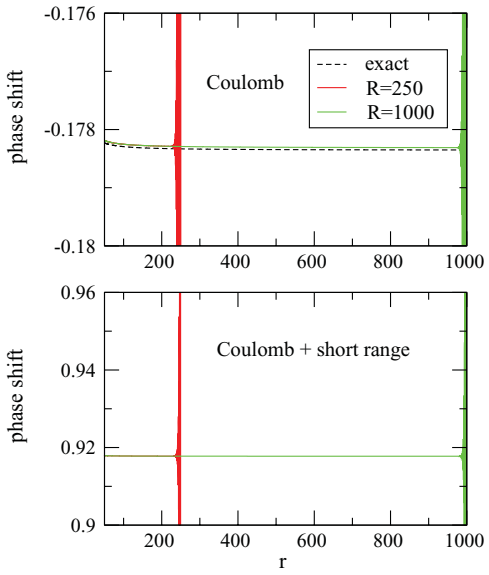

FIG. 2. (Color online) The local representation of the phase shift for a pure Coulomb potential (upper panel) and for the general case when a short-range potential is added to the Coulomb term (lower panel). In the first case, the exact solution (dashed black line) is also displayed. For the numerical solution, the boundary condition is imposed at $R = 250$ [red (dark gray) line] and $R = 1000$ [green (light gray) line]. A detailed discussion is given in the text.

The lower panel of Fig. 2 shows the results when the short-range potential is added to the Coulomb interaction. This modification does not change the previous observations. The lower panel of Fig. 2 clearly demonstrates each of the previous conclusions. The position of the boundary condition influences the value of the phase shift only around the point $r = R$. The phase shift calculated by the expression (51) is practically independent from the value of r. We note that apart from the oscillatory region around $r = 250$, the two numerical solutions

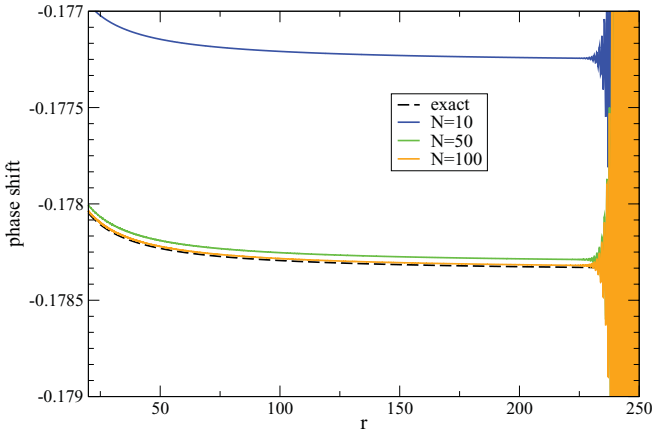

FIG. 3. (Color online) The local representation of the phase shift for a pure Coulomb potential. In the numerical solution, the boundary condition is imposed at $R = 250$. The exact solution and the numerical ones are displayed. In the numerical calculations, the number of the Lobatto shape functions (N) is varied.

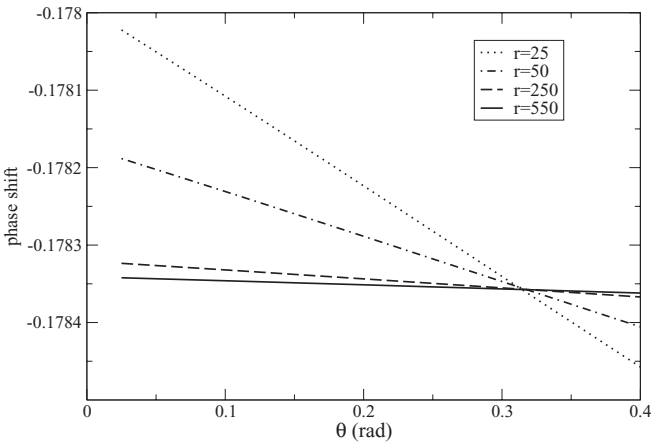

FIG. 4. The local representation of the phase shift for a pure Coulomb potential as a function of the complex-scaling parameter. Four different r values are considered and, in the local representation of the phase shift, the exact wave function is used.

corresponding to the choices $R = 250$ and $R = 1000$ coincide in the region $50 < r < 250$. In this region, in Fig. 2 the red (dark gray) and green (light gray) lines are indistinguishable on the used scale.

The calculations displayed in Fig. 2 have been carried out using 50 Lobatto shape functions on each element. We investigate the dependence of the local representation of the phase shift on the number of Lobatto functions used in the finite-element method. The boundary condition (58) is set up at $R = 250$. The results are depicted in Fig. 3. Apart from the region around $r = 250$, the exact phase shift is reproduced with three-digit accuracy with $N = 50$. The calculation with $N = 100$ very well reproduces the exact solution (where four-digit agreement is reached almost everywhere).

It remains to be checked how the complex-scaling parameter θ influences the calculated phase shift. Figure 4 displays the local representation of the phase shift as the function of the complex-scaling parameter. Four different r values are used. In these calculations, the exact wave function is used in (51). If the value of r is in the asymptotic region (e.g., $r = 550$), then the calculated phase shift is independent from the value of the complex-scaling parameter. For smaller r values, it is advantageous to use a larger θ value to get better agreement with the exact phase shift.

VII. SUMMARY

We have rigorously shown that the two-body scattering problem of the pure Coulomb interaction can be solved using the standard complex-scaling method. This is achieved without using any cutoff of the long-range interaction. The intricate scattering boundary condition is greatly simplified and so the numerical solution can be plainly achieved. It is obvious that the suggested driven Schrödinger equation can be solved by the use of the exterior complex-scaling method too. The advocated splitting of the total-wave function works for general circumstances. It can be applied not only for a pure Coulomb force, but also short-range interactions can be added to the Coulomb potential. We found that the splitting based on the Coulomb modified plane wave does not lead to simplification of the boundary condition from the point of view of complex scaling.

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APPENDIX A

In the case of the splitting (32), according to (31), the source term reads

$$\tilde{S}_l(k,r) = \left[-\frac{1}{2r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{2r^2} + \frac{\gamma k}{r} - \frac{k^2}{2}\right] \times [\omega_{i,l}(k,r) + \chi_l(k,r)]. \tag{A1}$$

Since $\omega_{i,l}(k,r)$ is just the Coulomb Jost solution [26,28], the contribution from $\omega_{i,l}(k,r)$ to the source is zero. By introducing a new variable $z = 2ikr$ and rewriting the summation in (16), we have

$$\tilde{S}_l(k,r) = \left[-\frac{k^2}{2} + \frac{2k^2}{z}\frac{d^2}{dz^2}z - \frac{2k^2 l(l+1)}{z^2} + \frac{2i\gamma k^2}{z}\right]\chi_l(z), \tag{A2}$$

where

$$\chi_l(z) = \frac{e^{\gamma\pi/2}}{\Gamma(1-i\gamma)}\frac{e^{z/2}}{z}\sum_{n=0}^{l}\frac{(l+1)_n(-l)_n(1)_n}{(1-i\gamma)_n}\frac{z^{-n}}{n!}. \tag{A3}$$

A direct calculation gives

$$\tilde{S}_l(k,r) = \frac{2k^2 e^{\gamma\pi/2}}{\Gamma(1-i\gamma)}\frac{e^{z/2}}{z^2}\sum_{n=0}^{l}\frac{(l+1)_n(-l)_n}{(1-i\gamma)_n} \times \left[i\gamma - n + \frac{n(n+1) - l(l+1)}{z}\right]z^{-n}. \tag{A4}$$

Rearranging the summation, we get

$$\tilde{S}_l(k,r) = \frac{2k^2 e^{\gamma\pi/2}}{\Gamma(1-i\gamma)}\frac{e^{z/2}}{z^2} \times \left\{i\gamma + \sum_{n=0}^{l-1}\left[\frac{(l+1)_n(-l)_n}{(1-i\gamma)_n}[n(n+1) - l(l+1)] + (i\gamma - n - 1)\frac{(l+1)_{n+1}(-l)_{n+1}}{(1-i\gamma)_{n+1}}\right]z^{-n-1}\right\}. \tag{A5}$$

Using the fact that the Pochhammer symbols satisfy the recursion $(a)_{n+1} = (a)_n(a+n)$, we can show that the expression inside the square bracket is zero, and so we have proven (33).

APPENDIX B

According to (13), in order to prove (52), it is enough to show that

$$\lim_{r\to 0} r^{l+1}\omega_{s,l}(k,r) = \lim_{r\to 0} r^{l+1}\chi_l(k,r). \tag{B1}$$

From definition (16), it follows that

$$\lim_{r\to 0} r^{l+1}\chi_l(k,r) = e^{\gamma\pi/2}\frac{(-1)^l}{(2ik)^{l+1}}\frac{\Gamma(2l+1)}{\Gamma(l+1-i\gamma)}. \quad \text{(B2)}$$

Considering (15), and the expression 7.2.2.3 from [29], the function $r^{l+1}\omega_{s,l}(k,r)$ is a sum of three terms,

$$r^{l+1}\omega_{s,l}(k,r) = A_l(k,r) + B_l(k,r) + C_l(k,r), \quad \text{(B3)}$$

where

$$A_l(k,r) = -K_l(k)\frac{M(l+1+i\gamma,2l+2;-2ikr)}{\Gamma(2l+2)\Gamma(i\gamma-l)} \times (-2ikr)^{2l+1}\ln(-2ikr)e^{ikr}, \quad \text{(B4)}$$

$$B_l(k,r) = -K_l(k)\frac{e^{ikr}}{\Gamma(2l+2)\Gamma(i\gamma-l)} \times \sum_{n=0}^{\infty} f_n^l \frac{(l+1+i\gamma)_n}{(2l+2)_n}\frac{(-2ikr)^{n+2l+1}}{n!}, \quad \text{(B5)}$$

and

$$C_l(k,r) = -K_l(k)\frac{(2l)!e^{ikr}}{\Gamma(l+1+i\gamma)}\sum_{n=0}^{\infty}\frac{(i\gamma-l)_n}{(-2l)_n}\frac{(-2ikr)^n}{n!}. \quad \text{(B6)}$$

The following abbreviations are used:

$$K_l(k) = \frac{(-1)^{l+1}}{(2ik)^{l+1}}e^{2i\sigma_l+\gamma\pi/2} \quad \text{(B7)}$$

and

$$f_n^l = \Psi(l+1+i\gamma+n) - \Psi(n+1) - \Psi(2l+2+n). \quad \text{(B8)}$$

The digamma function is denoted by $\Psi(z)$. From the expressions above, it is clear that $\lim_{r\to 0} A_l(k,r) = 0$ and $\lim_{r\to 0} B_l(k,r) = 0$. The limit value of $C_l(k,r)$ as $r \to 0$ is exactly the right-hand side of (B2), so we have proven (52).

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