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On the applicability of the exterior complex scaling method for scattering problems including Coulombic potentials

G. Gasaneo[1,2,a], L.U. Ancarani[3], and D.M. Mitnik[2,4]

[1] Departamento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Buenos Aires, Argentina
[2] Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina
[3] Laboratoire de Physique Moléculaire et des Collisions, UMR CNRS 7565, Université de Lorraine, 57078 Metz, France
[4] Departamento de Física, Universidad de Buenos Aires, and Instituto de Astronomía y Física del Espacio (IAFE), C.C. 67, Suc. 28, (C1428EGA) Buenos Aires, Argentina

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Abstract. We study some formal aspects of the exterior complex scaling (ECS) approach when implemented for both short and long-range potentials. In particular, we focus on the inconsistencies related to the requirement of an artificial cut-off of the potential in order to avoid exponential divergencies due to the complex rotation. For the pure two-body Coulomb potential we demonstrate analytically and numerically that the ECS inner solution is indeed the correct one, thus reinforcing the method; the extraction of the transition amplitude, however, remains problematic. We also show that a consistent application of the ECS method requires a distorted wave formulation, and two variants are proposed. Finally, we will propose an approach equivalent to the original ECS but that avoids all formal difficulties. It is based on performing the complex rotation on the basis functions rather than on the driven equation itself, and makes use of Sturmian functions with appropriately chosen outgoing boundary conditions. Our proposal differs from one of the original versions of the ECS method, through the use of physically based basis functions rather than pure numeric ones.

1 Introduction

The description of the collision processes between three particles presents significant difficulties both from the formal and numerical points of view. Different and successful time-independent methods as, e.g., the convergent close coupling [1,2], the J-matrix [3] and the exterior complex scaling (ECS) [4–6] have been developed to deal with them. In general these methods require an enormous amount of computational resources. The application of the same methods to the study of the next step, the four-body problem, is presently prohibitive or very difficult from the computational point of view (see, e.g., [7]). This is proved by the fact that none of the mentioned approaches have been applied as a pure ab initio treatment to the complete study of, e.g., double ionization of helium by electron impact; only S-wave models has been considered [8,9]. The reason is not the fact that they cannot be extended to deal with more particles, but because they demand such huge amounts of computational resources that their numerical implementation are presently impossible. For that reason it is important to clearly understand the advantages and drawbacks of different methods to be able to improve their efficiency and to extend them to the treatment of more complicated systems even with the computational resources available nowadays. In an attempt to improve the already existing methods, a modification of the original ECS has been implemented and successfully applied for electron-hydrogen collisions [10–12], the study of threshold behavior of e-H ionizing collisions [13] and electron-helium double ionization, single ionization with excitation, and double excitation within a S-wave model [14]. The main objective of the propagating exterior complex scaling method presented in references [10–12] is to maintain the efficiency of the original ECS approach and to reduce the computational requirements. It is within this framework and line of thinking that we present in this article a study of the ECS method when applied to scattering problems.

Complex scaling has been for a long time an important tool to study the structure of atomic systems as well as resonance states. This was mainly associated to the fact that only square integrable states could be treated within the framework of the method. The extension to collision problems was performed by Rescigno et al., see e.g. reference [15], for two-body problems. Since this first application to scattering, the ECS has proved to be one of the most successful methods to deal with a large variety

[a] e-mail: ggasaneo@gmail.com

of processes: the ionization of hydrogen by electron impact [4]; the double photo-ionization of helium [16]; the photo-ionization of molecules [17–19] (and further discussed using spheroidal coordinates [20,21]); even two-slit type of experiments were successfully described [22].

In this paper, we do not question the now well-established capabilities of the ECS approach and its computational technology; rather we concentrate on some theoretical and formal issues for scattering problems with long-range potentials. On page 2 of reference [23] Baertschy et al. stated that "*the fundamental correctness of our procedure relies on the empirical observation that the computed results are in perfect agreement with absolute experimental measurements*". Our work has the same philosophy as the recent works of Elander et al. [24], Volkov et al. [25] and Yakovlev et al.[26] who stated *"the definite success in applying this method to important and complicated problems ... makes a detailed study urgent"*. (p. 2 of Ref. [25]). We shall study the foundations of the method itself and also its implementation for long-range potentials, with a particular focus on its applicability to pure Coulomb potentials. Finally, we shall make a proposal to avoid formal difficulties associated to the recipe.

The implementation of the ECS method is based on the separation of the total wave function as the sum of an asymptotic (or approximated) solution of the problem and a scattering function [27,28] with, respectively, standing – and outgoing-wave behavior at large distances. This separation leads straightforwardly to a driven Schrödinger equation for the scattering part, the driven term being given by the product of the interaction potential and the asymptotic solution. Within the ECS method a complex rotation of the radial coordinate is performed on the driven equation. This enforces, at large distances, an exponentially decreasing behavior of the scattering wave function thus avoiding, according to the authors of reference [15], the imposition of asymptotic conditions. The complex rotation, however, introduces a problem on the driven term, as the latter becomes divergent due to the stationary character of the asymptotic solution. To circumvent this problem Rescigno et al. introduced – artificially – a cut-off on the interaction of the driven term, and at the same time used an exterior complex rotation of the coordinate. This cut-off is also used in the propagating ECS of Bartlett et al. [10] and Bartlett and Stelbovics [11,12]. This means that the rotation is effectively acting after a given value R_0 of the radial coordinate r and in this region the potential of the driven term is switched off. According to Baertschy et al. (p. 4 of Ref. [23]) "*[the cut-off] is the only source of systematic error in our scheme for calculating the scattered wave with exterior complex scaling*". As we shall discuss in more details in Sections 2.2 and 3, the ECS recipe leads to some formal difficulties. Some of the delicate issues/questions that appear are: (i) What are the consequences of cutting the potential only in the driven term? (ii) Does the wave function obtained in the region $r > R_0$ have any physical meaning? (iii) Is it really necessary to introduce a cut-off in the potential? We will investigate some of these questions and provide answers to some of them. Our work aims to contribute in understanding how and why the method works, independently of the fact that it is numerically very efficient as proved by the many important and successful results already presented to treat a large variety of processes [4,16–22]. In this report we shall deal only with the two-body case as it allows to illustrate all the ingredients and associated difficulties of the ECS method. Several results and observations to be presented are of general character and valid for any potential; however, the pure Coulomb case is fully treated here as it allows for an analytical study. A similar, though more cumbersome, analysis applies to three-body problems; it will be briefly discussed in Section 5.

Another major issue of the present paper is the applicability of the ECS method to the pure Coulomb potential. In reference [15], the authors showed how to deal with long-range potential, but explicitly mentioned in a note that the method does not apply for Coulomb potentials (note [28] of the cited paper: it is assumed the two-body "*potential should fall off more rapidly than* $1/|r|$ *at infinity*"). Recently, the Coulomb case has been under scrutiny since "*its extension to the Coulomb case remained questionable*" (p. 2 of [25]), and a series of papers have been dedicated to the ECS approach [24–26,29] aiming "*to set the... [ECS] approach on a mathematically solid basis*" (p. 2 of [25]). These facts motivated us to initiate a careful study of the ECS approach, since the Coulomb potential is the dominating interaction in atomic and molecular physics; the aim is to answer the question of whether the ECS method can be included into the formal scattering theory and applied to the pure two-body Coulomb potential.

The rest of the paper is arranged as follows. In Section 2 we present the two-body scattering formulation, the main ECS ingredients (Sect. 2.1), and several formal issues are discussed and questions are raised (Sect. 2.2). Section 3 is dedicated to understanding and reinforcing the method. In particular we will solve analytically the driven equation for the pure Coulomb case (with the ECS unbalanced treatment of the potential), demonstrate that the solution found in the inner region is indeed proportional to the correct one, and provide the proportionality coefficient. Next (Sect. 3.2) we show that when dealing with pure Coulomb potentials the use of a free-particle asymptotic initial state leads to a scattering problem which is not well defined. A Coulomb distorted initial state should be used instead in order to extract the transition matrix from the asymptotic behavior of the scattering wave function. We thus propose a reformulation within which the ECS approach could be equally applied to long-range potentials including the pure Coulomb case (note that the latter differs from the case of Coulomb plus short range potential which can be dealt with according to the description provided in section 4.2 of Ref. [5]). Section 4 presents an alternative approach based on the use of complex basis functions. We shall describe and illustrate how Sturmian functions with appropriately chosen outgoing behavior allow to avoid all of the formal difficulties encountered with

the ECS recipe using real basis functions. This alternative approach will be useful for the treatment of the three-body scattering problem. Finally, Section 5 presents a brief summary and a discussion with respect to the three-body case.

Atomic units ($\hbar = e = 1$) are used throughout.

2 Formulation of the scattering problem

Consider the scattering between two particles interacting via a spherically symmetric potential $V(r)$. The radial two-body Schrödinger equation describing the dynamics of the problem is

$$[\mathcal{T} + V(r) - E]\,\Phi(r) = 0, \tag{1}$$

where $\mathcal{T} = -\frac{1}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)$ is the full kinetic energy operator, μ the reduced mass, l the angular momentum eigenvalue and the energy $E = k^2/(2\mu)$ assumed positive. The transformations $\Phi(r) = \Psi(r)/r$ is usually introduced for convenience converting equation (1) into the following

$$[\mathcal{T}_l + V(r) - E]\,\Psi(r) = 0. \tag{2}$$

where $\mathcal{T}_l = -\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)$ represents the reduced kinetic energy operator.

The free-particle solution

$$\Psi_0(r) = kr j_l(kr), \tag{3}$$

of the simplified problem (without potential)

$$[\mathcal{T}_l - E]\,\Psi_0(r) = 0 \tag{4}$$

behaves at large distances as $\sin\left(kr - \frac{\pi}{2}l\right)$, and corresponds to a unitary flux; $j_l(z)$ represents the spherical Riccati-Bessel function of order l [30].

As done in standard textbooks (e.g., [27,28]), the solution of the scattering problem can be separated into two terms as follows

$$\Psi(r) = \Psi_0(r) + \Psi_{\rm sc}(r), \tag{5}$$

where $\Psi_0(r)$ is taken as initial – asymptotic – state (corresponding to no scattering) and $\Psi_{\rm sc}(r)$ is the scattering term describing the dynamics of the collision process. In principle, $\Psi_{\rm sc}(r)$ should have pure outgoing behavior, noted $\Psi^+_{\rm sc}(r)$; the corresponding wave function (5) is noted $\Psi^+(r)$. Replacing the decomposition (5) into equation (2) we get the following driven Schrödinger equation for $\Psi_{\rm sc}(r)$

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{\rm sc}(r) = -V(r)\Psi_0(r). \tag{6}$$

2.1 The ECS approach

The non-homogeneous equation (6) is the one solved within the context of the ECS [5,6,15]. The strategy used to solve it is based on two main ingredients: (i) an (exterior) complex rotation of the radial coordinate, such as the one proposed in reference [7,15]

$$r = q(r) = \begin{cases} r & r \le R_0 \\ R_0 + (r - R_0)e^{i\eta} & r > R_0 \end{cases} \tag{7}$$

where R_0 defines the radius within which the wavefunction will be the usual function of real valued coordinates, and $\eta > 0$ represents the scaling rotation angle on the complex plane; and (ii) a sharp cut-off of the potential $V(r)$ at the value $r = R_0$

$$V_{R_0}(r) = \begin{cases} V(r) & r \le R_0 \\ 0 & r > R_0, \end{cases} \tag{8}$$

for every potential excluding those decreasing exponentially or faster. According to the authors of reference [5,6,15], these two key bricks allow to affirm that the imposition of the asymptotic conditions is avoided. This is associated to the fact that, when the exterior complex rotation is performed, the wave function $\Psi^+(r)$ decreases to zero in the region $r > R_0$, and a *numerical zero* can be assumed for the function in, e.g., a numerical grid. Within the method, the amplitude A_l can be extracted from the function defined in the inner region ($r < R_0$) by taking the limit of the function for large r but smaller than R_0, or using the definition [6]

$$A_l = -\frac{2\mu}{k}\left\langle j_l(kr)\,|V(r)|\,\frac{\Psi^+(r)}{r}\right\rangle, \tag{9a}$$

$$= \frac{2\mu}{k}\left\langle j_l(kr)\,|\mathcal{T} - E|\,\frac{\Psi^+_{\rm sc}(r)}{r}\right\rangle_{R_0}, \tag{9b}$$

where the subscript R_0 in (9b) denotes the integration limited to the domain $0 \le r \le R_0$. The second equality (9b) is obtained using the Schrödinger equations (1) and (4), and assuming a vanishing contribution for $r > R_0$. (We should mention that in Ref. [6], equations (26), (27a) and (27b) are inconsistent with the definition (14); this, however, does not affect the rest of the review paper.)

2.2 Issues and difficulties associated to the ECS approach

Let us start by looking at the effect of performing the exterior complex rotation (7) of the radial coordinate on the solution of equation (6). Assuming that the wave function $\Psi_{\rm sc}(r)$ possesses pure outgoing behavior, the transformation $r \to q(r)$ given by (7) (actually, any general transformation similar to it) will give rise to an exponentially decreasing asymptotic behavior. On the other hand, the function $\Psi_0(r)$ appearing in the RHS of equation (6) has a standing wave behavior and becomes, for values of $r > R_0$,

$$\begin{aligned}\Psi_0(r) &\sim \sin\left(kre^{i\eta} - \frac{\pi}{2}l\right) \\ &\simeq \frac{1}{2i}\left[e^{ikr(\cos(\eta)+i\sin(\eta))} - e^{-ikr(\cos(\eta)+i\sin(\eta))}\right] \\ &\simeq -\frac{1}{2i}e^{-ikr\cos(\eta)}e^{kr\sin(\eta)}.\end{aligned} \tag{10}$$

Upon rotation of the coordinate, for $r > R_0$, the term with incoming behavior makes the standing wave function (10) – and hence the full wave function (5) – exponentially divergent. The non-homogeneity of equation (6) will be divergent unless the potential $V(r)$ on the RHS decreases fast enough to make it well defined and bound: this condition is met *only* for short-range potentials decreasing exponentially or faster. When $V(r)$ *is* already of that kind of short-range, then the potentials on the left and right-hand-sides of equation (6) are treated on equal footing. However, if $V(r)$ is not of short enough range, or is of long-range character (e.g., a Coulomb potential), something has to be done to avoid the difficulty and keep the non-homogeneous equation (6) well defined.

Within the standard ECS method [5,6,15], but also the propagating ECS [10–12], one – artificially – cuts the potential appearing on the RHS of equation (6) at a distance R_0 from the origin. Hence, the driven equation (6) is solved with the cut-off potential $V_{R_0}(r)$ defined through (8) on the RHS, but with $V(r)$ on the LHS, thus with an unbalanced treatment. This procedure is used in all the papers where the ECS method is presented and applied. In reference [15], the authors stated that "*by zeroing the potential on the complex portion of the contour, we eliminate any numerical difficulties associated with a less than exponential fall off of the potential at large distances, but have no measurable effect on the cross section*", and that "*we do not expect this remedy to come without a price.*" We want here to explore the price of doing that.

A first point is connected with the error introduced into the transition amplitude when using the cut-off potential $V_{R_0}(r)$. Indeed, starting from (9a) we have

$$A_l = \frac{2\mu}{k}\left\langle j_l(kr)\,|\,\mathcal{T}-E|\,\frac{\Psi^+_{\rm sc}(r)}{r}\right\rangle_{R_0} - \frac{2\mu}{k}\left\langle j_l(kr)\,|\,V(r)-V_{R_0}(r)|\,\frac{\Psi^+(r)}{r}\right\rangle. \quad (11)$$

Within the ECS framework, only the first term, i.e. equation (9b), is used to evaluate the transition amplitude as the potential is assumed to be cut, and hence $V(r)-V_{R_0}(r)$ is zero. Thus, an error (which decreases as R_0 increases) is introduced in the calculation by neglecting the external contribution of the potential. Of course if the energy $E \gg V(R_0)$ one can expect this approximation to be valid, as numerically verified in many applications.

Another price payed through the rotation to the complex plane is that the whole wave function (5) loses meaning in the outer region $r > R_0$ while quantum mechanics requires the wave function to be well defined and bound over the whole domain. Thus, to make the ECS work, one makes use of the artifice of cutting the potential. Two main questions then arise: (i) What is the real Schrödinger equation solved in that case? and (ii) What is the connection between the exact solution and the one obtained by this artificial cut-off? These two issues are essential to understand how, and why, the ECS approach leads numerically (as claimed by the authors in Refs. [5,6,15] and demonstrated through many numerical results) to the exact solution of two- and also three-body problems [6,7].

To address these two points let us suppose that, using the original decomposition (5), one solves the driven equation (6) with $V_{R_0}(r)$ on the RHS. Since the potential $V_{R_0}(r)$ is of short range it allows to mathematically impose to the solution, noted $\Psi^+_{{\rm sc},R_0}(r)$, a pure outgoing asymptotic behavior. Starting from equation (6), and using the fact that $\Psi_0(r)$ satisfies equation (4), it is rather easy to see that the full solution $\Psi_{R_0}(r) = \Psi_0(r)+\Psi^+_{{\rm sc},R_0}(r)$ satisfies the following equation

$$[\mathcal{T}_l + V_{R_0}(r) - E]\,\Psi_{R_0}(r) = -V_{\rm dis}(r)\Psi^+_{{\rm sc},R_0}(r). \quad (12)$$

where $V_{\rm dis}(r) = V(r) - V_{R_0}(r)$ is the tail (external) potential. This non-homogeneous equation (it is actually homogeneous up to the point $r = R_0$) is neither the Schrödinger equation corresponding to the full potential $V(r)$, nor the one corresponding to the truncated case $V_{R_0}(r)$. It is the Schrödinger equation solved by the ECS method as presented in references [5,6,15]. While it will coincide with the correct Schrödinger equation (2) in the limit of $R_0 \to \infty$, it is not clear if, and how, the solution of equation (12) will reach the exact solution. If the potential $V(r)$ is of short range, and if R_0 is located in a region where the potential is already negligible, then the procedure is justified since the Schrödinger equation is homogeneous beyond R_0. However, if the potential is of long range, then it is difficult to justify the use of equation (12), *unless one is able to demonstrate that the exact solution of the problem is found in the region* $r < R_0$. This issue is the subject of Section 3.1 where such a demonstration is provided analytically for the pure Coulomb problem.

As explained in reference [15], there are two alternative formulations of the ECS, one where the complex rotation is performed on the Hamiltonian and another where the complex rotation is performed on the basis set used to represent the operators and the wave functions. In most applications of the method the first one is used; this means one solves the equation resulting from changing r by $q(r)$ in equation (6). By writing the scattering wave function as $\Psi_{\rm sc}(r) = \sum a_i\chi_i(r)$ where $\chi_i(r)$ are, e.g., B-splines, the driven equation is reduced to the resolution of a set of linear equations for the a_i coefficients

$$[\mathcal{T}_{l,\eta} + \mathbf{V}_\eta - E\mathcal{O}]\,\mathbf{a} = \mathbf{b}_\eta, \quad (13)$$

where $\mathcal{T}_{l,\eta}$ and $\mathbf{V}_\eta$ are the matrices associated to the rotated kinetic energy and the rotated interaction potential represented on the basis; $\mathcal{O}$ is the overlap matrix. On the right hand side, the vector $\mathbf{b}_\eta$ is:

$$b_{\eta,i} = -\int_0^\infty \chi_i(r)V(q(r))\Psi_0(q(r))dr. \quad (14)$$

As explained before, the rotation applied to $\Psi_0(r) \to \Psi_0(q(r))$ produces a divergency for the initial function, and therefore of $\mathbf{b}$, requiring the cut-off of the potential $V(r)$. What is interesting here is that, assuming that an appropriated distorted wave approach is used, the LHS of equation (13) can be represented in the whole configuration space including the outer region $r > R_0$. This allows

for the inclusion of the correct asymptotic behavior. To see this we explore the problem by looking at the formal solution of the driven equation (6) through the full Green's function $G_l^+(r,r')$

$$\frac{\Psi^+(r)}{r} = \frac{\Psi_0(r)}{r} + \int_0^\infty r'^2 dr G_l^+(r,r') V(r') \frac{\Psi_0(r')}{r'}. \quad (15)$$

Taking the limit $r \to \infty$, expression (9a) results. To avoid the divergence, however, the potential underneath the integral symbol is cut

$$\frac{\Psi^+(r)}{r} = \frac{\Psi_0(r)}{r} + \int_0^{R_0} r'^2 dr G_l^+(r,r') V(r') \frac{\Psi_0(r')}{r'}, \quad (16)$$

so that the second term on the RHS is well defined; besides it possesses the correct asymptotic behavior provided by the Green's function since the latter is associated to the full potential kept in the LHS of the driven equation.

The basis representation of the operator $[\mathcal{T}_{1,\eta} + \mathbf{V}_\eta - E\mathcal{O}]$ up to the asymptotic region, allows one to provide the correct asymptotic behavior to the solution of equation (13) by using the inverse of the operator $(E-H)$. Again a fundamental issue surges: an appropriated distorted wave approach is required to be sure that the operator $(E-H)^{-1}$ will provide the correct asymptotic behavior to the wave function. But even when a scattering wave function similar to the correct one is obtained (it is not the exact one because the RHS in Eq. (16) is not the correct one), the divergence of (5) is still present and not removed by cutting the potential. We believe that these are *unnecessary inconveniences* created by the way in which the method is implemented. In Section 4, we will propose an approach as efficient as the original ECS but that avoids all the mentioned formal difficulties. It is based on performing the complex rotation on the basis functions rather than on the driven equation itself, and makes use of Sturmian functions with appropriately chosen outgoing boundary conditions.

3 Understanding and reinforcing the ECS approach, and adapting it for long-range Coulombic potentials

The separation of the wave function in two terms, as done in equation (5), is quite common in scattering theory. If the potential $V(r)$ is of short-range, the function $\Psi_{\rm sc}(r)$ may have outgoing wave behavior at large distances. Indeed, in this case, the RHS of the driven Schrödinger equation (6) is zero at large enough distances from the origin, and hence it becomes asymptotically homogeneous. A possible representation for the asymptotic form of $\Psi_{\rm sc}(r)$ is given by the Riccati-Hankel functions, noted $H_l^\pm(0,r)$, which are irregular at the origin and behave asymptotically as $e^{\pm i\left(kr-\frac{\pi}{2}l\right)}$ (see Eq. (A.8) in Appendix A). If the outgoing (+ sign) behavior is imposed onto $\Psi_{\rm sc}(r)$, then the solution $\Psi^+(r)$ of the full Schrödinger equation (2) will behave at large distances as follows

$$\Psi^+(r) = \Psi_0(r) + \Psi_{\rm sc}^+(r)$$
$$\to \frac{1}{2i}\left[-e^{-i\left(kr-\frac{\pi}{2}l\right)} + e^{i\left(kr-\frac{\pi}{2}l\right)}\right] + A_l\, e^{i\left(kr-\frac{\pi}{2}l\right)} \quad (17a)$$
$$= e^{i\delta_l}\sin\left(kr - \frac{\pi}{2}l + \delta_l\right). \quad (17b)$$

Thus, for short range potentials it is possible to expect for a scattering solution $\Psi_{\rm sc}^+(r)$ which provides asymptotically the transition matrix $A_l = e^{i\delta_l}\sin(\delta_l)$ (or the scattering matrix $S_l = e^{2i\delta_l}$) in terms of the scattering phase-shift δ_l.

When dealing with long-range potentials, however, the treatment should be different. As it is well known, the distorted wave theory can be applied in this case. Within the ECS, a reformulation of the scattering driven equation allowing for an outgoing spherical wave has been proposed (see section 4.2 of Ref. [5]). The interaction potential can be separated into two terms $V(r) = V_1(r) + V_2(r)$ where $V_1(r)$ is of long range, including the Coulomb case, and $V_2(r)$ of short range. The regular solution of $V_1(r)$ is then taken as initial state and the scattering is associated to $V_2(r)$. However, the case of the pure Coulomb potential $V(r) = z_1 z_2/r$ has not been considered in [5,6], and it had been explicitly excluded in reference [15] which was dedicated to long-range potentials. We should also mention that a distorted wave approach was discussed in the context of molecular ions [18,20]. A practical (but not formal) way to apply right boundary conditions to the incoming wave was put forward; however, no explicit recipe is proposed for the pure two-body Coulomb case. In Section 3.2, we shall show how that case can be dealt with within a distorted wave formulation (actually, our analysis is of general character and is valid for any type of potential); two proposals will be put forward. One of them is equivalent to that presented by Elander et al. [24] and Volkov et al. [25]. We shall emphasize that, within a distorted wave approach in ECS, it is essential to get an exponentially decreasing or strictly zero driven term in the asymptotic region.

Before doing that we present a fully analytical investigation of the driven equation (6) for the pure Coulomb case to answer the following two questions: Is it possible to define a ECS procedure in this case? and: Can the transition amplitude be extracted from the inner part of the wave function at large distances, or using equation (9b)?

3.1 Reinforcing the ECS method: the pure Coulomb potential

Consider the pure Coulomb potential $V(r) = z_1 z_2/r$ and let $\alpha = z_1 z_2 \mu/k$ define the Sommerfeld parameter. We want to present the exact solution obtained when the standard recipe of the ECS is used to solve the problem, i.e., to cut the potential on the RHS of (6). We will show, on one hand, that the exact solution of the (Coulomb) problem is not obtained on the whole domain but, on the

other hand, that the solution obtained in the inner region is correct thus reinforcing the ECS approach.

According to the standard theory of differential equations [31] the general solution of equation (6) is given by the sum of the linearly independent solutions (A.1a) and (A.1b) of the corresponding homogeneous equation and of the particular solution $\Psi^P(r)$ of the non-homogeneous equation:

$$\Psi^G_{\rm sc}(r) = A^{Reg} v^{Reg}(r) + A^{Irreg} v^{Irreg}(r) + \Psi^P(r), \quad (18)$$

where the coefficients A^{Reg}, A^{Irreg} are chosen according to the boundary conditions one wants to impose to the scattering problem. The particular solution $\Psi^P(r)$ is provided in Appendix B. Let us solve equation (6) where the potential $V(r)$ is truncated only on the RHS. The solution, regular at the origin, in the inner region (I), reads

$$\Psi^G_{{\rm sc},I}(r) = A_I v^{Reg}(r) + \Psi^P(r). \quad (19)$$

In the outer region (II), the RHS of equation (6) is equal to zero, and a solution possessing outgoing asymptotic behavior is simply

$$\Psi^G_{{\rm sc},II}(r) = A_{II} H_l^+(\alpha, r), \quad (20)$$

where $H_l^+(\alpha, r)$ is defined through equation (A.6). Imposing continuity at $r = R_0$ of the logarithmic derivative of the wave function leads to

$$A_I = -\left(\frac{\gamma^P - \gamma_C^+}{\gamma^{Reg} - \gamma_C^+}\right) \frac{\Psi^P(R_0)}{v^{Reg}(R_0)}, \quad (21)$$

where $\gamma^{Reg} = [(dv^{Reg}(r)/dr)/v^{Reg(r)}]_{r=R_0}$, $\gamma^P = [(d\Psi^P(r)/dr)/\Psi^P(r)]_{r=R_0}$ and $\gamma_C^+ = [(dH_l^+(\alpha, r)/dr)/H_l^+(\alpha, r)]_{r=R_0}$. Note that γ^{Reg} and γ^P are real, while γ_C^+ is complex; thus A_I will be a complex constant. The constant A_{II} of the external region is complex and given by

$$A_{II} = \frac{\Psi^G_{\rm sc,I}(R_0)}{H_l^+(\alpha, R_0)}. \quad (22)$$

The solution $\Psi^G_{\rm sc}(r)$ and its derivative are continuous on the full domain $[0, \infty)$. This is what typically is expected for a scattering wave function. The ECS method (with sharp rotation [6,15]) provides a solution having a discontinuity on the first derivative at $r = R_0$. Therefore, a question arises: Is our solution $\Psi^G_{\rm sc}(r)$ equivalent to the ECS solution? It is not clear to us what is the limit of the function provided by ECS when the rotation angle η tends to zero. On the other hand, $\Psi^G_{\rm sc}(r)$ should be the right solution at this limit.

The next step is to explore the behavior of the full solution of the Schrödinger equation (2). In the inner region (I) we have

$$\begin{aligned}\Psi(r) &= kr j_l(kr) + \Psi^G_{{\rm sc},I}(r) \\ &= kr j_l(kr) + A_I v^{Reg}(r) + \Psi^P(r). \end{aligned} \quad (23)$$

With the property (B.3), we get

$$\Psi(r) = \left(A_I + \frac{k^{l+1} N_C(l)}{(2l+1)!!}\right) v^{Reg}(r), \quad (24)$$

that is to say a function proportional (with a complex constant) to the exact solution of the Coulomb potential. In order to obtain exactly $v^{Reg}(r)$, we can renormalize the whole wave function $\Psi(r)$ simply by dividing it by a complex constant. This is a very important result and, we believe, it could be the cornerstone of the ECS methodology. We presented the results for the Coulomb potential, but the same conclusion will result for any type of potential (though it is generally difficult to demonstrate analytically).

For the truncated Coulomb potential $V_{R_0}(r)$, we have fixed the constant A_I of equation (19) by asking at $r = R_0$ for continuity of the function and its derivative. However, any other condition applied at that coordinate will lead to the same conclusion, i.e., a Coulomb wave function $v^{Reg}(r)$ multiplied by constant. This implied no necessity of imposing any boundary condition as stated in the ECS approach. Again, this conclusion applies for any type of potential. *The problem is to find appropriately the renormalization constant.*

In Figure 1a, respectively Figure 1b, we plot (solid line) as a function of r the real (respectively imaginary) part of the function $\Psi(r)$, given by equation (23), and renormalized using the constant provided in equation (24). The plot is performed up to $r = 200$ and with $R_0 = 100$; we have taken $z_1 z_2 = -1$, $k = 1$, $\mu = 1$ and hence $E = k^2/2\mu = 1/2$. For comparison $v^{Reg}(r)$ is included (dotted line), allowing the observation of differences between our total solution and the exact solution of the Coulomb problem. In the inner region the functions are equal (for both the real and imaginary parts), but in the outer region they clearly disagree. This illustrates the differences between solving the driven Schrödinger equation (6) with the full potential $V(r)$ or with a cut-off potential $V_{R_0}(r)$.

In principle, since the potential $V_{R_0}(r)$ is of short range, we can try to extract the transition matrix from the asymptotic limit of the wave function in the region where the potential becomes negligible. In the outer region (II), we have the complex solution $\Psi_0(r) + A_{II} H_l^+(\alpha, r)$. Assuming the limit is taken for $r > R_0$, we find

$$\begin{aligned}\Psi^+(r) &\to kr j_l(kr) + A_{II} H_l^+(\alpha, r) \\ &= \frac{1}{2i}\left(-e^{-i(kr - \frac{\pi}{2}l)} + e^{i(kr - \frac{\pi}{2}l)}\right) \\ &\quad + \frac{\Psi^G_{{\rm sc},I}(R_0)}{H_l^+(\alpha, R_0)} e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right]}. \end{aligned} \quad (25)$$

The resolution of the Coulomb problem with the truncated potential $V_{R_0}(r)$ on the RHS of (6) clearly shows that the initial state is not compatible with the Coulomb distorted outgoing state, and a proper transition matrix (as shown by Eq. (17a) for a short-range potential) cannot be extracted. As described in the next subsection, a

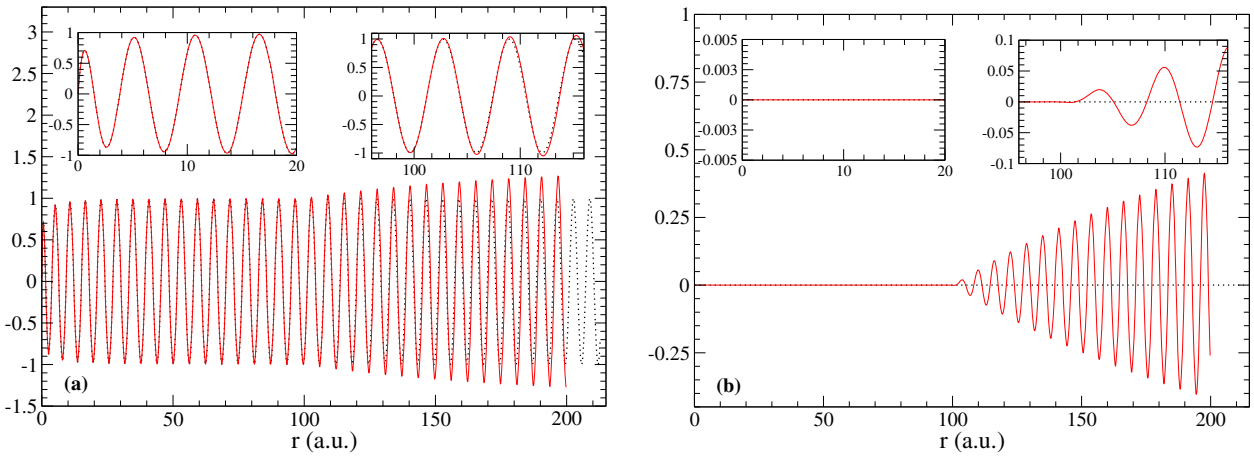

Fig. 1. (Color online) In part (a), the real part of the rescaled function $\Psi(r)$ studied in Section 3.1 is plotted (solid line) as a function of the radial coordinate r. The scaling factor, given by equation (24), was used to have complete agreement in the inner region I, up to $r = R_0 = 100$, with the exact Coulomb function $v^{Reg}(r)$ (dotted line). We have taken an angular momentum $l = 0$, a momentum $k = 1$, a reduced mass $\mu = 1$, and charges $z_1 z_2 = -1$. The insets show the behavior of the functions with more details in the inner (I) and outer (II) regions; in the latter the disagreement with the Coulomb function starts to appear. In part (b) the imaginary part of the function is shown. It is zero up to $r = R_0$ and then increases leading, as in the real part, to a disagreement with the exact Coulomb wave function in the outer region.

distorted initial state, $\Psi_{0,\mathrm{dis}}(r)$, with proper Coulombic asymptotic behavior (A.7) should be used. We are studying here the Coulomb case, but the same difficulty would appear for any type of long-range potential. Thus, cutting the potential only on the RHS of (6) leads to this type of incompatibilities.

Following a similar analytical investigation one may consider the artificial scattering problem where the cut-off potential $V_{R_0}(r)$ is set on both sides of the driven equation (6). Such a balanced treatment of the cut-off leads to a well defined scattering problem, since the transition amplitude can be obtained from the wave function in the region where the interaction potential is negligible; however, this implies working with an approximated short-range potential instead of dealing with the real long-range potential.

3.2 Distorted wave proposals for the pure Coulomb potential

The pure Coulomb potential case is now treated formally within a distorted wave approach. If the free-particle solution (3) is used as initial state $\Psi_0(r)$, then the solution $\Psi_{\mathrm{sc}}(r)$ of the driven equation (6) *must* contain corrections to it, in order to build the well known asymptotic logarithmic phase $\alpha \ln(2kr)$ produced by the long-range of the Coulomb potential. In other words, as $\Psi_0(r)$ is a free-particle standing-wave while a Coulomb-like behavior should be observed, the corrections should come from $\Psi_{\mathrm{sc}}(r)$. Thus, the scattering function $\Psi_{\mathrm{sc}}(r)$ *can not* possess pure outgoing wave behavior. This is actually a consequence of the fact that the decomposition (5) is not well formulated from the very beginning (a connected analysis has been presented in details in a recent paper [32]). To avoid this difficulty, and to be sure that pure outgoing wave behavior can be imposed to the solutions of equation (6), a (Coulomb) distorted initial state – noted $\Psi_{0,\mathrm{dis}}(r)$ – should be used instead of $\Psi_0(r)$. We now present two possible ways to introduce such a function $\Psi_{0,\mathrm{dis}}(r)$ which "diagonalizes" the Coulomb potential at large distances. One of them leads to a distorting potential falling as $\mathcal{O}\left(\frac{1}{r^2}\right)$, while the second produces a distorting potential being strictly zero at large distances.

Our first proposal is

$$\Psi_{0,\mathrm{dis}}(r) = \sin\left[kr - \left(\alpha \ln(2kr) + \frac{\pi}{2} l\right) g(r)\right] \xrightarrow{r \to \infty} \frac{1}{2i}\left(-e^{-i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]} + e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]}\right), \tag{26}$$

where $g(r)$ can be any function growing faster than r at the origin and going to one at large distances as, e.g., $g(r) = 1 - e^{-ar^2}$ (a is a positive real constant). The function $\Psi_{0,\mathrm{dis}}(r)$ solves, asymptotically, the Schrödinger equation

$$\left[\mathcal{T}_l + V(r) - E\right] \Psi_{0,\mathrm{dis}}(r) = \mathcal{O}\left(\frac{1}{r^2}\right). \tag{27}$$

By using $\Psi_{0,\mathrm{dis}}(r)$ instead of the free-particle function $\Psi_0(r)$ given by (3), we may redefine the decomposition of $\Psi(r)$ as

$$\Psi(r) = \Psi_{0,\mathrm{dis}}(r) + \bar{\Psi}_{\mathrm{sc}}(r), \tag{28}$$

and the standard scattering theory can then be recovered. Indeed, instead of equation (6), the Schrödinger equation (2) becomes

$$\left[\mathcal{T}_l + V(r) - E\right] \bar{\Psi}_{\mathrm{sc}}(r) = \left(E - \mathcal{T}_l - V(r)\right) \Psi_{0,\mathrm{dis}}(r). \tag{29}$$

According to equation (27), the RHS of (29) goes as $1/r^2$ at large distances, so that one may ask $\bar{\Psi}_{\mathrm{sc}}(r)$ to have outgoing behavior $A_l e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]}$ (see Eq. (A.7)), as the

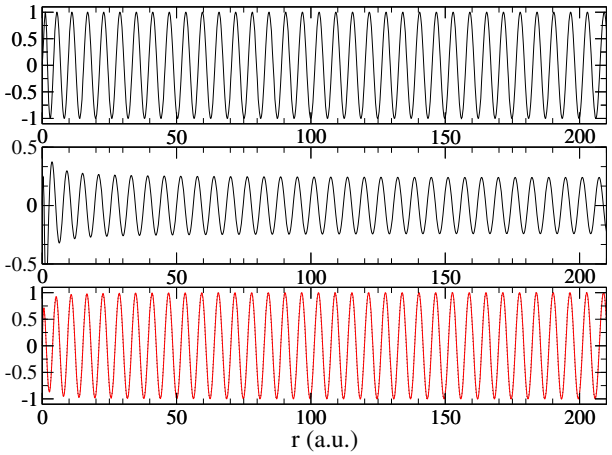

Fig. 2. (Color online) The functions $\Psi_{0,\mathrm{dis}}(r)$ (top panel), $\bar{\Psi}_{\mathrm{sc}}(r)$ (middle panel) and $\Psi(r)$ (botton panel) of, respectively, equations (26), (29) and (28) are plotted as a function of the radial coordinate r; we have taken $l = 0$, $k = 1$, $\mu = 1$ and $z_1 z_2 = -1$ (as in Fig. 1), and $a = 0.5$ in equation (26). In the bottom panel, the Coulomb wave function $v^{Reg}(r)$ is included (dotted line) for comparison. The numerical solution for $\bar{\Psi}_{\mathrm{sc}}(r)$ is obtained using Sturmian functions with outgoing asymptotic behavior.

scattering theory establishes, and a transition amplitude may be extracted. At large distances, we have

$$\Psi^{+}(r) \to \frac{1}{2i}\left(-e^{-i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}+e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}\right) + A_l\; e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}, \tag{30}$$

where the transition matrix $A_l = e^{i\delta_l}\sin(\delta_l)$ will result from solving equation (29) for $\bar{\Psi}_{\mathrm{sc}}(r)$. This type of approach was not considered in references [24–26,29] and does not require an exact asymptotic solution of the scattering problem.

To illustrate the proposal we have solved numerically (using Generalized Sturmian tools, see [33–37] and references therein) the distorted wave driven equation (29) in the case of the Coulomb potential. In the top and middle panels of Figure 2, we plot the functions $\Psi_{0,\mathrm{dis}}(r)$ and $\bar{\Psi}_{\mathrm{sc}}(r)$. In the bottom panel the function $\Psi(r)$, as given by the sum of equation (28), is compared with the exact Coulomb wave function (dotted line) $v^{Reg}(r)$. We have taken $z_1 z_2 = -1$, $k = 1$, $\mu = 1$ (as in Fig. 1), and $a = 0.5$ in equation (26). The facts that $\Psi_{0,\mathrm{dis}}(r)$ possesses the appropriated Coulomb distortion and that the sum (28) leads to the correct result, show that the driven equation (29) is well formulated and in accordance with the scattering theory.

Our second proposal is

$$\Psi_{0,\mathrm{dis}}(r) = \begin{cases} krj_l(kr) = \Psi_0(r) & r \le R_0 \\ \frac{1}{2i}\left(e^{i\delta_{\mathrm{dis},l}}F_l^{+}(\alpha,r) - e^{-i\delta_{\mathrm{dis},l}}F_l^{-}(\alpha,r)\right) & \\ & r > R_0, \end{cases} \tag{31}$$

where the functions

$$F_l^{\pm}(\alpha,r) = e^{\pm i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}\left[\sum_{n=0}^{N}\frac{A_n^{\pm}}{r^n}+\mathcal{O}\left(\frac{1}{r^{N+1}}\right)\right] \quad (A_0 = 1), \tag{32}$$

have a Coulombic asymptotic form and the series constructs the correct solution to increasing orders in $1/r$ (see, e.g., Ref. [38]). The function $\Psi_{0,\mathrm{dis}}(r)$ solves the Schrödinger equation

$$\left[\mathcal{T}_l + V_{\mathrm{dis}}(r) - E\right]\Psi_{0,\mathrm{dis}}(r) = 0, \tag{33}$$

where $V_{\mathrm{dis}}(r) = V(r) - V_{R_0}(r)$; in our case, $V_{\mathrm{dis}}(r)$ is simply the Coulomb potential in the external region ($r > R_0$) and zero internally.

Here, it is assumed that the functions $F_l^{\pm}(\alpha,r)$ are solutions of the Coulomb problem from $r = R_0$ and up to ∞; if this is not fulfilled then the RHS of (33) will be zero to a given order $\mathcal{O}(1/r^n)$ with $n > 2$. The phase-shift $\delta_{\mathrm{dis},l}$ in equation (31) is determined in such a way that the logarithmic derivative of the wave function is continuous at R_0, i.e.,

$$e^{2i\delta_{\mathrm{dis},l}} = \frac{\gamma_F^{-}-\gamma_0}{\gamma_F^{+}-\gamma_0}\,\frac{F_l^{-}(\alpha,R_0)}{F_l^{+}(\alpha,R_0)}, \tag{34}$$

where $\gamma_0 = \left[(d\Psi_0(r)/dr)/\Psi_0(r)\right]_{r=R_0}$ and $\gamma_F^{\pm} = \left[\left(dF_l^{\pm}(\alpha,r)/dr\right)/F_l^{\pm}(\alpha,r)\right]_{r=R_0}$. The function $\Psi_{0,\mathrm{dis}}(r)$ may be defined as having unit flux at infinity, i.e., behaving as $\sin\left[kr-\alpha\ln(2kr)-l\pi/2+\delta_{\mathrm{dis},l}\right]$. As in the previous proposal, we may use the new decomposition (28) and, instead of equation (6), the Schrödinger equation (2) becomes

$$\left[\mathcal{T}_l + V(r) - E\right]\bar{\Psi}_{\mathrm{sc}}(r) = -V_{R_0}(r)\Psi_{0,\mathrm{dis}}(r). \tag{35}$$

Since the RHS is again of short range, one may ask $\bar{\Psi}_{\mathrm{sc}}(r)$ to have outgoing behavior $\bar{A}_l e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}$ where $\bar{A}_l$ will result from solving equation (35) for $\bar{\Psi}_{\mathrm{sc}}(r)$. Thus, from the wave function at large distances $r > R_0$,

$$\Psi^{+}(r) \to -\frac{e^{i\delta_{\mathrm{dis},l}}}{2i}e^{-i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]} + A_l e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}, \tag{36}$$

one may extract the transition amplitude $A_l = e^{i\delta_l}\sin(\delta_l) = \frac{1}{2i}e^{i\delta_{\mathrm{dis},l}} + \bar{A}_l$. Note that in this case, the potential in the external region is *zero* (as the ECS recipe requires) as it is naturally imposed by using a distorting potential. This procedure could be used in general to make zero, or exponentially decreasing, the RHS of the driven equation (6) thus avoiding the problems related to the ECS standard procedure. Our second proposal is equivalent to the one discussed in the work of Elander et al. [24] and Volkov et al. [25]. It allows for a direct implementation of the original ECS recipe, but requires the knowledge of the exact asymptotic solution of the problem under consideration. While this is fine for the pure

two-body Coulomb problem, it is not for a general potential; we should add that for the three-body problem similar arguments apply, and the asymptotic solution is not known.

Up to this point we just remarked something which is well known: to formulate appropriately a scattering problem the driven term *must* be of short range. If the potential is not of that nature, a distorted wave formulation must be implemented. Another issue that we wanted to emphasize is that there exists infinite distorted wave formulations; however, only the one based on the exact asymptotic solution of the problem (second proposal) leads to a zero driven term in the asymptotic region. This is crucial, not only for the two-body problem, but also for the extension of the ECS theory to three- and n-body problems.

The previous analysis permits to formulate the scattering problem for both short – and long-range (including the pure Coulomb) potentials. With the above proposals, the driven equation admits a true outgoing solution as required for the ECS to work. However, even when the ECS method can be applied, the introduced artificial cut-off gives rise to a new issue: the driven Schrödinger equation leads to a meaningless solution for $r \geq R_0$. From the scattering theory formal point of view, the complex rotation cannot be applied in general to full scattering type wave functions because it leads to a divergent total wave function. This said, if R_0 is taken sufficiently large to ensure that the outgoing asymptotic behavior is reached, then the method will provide numerically acceptable transition amplitudes since the neglected part in equation (11) will be negligible. This is what Baertschy et al. observed, and clearly stated, e.g., on page 2 of reference [23]: "*The physically correct results are then recovered by extrapolating the computed values to infinite box size. Because we cannot offer a strict mathematical proof that this extrapolation yields the exact value, we have carried out a number of numerical tests to show that the procedures employed are in fact producing the correct result.*"

4 Alternative approach: use of complex basis

As shown in Section 3, the divergency associated to the (incoming part of the initial wave function in the) driven term is artificially created, within the ECS, when performing the complex rotation (exterior or standard) of the coordinate. In general, in atomic scattering problems, the driven term should be mathematically well behaved, meaning that after a given distance it must be zero, in such a way that pure outgoing behavior can be set to the solution of equation (6), or equation (29) or (35) when dealing with the Coulomb potential. The divergence appearing in the driven term can be circumvented by an artificial potential cut-off. This trick brings in some other issues on the interpretation of the solution in the outer part of the scattering wave function, where it is supposed that the information about the scattering process has to be extracted, as provided by the asymptotic form of the Green's function (see Eq. (15)). All these difficulties are completely avoided if a set of complex basis functions possessing pure outgoing behavior is used. The exterior (or even standard) complex rotation can then be performed on the basis as explained in this section, leading to a formulation which, from the theory point of view, is more adequate. This approach supports the proposal made in reference [15] where the authors studied with some details the equivalence between solving the driven Schrödinger equation resulting after performing a complex rotation of the coordinate and solving the same equation with a real coordinate, i.e., a real Hamiltonian, but using L^2 basis sets with a complex rotation of the coordinate. We believe that this is a clue point.

The basic idea of the ECS is to find a matrix representation of the operator $(E - h_l)$ and its inverse $(E - h_l)^{-1}$, the Green function; here $h_l = \mathcal{T}_l + V(r)$. In reference [15], Rescigno et al. instead of representing the real Hamiltonian h_l on a L^2 basis set, they used an Hamiltonian $h_{\eta,l}$ where the coordinate is rotated to the complex plane by an angle η. This procedure is adequate for the LHS of, e.g., equation (6) but brings in the problems in the RHS as already explained.

Sturmian functions $S_{n,l}(r)$ may be used as an appropriate basis to deal with scattering problems (see [33,34,37] and references therein). These functions satisfy the equation

$$[\mathcal{T}_l + \mathcal{U}(r) - E]\, S_{n,l}(r) = -\beta_n \mathcal{V}(r) S_{n,l}(r). \tag{37}$$

where $\mathcal{U}(r)$ and $\mathcal{V}(r)$ are, respectively, the *auxiliary* and a short-range *generating* potentials, and β_n are the eigenvalues; here the energy E is taken as an externally fixed value ($E \geq 0$ for scattering problems). Assuming $r = x$ is a point located in a region where the generating potential is negligible, Sturmian functions are associated with the two-points boundary conditions: $S_{n,l}(r = 0) = 0$ and $S_{n,l}(r = x) \to f_l^{\pm}(x)$, where $f_l^{\pm}(x) = H_l^{\pm}(\alpha, x)$ if $\mathcal{U}(r)$ is dominated by a Coulomb character ($\alpha \neq 0$) and $f_l^{\pm}(x) = H_l^{\pm}(0, x)$ if $\mathcal{U}(r)$ is of short range. As in all two-point boundary value problem, the Sturmian functions $S_{n,l}(r)$ form a complete and orthogonal set (with respect to the generating potential $\mathcal{V}(r)$).

All the Sturmian functions possess the same energy and the same (e.g., outgoing) asymptotic behavior ruled by $\mathcal{U}(r)$. These properties allow to define an appropriate basis set to deal with scattering problems, and we can use it to solve the driven equation (6). Indeed, setting $\Psi_{\rm sc}(r) = \sum_n a_n S_{n,l}(r)$, the scattering problem is converted into a matrix problem which can be easily solved by standard matrix methods. Taking the asymptotic limit of $\Psi_{\rm sc}(r)$ yields

$$\begin{aligned}\Psi_{\rm sc}(r) &\to \sum_n a_n e^{\pm i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]} \\ &= T_l e^{\pm i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]}\end{aligned} \tag{38}$$

which provides directly the transition amplitude $T_l = \sum_n a_n$.

The Sturmian basis functions transformed the operator $(h_l - E)$ into a diagonal matrix whose elements are

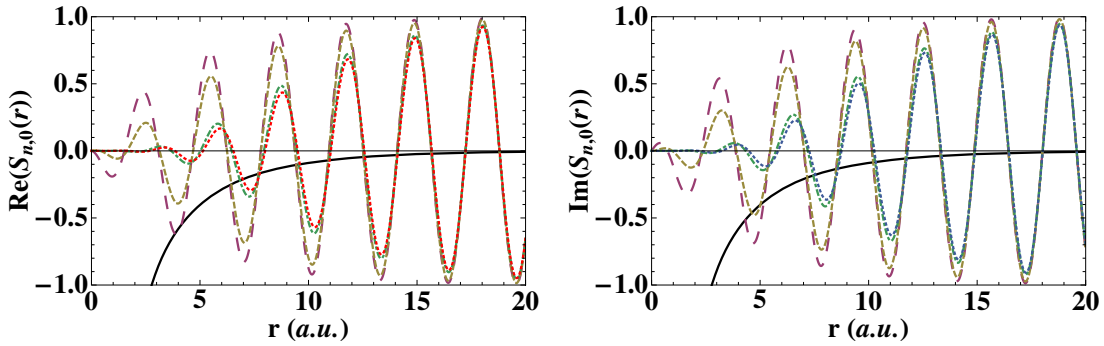

Fig. 3. Real and imaginary parts of four Hulthén Sturmian functions $S_{n,0}(r)$ ($n = 1, 2, 6, 7$) for angular momentum $l = 0$, range $r_0 = 4$ and energy $E = 2$. The Hulthén potential (solid line) is also shown.

simply the Sturmian eigenvalues. The ECS uses also spectral methods to represent $(h_l - E)$, however the main difference with our proposal is that we are using here basis functions that diagonalize the dominant Coulomb interaction and the kinetic energy. Besides, the generating potential $\mathcal{V}(r)$ can be defined as having the range of the driven term, implying that all the basis functions are concentrated in the region where the driven term $V(r)\Psi_0(r)$ is not negligible. This is illustrated in Figure 3 where we plot versus r the real and imaginary parts of the Sturmian functions corresponding to the Hulthén potential $\mathcal{V}(r) = -e^{-r/r_0}/(1 - e^{-r/r_0})$ with $r_0 = 4$ and $\mathcal{U}(r) = 0$ [37] with $n = 1, 2, 6$ and 7. One can easily observe that all the basis functions possess the same asymptotic behavior for values of r where the potential can be assumed to be zero; all of them have the same energy, here $E = 2$. If we assume that the range R_0 of the driven term is that of the the generating potential, then it is clear that the efficiency of the basis is increased because all the nodes are located in that region, the convergence rate of the expansion of $\Psi_{\rm sc}(r)$ is accelerated, the convergence itself being guaranteed by the fact that $V(r)\Psi_0(r)$ is of short range. We should mention that, generally, one should be careful when using complex basis as they can provide convergence problems and even lead to wrong results [39] (see also [40]). However, as our Sturmian functions are constructed to contain most of the physics of the problem, no convergence problems arise; this was illustrated, for example, in reference [34] for two-body and in reference [33] for three-body problems where a very fast convergence to the correct collision result was observed.

The previous description of the Sturmian method implemented to deal with scattering problems shows that it is equivalent to the ECS in the sense that a matrix representation of $(h_l - E)$ and $(h_l - E)^{-1}$ is used to solve the problem, and a similar type of linear system of equations appears. In the Sturmian case the basis is optimized to have not only the energy of the problem but also the appropriate asymptotic behavior; besides, it is localized in the region where the interaction potential appearing in the driven term is not negligible. The difference with the ECS approach is, up to this point, that we are not performing a rotation of the coordinate. However, we can do it. Consider a smooth exterior complex rotation of the coordinate, noted $\tau(r, \eta)$, which at the origin and until a point close to R_0 behaves as r and for large $r > R_0$ as $re^{i\eta}$. For $r > R_0$ this rotation will transform all the basis functions with, e.g., outgoing behavior into

$$S_{n,l}(\tau(r, \eta)) \to H_l^+(\alpha, re^{i\eta}). \tag{39}$$

For large values of r we have $H_l^+(\alpha, re^{i\eta}) \to e^{\pm i\left[kre^{i\eta} - \alpha \ln\left(2kre^{i\eta}\right) - \frac{\pi}{2}l\right]} \to 0$ as desired.

A complete connection between the ECS and the Sturmian approaches can be established if the set of Sturmian functions is derived from the equation

$$\begin{aligned}[h_0(\tau(r, \eta)) + \mathcal{U}(\tau(r, \eta)) - E]\, \bar{S}_{n,l}(\tau(r, \eta)) \\ = -\beta_n \mathcal{V}(\tau(r, \eta))\bar{S}_{n,l}(\tau(r, \eta)),\end{aligned} \tag{40}$$

with the two-points boundary conditions: $\bar{S}_{n,l}(r = 0) = 0$ and $\bar{S}_{n,l}\,[\tau(r, \eta) = \tau(x, \eta)] \to f_l^{\pm}(x)$. The boundary condition at large values of the coordinate is imposed for a real value x of the radial coordinate and the parameter η enters parametrically through the relation $\tau(r, \eta) = \tau(x, \eta)$. Here, we are giving not only the optimal basis functions to be used in scattering problems, but also the way of obtaining them. All the methods discussed in references [33,34,37] (and references therein) can be applied to solve the complex rotated Sturmian equation. The limit $\eta \to 0$ can be easily taken and will lead to Sturmian functions obtained over the real axis of the coordinate. The use of a smooth exterior complex rotation of the coordinate avoids the occurrence of a discontinuity of the Sturmian functions derivative contrary to the ECS proposal [6].

The proposed formulation is formally more adequate than the commonly used ECS: the divergency of the driven term is completely avoided when Sturmian functions with outgoing behavior are used. Besides, the use of this basis for solving the driven Schrödinger equation can considerably increase the efficiency of the standard ECS approach as indicated in, e.g., reference [15]. Numerical results for different scattering problems will be presented elsewhere.

For completeness, we should mention that the idea of combining Sturmian functions and complex scaling has been used before in several occasions and by different authors. As an example we can mention the use of Sturmian functions in perimetric coordinates [41]; in

that work, however, the basis functions had no clear connection with the physical problem under consideration. Eiglsperger et al. have performed many different calculations using Sturmian functions and complex rotation (see, e.g., [42]). In all these publications, use was made of Coulomb-*like* Sturmian functions which are not necessarily the most adequate for solving the considered physical problems (they have though the advantage of being analytic, and allow for precise evaluation of all the matrix elements required). To the best of our knowledge there is no discussion in the literature about how to define Generalized Sturmian functions in combination with the complex rotation technique. This was the aim of the present section.

5 Summary and three-body problem considerations

In this contribution we performed a careful analysis of the foundations of the exterior complex scaling method applied to two-body scattering problems. We studied some difficulties appearing in its formulation from the theoretical point of view and from the scattering theory itself.

We recalled in the introduction that even when complex rotation is well known since years now, it was for the first time implemented in scattering theory by Rescigno et al. in 1997 [15]. The main problem encountered in such applications was due to the fact that standing wave functions turn divergent when rotated to the complex plane. Even when a strategy can be defined to obtain the scattering part of the solution, the total wave function is divergent and thus looses physical meaning. What Rescigno et al. found is a way to avoid the consideration of the full wave function and to work out the full problem as depending only on the scattering part; in other words, only the physical part ($r < R_0$) is used to extract scattering amplitudes. However, here two ingredients are crucial. The first ingredient is that the complex rotation has to be performed in a region of the configuration space where the asymptotic behavior of the wave function is already reached. The second one is that the driven equation defining the scattering part has to be well defined. For long-range potentials it is indispensable to use a distorted wave approach to ensure that a pure outgoing wave will be admissible as solution of the driven equation. While this statement is quite general, we showed that, for the Coulomb case, if this approach is not used, wrong results will come from the procedure; the work presented here complements the one of reference [5]. With these two ingredients, the extraction of the information, as implemented by the ECS method, will bring the correct result.

The treatment of the pure two-body Coulomb potential is perfectly possible within the ECS if an appropriated distorted wave approach is implemented; the only admissible way requires the use of the exact asymptotic solution. If not, a cut-off will be necessary. In that case, we showed that while the outer solution has no physical meaning, the inner solution is indeed proportional – with known constant – to the exact solution. This proof reinforces the ECS approach as the property is a cornerstone for the method to work. While this is fine for the two-body case, it is important to underline here that such a demonstration for the three-body case is not possible as the exact solution is not known.

A very interesting conclusion can be extracted from reference [15]: the use of complex basis avoids all the mentioned problems. It is not necessary to rotate the original Schrödinger equation or the driven one, and it is not necessary to cut-off the potential in the driven term. If one still wants to use the efficient technique of complex scaling, a complex rotation, uniform or exterior, can be applied on the basis functions. We presented here the use of Sturmian functions as a very convenient basis set to solve scattering problems both with or without complex scaling.

Similar difficulties as those discussed for the two-body case appear when dealing with three-body problems. Again, the full wave function is separated into the sum, $\Psi = \Psi_0 + \Psi_{\rm sc}$, of an initial channel Ψ_0 with standing-wave character and a scattering part $\Psi_{\rm sc}$ with, e.g., outgoing character; a partial wave expansion is generally performed. The replacement of this ansatz into the Schrödinger equation leads to a driven equation for $\Psi_{\rm sc}$, $(H - E)\Psi_{\rm sc} = -V_{\rm in}\Psi_0$ where H is the full Hamiltonian. Generally, the initial state does not include correlation between all the particles and $V_{\rm in}$ is of long-range [4]. For example, for the study of ionization of hydrogen by electron impact, Ψ_0 is constructed as a symmetrized product of a plane wave for the projectile and a hydrogen bound state. In the region where both electrons are close to each other and far from the nucleus, the interaction results to be of long range. When solving this problem by complex rotation of the coordinate again surges the problem that divergencies are observed due to the stationary character of part of the initial state. The cut-off in a long range interaction is then required with the inconveniences discussed in Section 2 for the two-body case. According to the results provided by using the ECS method these difficulties are not numerically appreciable even when they are present. We should mention that, contrary to the electron impact case, for double photoionization by a single photon no difficulties appear as the driven term is exponentially bounded [6,18,20,21].

The ECS representation of the three-body problem implies also some issues not present in the two-body case. There are various asymptotic conditions to be fulfilled and they depend on the channel to be analyzed. However, when using the ECS method, all the channels are coupled and simultaneously present. As in the two-body case, use is made of a numerical representation of $(H-E)$ and the Green's function $G = (E-H)^{-1}$ on a grid or in a numerical basis (as, e.g., B-splines). The Hamiltonian H is rotated to the complex plane and a zero is forced on a square box of size R_0, meaning that a "square" boundary condition is imposed. However, it is well known that the asymptotic behavior for ionization or ionization-excitation channels possess outgoing hyper-spherical wave forms [43]. The complex rotation of the Hamiltonian and the imposition of box type condition force the solution of the driven

equation $(H-E)\Psi_{sc} = -V_{in}\Psi_0$ to possess outgoing flux on both coordinates r_1 and r_2. This in turn creates purely outgoing flux on the hyper-spherical coordinate ρ (this is supported also by the work presented in Ref. [33]), but the reason why this is so is unclear and it is a subject of our present investigations. The complex rotation of the Hamiltonian on both coordinates induces on the Green's function G an outgoing flux, leading to a good representation of the channels associated to continuum spectra. We wonder how this could be mathematically explained and it would be interesting to seek a mathematical way of evaluating the error appearing through such type of representations. Besides, it is not clear if and how the appropriate logarithmic Coulomb phase (see Ref. [43]) is produced through the numerical implementation. According to the study presented in reference [23] a phase proportional to the correct one is obtained, but as far as we know no general and formal – or even numerical – study has been performed on this point.

An additional issue to observe is that the cut-off imposed on the RHS of the driven equation affects mostly the excitation channels which are more strongly coupled to the initial state Ψ_0. When numerically solving the problem, all channels are included in Ψ_{sc}, but because of the flux conditions imposed on a square contour the double continuum is expected to be the best channel represented. It is clear, however, that even when the three-body Green's function – and its numerical representation – includes all the interactions, the implementation of the ECS leads to an approximate solution (whose convergence to the exact solution can in principle be reached). However, it is not clear up to now, how to evaluate the error introduced by the cut-off performed on a square contour. A procedure similar the ECS which avoids all these problems associated with the complex rotation is the one presented in reference [33]. In connection with that work, we again suggest that the use of complex Sturmian basis would be well adapted to the problem because it avoids the potential cut-off and possible – unnecessary – sources of errors. It has been already demonstrated [33,34] that the Generalized Sturmian method works in spherical coordinates, with no convergence difficulties as those observed by Baumel et al. [39]. All the matrix elements required to evaluate the wave functions and transition amplitudes are well defined, and the method converges towards the correct results. This is due to the built in properties of the basis functions, and in particular to the unique and common asymptotic behavior. We are currently working on the implementation of a Sturmian method to solve three-body problems in hyper-spherical coordinates including the suitable asymptotic conditions into the basis functions. The study of double ionization of helium by electron and photon impact will soon be presented.

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Appendix A

For the Coulomb potential $V(r) = z_1 z_2/r$, the solutions $v^{Reg}(r)$ and $v^{Irreg}(r)$ of the Coulomb Schrödinger equation (2) are well known [28]. They are given by

$$v^{Reg}(r) = N_C(l) r^{l+1} e^{ikr}\ {}_1F_1\left(\begin{matrix} i\alpha + l + 1 \\ 2l+2 \end{matrix}\middle| ; -2ikr\right) \tag{A.1a}$$

$$v^{Irreg}(r) = N_C(l) r^{l+1} e^{ikr}\ U\left(\begin{matrix} i\alpha + l + 1 \\ 2l+2 \end{matrix}\middle| ; -2ikr\right), \tag{A.1b}$$

where $\alpha = z_1 z_2 \mu/k$ defines the Sommerfeld parameter, ${}_1F_1(a,b;z)$ and $U(a,b;z)$ represent the regular and irregular solutions of the Kummer equation [30]. Both solutions, regular $[v^{Reg}(r)]$ and irregular $[v^{Irreg}(r)]$ at the origin, are real functions. The normalization constant

$$N_C(l) = \frac{(2k)^{l+1}}{2} \frac{|\Gamma(i\alpha + l + 1)|}{\Gamma(2l+2)} e^{-\frac{\pi}{2}\alpha}, \tag{A.2}$$

is chosen in such a way to have the following (unit flux) large distances behavior

$$v^{Reg}(r) \longrightarrow \sin[\Phi_C(l) + \sigma_C(l)] \tag{A.3a}$$

$$v^{Irreg}(r) \longrightarrow \cos[\Phi_C(l) + \sigma_C(l)] \tag{A.3b}$$

where

$$\Phi_C(l) = kr - \alpha \ln(2kr) - \frac{\pi}{2} l \tag{A.4}$$

$$\sigma_C(l) = \mathrm{Arg}[\Gamma(i\alpha + l + 1)]. \tag{A.5}$$

Close to the origin, the function $v^{Reg}(r)$ behaves as $N_C(l) r^{l+1}$.

From the standing-wave behaviors (A.3a) and (A.3b) one may construct solutions with incoming $(H_l^-(\alpha,r))$ or outgoing $(H_l^+(\alpha,r))$ asymptotic behaviors, namely

$$H_l^{\pm}(\alpha,r) = \left[v^{Irreg}(r) \pm i v^{Reg}(r)\right] e^{\mp i\sigma_C(l)}, \tag{A.6}$$

which are irregular close to the origin, and at large distances behave as

$$H_l^{\pm}(\alpha,r) \longrightarrow H_{l,as}^{\pm}(\alpha,r) = e^{\pm i\Phi_C(l)}. \tag{A.7}$$

For the free particle case, $\alpha = 0$, these solutions reduce to the Riccati-Hankel functions, noted $H_l^{\pm}(0,r)$, which behave asymptotically as

$$H_l^{\pm}(0,r) \longrightarrow H_{l,as}^{\pm}(0,r) = e^{\pm i\left(kr - \frac{\pi}{2}l\right)}. \tag{A.8}$$

Appendix B

A particular solution $\Psi^P(r)$ of the Coulomb driven Schrödinger equation (6) is readily available in closed form and is given by [32]

$$\Psi^P(r) = (-2\mu)(-z_1 z_2)\frac{k^{l+1}}{(2l+2)(2l+1)!!} \times e^{ikr} r^{l+2} \Theta^{(1)}\left(\begin{array}{c} 1,1|\, l+1, i\alpha+l+2 \\ i\alpha+l+2|\, 2, 2l+3 \end{array}\middle|\, ; -2ikr, -2ikr\right), \tag{B.1}$$

where $\Theta^{(1)}$ represents a two-variable hypergeometric function (convergent for all values of r)

$$\Theta^{(1)}\left(\begin{array}{c} a_1, a_2|\, b_1, b_2 \\ c_1|\, d_1, d_2 \end{array}\middle|\, ; x_1, x_2\right) = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} \frac{(a_1)_{m_1}(a_2)_{m_2}(b_1)_{m_1}(b_2)_{m_1+m_2}}{(c_1)_{m_1}(d_1)_{m_1+m_2}(d_2)_{m_1+m_2}} \frac{x_1^{m_1} x_2^{m_2}}{m_1! m_2!} \tag{B.2}$$

introduced and studied in reference [44]. It can be verified that $\Psi^P(r)$ satisfies

$$krj_l(kr) + \Psi^P(r) = v^{Reg}(r)\; k^{l+1}/(N_C(l)(2l+1)!!), \tag{B.3}$$

and hence possesses the following behavior at large distances

$$\Psi^P(r) \to \frac{1}{N_C(l)}\frac{k^{l+1}}{(2l+1)!!}\sin\left(\Phi_C(l)+\sigma_C(l)\right) - \sin\left(kr - \frac{\pi}{2}l\right). \tag{B.4}$$

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