Application of the complex scaling method in solving three-body Coulomb scattering problem

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Abstract

The three-body scattering problem in Coulombic systems is a widespread, yet unresolved problem using the mathematically rigorous methods. In this work this long-term challenge has been undertaken by combining distorted waves and Faddeev–Merkuriev equation formalisms in conjunction with the complex scaling technique to overcome the difficulties related with the boundary conditions. Unlike the common belief, it is demonstrated that the smooth complex scaling method can be applied to solve the three-body Coulomb scattering problem in a wide energy region, including the fully elastic domain and extending to the energies well beyond the atom ionization threshold. A newly developed method is used to study electron scattering on the ground states of hydrogen and positronium atoms as well as a $e^+ + H(n = 1) \rightarrow p + Ps(n = 1)$ reaction. Where available, obtained results are compared with the experimental data and theoretical predictions, proving the accuracy and efficiency of the newly developed method.

Keywords: scattering, inelastic scattering, ionization, three-body Coulomb problem

(Some figures may appear in colour only in the online journal)

1. Introduction

The Coulomb force is at the origin of all vital processes in nature. It is the dominant interaction from the nanometer to the millimeter scale. Therefore the ability to treat quantum Coulombic systems represents substantial interest for a large community of scientists. Unfortunately analytical solutions exist only for two interacting charged particles and accounts for only a negligible part of the Coulombic systems. Three interacting charges constitute therefore the simplest Coulombic problem, which cannot be solved analytically. The solution of a bound state problem in systems of three charges is well advanced and now reaches impressive accuracy, which enables one to test the tiniest effects related to relativistic and QCD corrections [1]. Nevertheless a description of the inelastic collisions remains problematic and yet unresolved by the mathematically rigorous methods. The inelastic scattering process and particularly three-body break-up (atom ionization by a charged particle) remains very challenging. The main complications arise due to the long-range nature of the Coulomb interaction and are reflected in the presence of the infinite number of reaction channels, existence of long-range couplings between the separate reaction channels (in particular degenerate ones) and finally the inability to construct three-particle break-up asymptotes.

The aforementioned complications naturally emphasize the need to develop a method of the scattering theory, which does not rely on a good knowledge of wave function behavior in far asymptotes. Such methods exist and are in particular successful in describing collisions dominated by the short-range interactions [2]. One such method, complex scaling, has been proven to be very efficient in describing resonance phenomena for atomic systems [3, 4]. The unique asset of the complex scaling method is that it presents a unified formalism enabling one to treat bound, resonant and scattering states. Nevertheless, an originally formulated [5] smooth complex scaling method is not directly applicable in solving scattering problems with long-range interactions. For this purpose the
exterior complex scaling method has been proposed [6]. This method has been successfully implemented in describing the scattering of electrons on hydrogen atoms [7–9] and recently for describing fully elastic scattering in the systems of three different charged particles [10]. Nevertheless the exterior complex scaling method contains several drawbacks from a formal as well as practical point of view, which impedes its further development. In particular, exterior complex scaling is:

- limited to a case of central and local interaction
- difficult to use together with partial-wave expansion
- difficult to generalize for \( N > 3 \) particle system

On the other hand, the smooth complex scaling method is not affected by the aforementioned complications. The goal of this work is to demonstrate that the smooth complex scaling method can be successfully employed in describing Coulombic three-body collisions, thus overcoming its original limitation to the scattering dominated by the short-range interactions.

Technically the most advanced methods of atomic collisions evolved from the close coupling (CC) expansion introduced by Massey and Mohr [11], which is based on the expansion of the system’s wave function in terms of the eigenstates of the target atom. The success of these techniques relies on the simplicity of the hydrogenic wave functions and the ability to find analytical expression for the matrix elements involved in the numerical solution. Techniques based on CC expansion have also proven to be successful in solving the e-H scattering problem in a wide range of energies, which also allows one to evaluate ionization cross sections [12, 13]. For this aim the positive-energy pseudostates of the H atom should be included in the wave function expansion [13]. Given a sufficiently large basis and successful parameterizations of pseudostates, these methods become very efficient and provide very accurate solutions. The clear advantage of the pseudostate methods is due to the fact that they allow one to perform calculations by keeping the analytical part of the problem almost unchanged.

The presence of three different charged particles reveals more severe formal difficulties for the conventional CC methods. For this aim two-center CC expansion has been introduced [14]. The drawback of the last method is that the two-center CC basis becomes overcomplete and results in a mathematically ill-conditioned problem [15]. Nevertheless by well mastering the parameter space this method turns into a very efficient tool.

The complex scaling technique by itself is just a tool, which allows one to avoid the complications related with complex wave function behavior in the far asymptotes, and might be used successfully in conjunction with CC expansion. In this work I have however decided to apply the complex scaling method in conjunction with Faddeev–Merkuriev (FM) equations. FM equations present a mathematically rigorous formulation of the three-body Coulombic problem. When exploring the potential of the complex scaling technique this presents one clear advantage, since mathematically well-conditioned formulation of the problem should guarantee convergence of the basis expansion, regardless of the fact that a chosen basis is not optimized. The drawback to using FM equations, compared to the CC approaches, is the appearance of some complicated integrals, which are not possible to perform analytically and numerical approximations should be used.

2. The formalism

2.1. FM equations

In the many-particle scattering theory Jacobi coordinates represent the natural choice, which permits one to simplify mathematical formulation. For a three-body system three independent Jacobi coordinate sets \((\xi_a, \xi_b, \xi_c)\) exist

\[
\xi_a = \sqrt{\frac{2m_\alpha m_\gamma}{(m_\beta + m_\gamma)m}} (\vec{r}_a - \vec{r}_\gamma); \quad \xi_b = \sqrt{\frac{2m_\beta m_\gamma}{(m_\alpha + m_\gamma)m}} (\vec{r}_b - \vec{r}_\gamma),
\]

where \(m_\alpha\) and \(\vec{r}_\alpha\) are respectively a mass and position of particle \(\alpha\). Particle indexation \((\alpha/\beta/\gamma)\) represents a cyclical permutation of particle indexes \((123)\), whereas a mass-factor \(m\) of free choice is introduced into the former equations in order to retain the proper unities of the distances. When studying atomic systems it is convenient to identify this mass with the mass of an electron \(m = m_e\).

In the 1960s L.D. Faddeev formulated a set of equations [16] to solve the three-particle scattering problems with short-range potentials. Some 20 years later the original Faddeev equations have been elaborated by SP Merkuriev [17] to treat long-range interactions. Merkuriev proposed splitting the Coulomb potential \(V_0\) into two parts (short and long range), \(V_0 = V_0^s + V_0^l\), by means of some cut-off function \(\chi_\alpha\).

\[
V_0^s(x_\alpha, y_\alpha) = V_0(x_\alpha) \chi_\alpha(x_\alpha, y_\alpha); \quad V_0^l(x_\alpha, y_\alpha) = V_0(x_\alpha)[1 - \chi_\alpha(x_\alpha, y_\alpha)].
\]

Using the last identity a set of three Faddeev equations is rewritten:

\[
(E - H_0 - V_\alpha - W_\alpha)\Psi_\alpha = V_\alpha^s \sum_{\beta=1}^{3} \Psi_\beta^s; \quad W_\alpha = V_\beta^l + V_\gamma^l
\]

Here \(E\) is a center of mass energy and \(H_0\) is a free Hamiltonian of a three-particle system. In these equations the term \(W_\alpha\) represents a non-trivial long-range three-body potential. This term includes residual long-range interaction between the projectile particle \(\alpha\) and the target composed of particles \((\beta/\gamma)\). In order to obtain a set of equations with compact kernels and which efficiently separate wave function asymptotes of different binary particle channels, the function \(\chi_\alpha\) should satisfy certain conditions [17]. To satisfy these conditions Merkuriev
proposed a cut-off function in the form:

\[
\chi_{\alpha}(x_\alpha, y_\alpha) = \frac{2}{1 + \exp\left(\frac{x_{\alpha} - x_0}{\mu}\right)},
\]

(5)

with parameters \(x_0, \mu\), which can be chosen to be different in each channel \(\alpha\). A constrain \(\mu > 2\) should be however respected, while the choice of \(x_0\) and \(\mu\) remains arbitrary. From the perspective of a physics parameter \(x_0\) is associated with the effective size of the two-body-interaction; it therefore makes sense to associate this parameter with the size of two-body bound state. On the other hand parameter \(x_0\) is associated with the size of a three-body region, where three-particle overlap is important.

FM equations, as formulated in equation (4), project the wave function’s asymptotes of the \(\alpha\)-\(\beta\gamma\) particle channels to component \(\Psi_{\alpha}\). The total system’s wave function is recovered by summing the three FM components \(\Psi(x, y) = \Psi_1(x, y) + \Psi_2(x, y) + \Psi_3(x, y)\). Similarly, by summing up three equations equation (4), formulated for each component \(\Psi_{\alpha}\), the Schrödinger equation is recovered.

In order to solve FM equations numerically, it is convenient to express each FM component \(\Psi_{\alpha}\) in its proper set of Jacobi coordinates \((\vec{x}_\alpha, \vec{y}_\alpha)\). Further it is practical to employ partial waves to describe the angular dependence of these components:

\[
\Psi_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha) = \sum_{l\ell_x, l\ell_y} \left\{ Y_{\ell_x}(\vec{x}_\alpha) \otimes Y_{\ell_y}(\vec{y}_\alpha) \right\}_{LM},
\]

(6)

here \(\ell_x\) and \(\ell_y\) are partial angular momenta associated with the Jacobi coordinates \(\vec{x}_\alpha\) and \(\vec{y}_\alpha\), respectively. Naturally, total angular momentum \(\vec{L} = \vec{l}_x + \vec{l}_y\) of the system should be conserved.

Let us select an initial scattering state \(\Psi^{(in)}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha)\), proper to the Jacobi coordinate set \(\alpha\) (this feat will be expressed by the Kroneker \(\delta_{\alpha, \beta}\) function). The scattering state \((\alpha)\) is defined by a particle \(\alpha\), which with momentum \(q_\alpha = \frac{m_e}{\hbar} \sqrt{E - E_\alpha}\) impinges on a bound particle pair \((\beta\gamma)\). This bound state is defined by a proper angular momentum quantum number \(l_{\alpha}^{(a)}\) and binding energy \(E_\alpha\). The relative angular momentum quantum number \(l_{\beta\gamma}^{(a)}\) should satisfy triangular conditions, related with the angular momenta conservation condition:

\[
l_{\beta\gamma}^{(a)} + l_{\alpha}^{(a)} = \vec{L} = \vec{I}_x + \vec{I}_y.
\]

(7)

Then

\[
\Psi^{(a)}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha) = \Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha) \delta_{\alpha, \beta} + \Psi_{\beta\gamma}^{(a)}(\vec{x}_\alpha, \vec{y}_\alpha)\]

(7)

The standard procedure is to consider for \(\Psi_{\beta\gamma}^{(a)}(\vec{x}_\alpha, \vec{y}_\alpha)\) a free incoming wave of particle \(\alpha\) with respect to a bound pair of particles \((\beta\gamma)\). Nevertheless the Coulomb field of particle \(\alpha\) easily polarizes and excites the target, resulting in long-range coupling between different target configurations [18, 19]. As a result, the scattering wave function in its asymptote may approach a free-wave solution only in far asymptotes, beyond the region covered by the numerical calculation. It might be useful to represent the incoming wave function by distorted waves, which describe more accurately an asymptotic solution. That is, the incoming wave may be generalized to satisfy a three-body Schrödinger equation:

\[
(E - H_0 - V_\alpha - \tilde{W}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha)) \Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha) \equiv 0
\]

(8)

with some auxiliary long-range potential \(\tilde{W}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha)\). This potential is exponentially bound in the \(x_\alpha\) direction and therefore does not contribute to the particle recombination process. Nevertheless it may couple different target states. Such an auxiliary potential can be conveniently expressed by employing a separable expansion:

\[
\tilde{W}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha) = \sum_{a,b} |\varphi_{a,l_a}(\vec{x}_\alpha)| \lambda_{ab}(\vec{x}_\alpha) \varphi_{b,l_b}(\vec{y}_\alpha) l_{ab}(\vec{x}_\alpha) \equiv \lambda_{ab}(\vec{x}_\alpha) \varphi_{b,l_b}(\vec{y}_\alpha)
\]

(9)

Radial amplitudes representing a distorted incoming wave \(\Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha)\) satisfy the standard boundary condition:

\[
\int_{a,b,l_a,l_b} (x_\alpha, y_\alpha \to \infty) \bar{\lambda}_{a,b}(\vec{x}_\alpha) \bar{\varphi}_{b,l_b}(\vec{y}_\alpha) = \frac{\bar{q}_a}{q_a} \bar{\varphi}_{b,l_b}(\vec{x}_\alpha) \times \exp(iq_{\alpha} y_\alpha - il_l \pi/2) \delta_{l_{a,b},0},
\]

(10)

where \(\bar{\lambda}_{a,b}(\vec{x}_\alpha)\) is the scattering amplitude due to the auxiliary long-range potential \(\tilde{W}_{\alpha}(\vec{x}_\alpha, \vec{y}_\alpha)\). Equation (8) is easy to solve numerically using close coupling expansion [11]. The close coupling procedure allows one to eliminate the dependence on \(\vec{x}_\alpha\), thus leading to a standard two-body coupled channel problem. By solving equation (8) the incoming wave \(\Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha)\) is obtained numerically and may be further employed to solve three-body FM equations. By setting expressions (7) and (8) into the original FM equation (4), one obtains:

\[
(E - H_0 - V_\alpha - W_\alpha) \Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha) = \sum_{\alpha, \beta, \gamma} \lambda_{\alpha, \beta\gamma}(\vec{x}_\alpha, \vec{y}_\alpha) \bar{\Psi}_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha) + \bar{\lambda}_{\alpha, \beta\gamma}(\vec{x}_\alpha, \vec{y}_\alpha) \bar{\Psi}_{\beta\gamma}^{(a)}(\vec{x}_\alpha, \vec{y}_\alpha)
\]

(11)

The FM amplitude \(\int_{a,b,l_a,l_b} (x_\alpha, y_\alpha \to \infty)\) associated with the component \(\Psi_{\alpha}^{(in)}(\vec{x}_\alpha, \vec{y}_\alpha)\), in the asymptote contains only outgoing waves. It may contain two types of outgoing waves: those representing binary process where a particle \(\alpha\) is liberated but a pair of particles \((\beta\gamma)\) remains bound and outgoing waves representing the break-up of the system into three free particles:

\[
\int_{a,b,l_a,l_b} (x_\alpha, y_\alpha \to \infty) = \sum_{l_a, l_b, l_c} \lambda_{a,b,c}(E, \frac{x_\alpha}{\sqrt{\sqrt{x_\alpha^2 + y_\alpha^2}^2}}, \sqrt{\sqrt{x_\alpha^2 + y_\alpha^2}}) \times \exp\left[iq_{\alpha} y_\alpha - il_l \pi/2\right] \delta_{l_{a,b},0}
\]

(12)
solution \( \tilde{\Psi}_b^{(a)} \) of the FM equations by applying Green’s theorem. In this study, I will concentrate only on scattering amplitudes related to the rearrangement reactions. The amplitude \( A_{b,a}(E) \) is given as:

\[
\begin{align*}
A_{b,a}(E) &= \sqrt{\frac{m_e}{\hbar^2}} \left( \langle \Psi_b^{(a)} | E - H_0 | \Psi_b^{(in)} \rangle - \langle \Psi_b^{(in)} | E - H_0 | \Psi_b^{(a)} \rangle \right) \\
&= \sqrt{\frac{m_e}{\hbar^2}} \left( \sum_{\alpha} \left( V_{\alpha} + \tilde{W}_b \right) \delta_{\alpha,b} - V_{\alpha} \right) \langle \Psi_b^{(in)} | \Psi_b^{(a)} \rangle 
\end{align*}
\]

The total scattering amplitude is given by:

\[
A_{b,a}(E) = \bar{A}_{b,a}(E) + \tilde{A}_{b,a}(E). 
\]

In terms of this full amplitude partial scattering cross section for a process \( b \rightarrow a \) and a partial wave \( L \) is defined by:

\[
\sigma_{ab}^L(E) = \frac{2\pi a_0^2}{(m_a m_b + m_0)^2} (2L + 1) |A_{a,b}(E)|^2. 
\]

One may also define the total inelastic cross section for a collision \( (a) \):

\[
\sigma_{a,\text{inel}}^L(E) = \frac{2\pi a_0^2}{(m_a m_b + m_0)^2} (2L + 1) (1 - 1 + 2iA_{a,d}(E))^2. 
\]

2.1.1. Complex scaling. The next step is to perform the complex scaling transformation on the radial parts of the Jacobi coordinates. Conventional complex scaling is considered here, defined by a smooth complex scaling transformation:

\[
\tilde{S}_p = e^{i\theta_p \frac{a_0}{m_0}} = e^{i\theta (\frac{x_1}{x_0} + \frac{x_2}{x_0})},
\]

where parameter \( \theta \) is often referred as the complex scaling angle. The free Hamiltonian after the complex scaling operation is simply expressed as:

\[
H_0^\theta = \tilde{S}_p H_0 \tilde{S}_p^{-1} = e^{-2i\theta} H_0.
\]

An action of a complex scaling operator on some radial function \( f(x_1, x_2) \) gives:

\[
\tilde{S}_p f(x_1, x_2) = f(x_1 e^{i\theta}, x_2 e^{i\theta}).
\]

Complex scaling transformation efficiently handles outgoing waves, by transforming them into exponentially bound functions. On the other hand incoming waves become exponentially divergent. In equation (11) the incoming wave appears only as an inhomogeneous term premultiplied with a term containing potential. Thus for the exponentially bound interactions the equation kernel remains compact even after performing an complex scaling operation. The situation is quite different for the case of Coulomb interaction. In this case the residual interaction term \( (W_0 - \tilde{W}_0) \) converges only as a power series in \( 1/x_0 \), and is not able to compensate for the exponential divergence of the incoming wave.

Nevertheless, it is expected that a key part of the collision happens when a projectile is close to a target, whereas the asymptotic part of the residual interaction plays only a minor role in the elastic process. Therefore one may try to screen the residual interaction term at long distances without expecting a sizeable effect on the scattering observables. Furthermore an impact of the residual term may be minimized by considering the long-range auxiliary potential \( \tilde{W}_b(x_1, x_2) \), which includes higher order corrections of the full residual interaction \( W_b \). This feat will be explored in this paper.

Technically, the complex scaled FM equations are solved to determine the complex scaling transformed FM components \( \tilde{\Psi}_a^{(a)} = \tilde{S}_p \Psi_a^{(a)} (x_1, x_2) \) and \( \tilde{\Psi}_a^{(in)} = \tilde{S}_p \Psi_a^{(in)} \). When complex scaling distorted incoming waves are necessary \( \tilde{\Psi}_a^{(in)} = \tilde{S}_p \Psi_a^{(in)} \), they can be calculated numerically by solving the complex scaling system of coupled equations corresponding to equation (8).

To keep the kernels of the complex scaled FM equations compact the term \( \tilde{S}_p(W_0 - \tilde{W}_0) \tilde{S}_p^{-1} \) is screened beyond some fixed radius \( x_0 \), using the following expression:

\[
\tilde{S}_p(W_0 - \tilde{W}_0) \tilde{S}_p^{-1} \exp \left( \left( \frac{x_1 - x_c}{x_0} \right)^n \right) ; \quad y < x_c
\]

\[
\tilde{S}_p(W_0 - \tilde{W}_0) \tilde{S}_p^{-1} \exp \left( \left( \frac{x_1 - x_c}{x_0} \right)^n \right) ; \quad y > x_c
\]

with \( n > 1 \). In this work the parameter \( x_c \) is chosen in a range 30–35 a.u., whereas \( x_c \in (5–6) \) a.u. Then:

\[
\tilde{S}_p(E - H_0 - V_r - W_0) \tilde{S}_p^{-1} \tilde{\Psi}_a^{(a)} = V' \sum_{\alpha} \left( \tilde{\Psi}_b^{(a)} + \tilde{\Psi}_a^{(m)} \delta_{\alpha,a} \right) + \tilde{S}_p(W_0 - \tilde{W}_0) \tilde{\Psi}_a^{(in)} \tilde{\Phi}_a^{(a)} \tilde{\delta}_{\alpha,a}.
\]

The scattering amplitudes are calculated by modifying the integration contour in (14) along the complex rotation line, giving [20, 21]:

\[
\begin{align*}
\bar{A}_{b,a}(E) &= \sqrt{\frac{m_e}{\hbar^2}} \left( \langle \Psi_b^{(a)} | E - H_0 - V_r - W_0 | \Psi_b^{(in)} \rangle - \langle \Psi_b^{(in)} | E - H_0 - V_r - W_0 | \Psi_b^{(a)} \rangle \right) \\
&= \sqrt{\frac{m_e}{\hbar^2}} \left( \sum_{\alpha} \left( V_{\alpha} + \tilde{W}_b \right) \delta_{\alpha,b} - V_{\alpha} \right) \langle \Psi_b^{(in)} | \Psi_b^{(a)} \rangle \\
&= \sqrt{\frac{m_e}{\hbar^2}} \left( \langle \tilde{\Psi}_b^{(a)} | (x_1, y_1) \nabla | \tilde{\Psi}_b^{(in)} \rangle \right). 
\end{align*}
\]

Here the expression \( \langle \tilde{\Phi}_a^{(a)}(x_1, y_1) \rangle \) represents a biconjugate function of \( \tilde{\Phi}_a^{(a)}(x_1, y_1) \). There is no need to recalculate these biconjugate functions, they are easily obtained from the expression of the biconjugate partner, via relation:

\[
\begin{align*}
\langle f(x, y) | \tilde{Y}_a(\tilde{x}_a) \rangle &\equiv \langle \tilde{Y}_a(\tilde{x}_a) | f(x, y) \rangle_{\text{LM}} \\
&= \langle f(x, y) | \tilde{Y}_a(\tilde{x}_a) \rangle_{\text{LM}} 
\end{align*}
\]
2.1.2. Numerical solution using Lagrange-mesh technique. The functions $f^{(a,\theta)}_{\alpha,\lambda,J}(x_a, y_a)$, representing the radial dependence of complex scaled FM components $\Phi^{(a,\theta)}_i$, are expanded using a Lagrange-mesh basis [22]:

$$f^{(a,\theta)}_{\alpha,\lambda,J}(x_a, y_a) = \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} C_{\alpha,\lambda,i}^{(a,\theta)} F_{i,j}(x_a/h_{i,j}, y_a/h_{i,j})$$

(25)

with $C_{\alpha,\lambda,i}^{(a,\theta)}$ representing the complex expansion coefficients to be determined. The $h_{i,j}$ and $h_{i,j}$ are the scaling parameters for the basis functions defined as

$$F_{i}(x) = (-1)^i c_i \frac{x L_N(x)}{x_i x} e^{-x/2},$$

(26)

In this expression $L_N(x)$ represents a $N^{th}$ degree Laguerre polynomial, whereas $x_i$ are its zeroes. The coefficients $c_i$ are fixed by imposing the basis functions to be orthonormal, namely:

$$\int_0^{\infty} F_i(x) F_j(x) \, dx = \delta_{ij},$$

(27)

The set of differential equations (22) is transformed into a linear algebra problem by projecting their angular dependence on a partial wave basis, defined in equation (6). The radial parts are projected on Lagrange-mesh basis, defined in equation (25). The coefficients $C_{\alpha,\lambda,i}^{(a,\theta)}$ are obtained after solving the linear algebra problem:

$$(H^\theta - E) C_{\alpha,\lambda,i}^{(a,\theta)} = b^{(in,\theta)}$$

(28)

Here $(H^\theta - E)$ represents a part of a complex scaled Hamiltonian acting on the wave function’s component $\Phi^{(a,\theta)}_i$, represented by the coefficients $C_{\alpha,\lambda,i}^{(a,\theta)}$. The inhomogeneous term $b^{(in,\theta)}$ is obtained after projecting into equation (22) terms containing the incoming wave term $\Phi^{(a,\theta)}_i$. Finally, the transformed components $\Phi^{(a,\theta)}_i$ serve to retrieve scattering amplitudes employing the integral relation (23). One may refer to [22, 23] for a more detailed description of the numerical methods used in this work.

3. Results

3.1. Bound state input

The first step in performing any many-body scattering calculations is determining projectile (target) bound state wave functions from which free-wave solutions are constructed. Clearly the accuracy of any scattering calculation critically depends on this input. Lagrange–Laguerre quadrature, being based on Laguerre polynomial basis, is naturally well fit to describe hydrogenic wave functions. Numerical calculations exist proving the accuracy of this method in solving Coulombic bound state problems [24]. Nevertheless it is not obvious how this basis complies with complex scaling transformation.

In table 1 the accuracy in determining positronium binding energies are presented. The parameters of the Lagrange–Laguerre quadrature and complex scaling angles are chosen to comply with the parameters of the three-body scattering calculations (presented in the following subsections). These parameters were not optimized to reproduce the excited states of the positronium. Due to the complex scaling operation binding energies are obtained as complex numbers, contaminated by a small imaginary part—reflecting numerical artifacts of the complex scaling transformation. As one can see the ground state binding energy of the positronium is quasi-exact already when using a modest quadrature of 15 points. The inaccuracy of the calculated ground state energy is due to the dominance of machine round off error, rather than the numerical method. The accuracy of the excited states is also quite satisfactory and systematically improves by increasing the number of quadrature points (basis size). Naturally more accurate values are obtained when small complex scaling angles are employed, resulting in a weaker overall effect of the complex scaling transformation on the positronium’s wave function.

There is no point in repeating the same analysis for the hydrogen atom, since its bound state wave functions coincide with Positronium ones after a trivial coordinate scaling.

Positions of three-body bound and resonant states influence strongly the scattering observables. In this work I will not discuss ability of the complex scaling method to reproduce resonant states, there is rich literature on it proving efficiency of complex scaling [3, 4]. In order to demonstrate level of accuracy of the numerical technique used in this work in table 2 convergence of the ground state of the positronium ion $(e^- e^- e^+)$ is presented. The positronium ion is a relatively weakly bound structure and thus is a suitable test ground for three-body calculations. The calculations presented in table 2 were performed using the same configuration as in the scattering calculations of the next subsection. The partial wave expansion has been limited to $l_x, l_y \leq 9$, whereas convergence has been studied as a function of the Lagrange–Laguerre quadrature size $(N_x = N_y = N_z)$ employed in expanding the radial parts of the FM components. One may see that already a moderate basis of $20 \times 20 \times 20$ points (functions) provides an accuracy of six significant digits, further improvement of the calculation is impeded and would require the enlargement of the partial-wave basis. The presence of the complex scaling transformation has only a limited impact on the calculated binding energies. The smallness of the spurious imaginary part of the binding energy as well as weak deterioration of the calculated values when increasing the complex scaling parameter $\theta$ proves this point.

3.2. $e^- + Ps(n = 1)$ scattering

Electron scattering on the positronium constitutes probably the simplest realistic Coulombic three-body system. This system has been well explored at low energies, below the first

1 It is well known that convergence of the partial-wave series is slow for Coulombic problems due to awkward ’cusp’ behavior at the two-particle collision points.
postiontronium excitation threshold [26–31]. Above the postiontronium excitation threshold only calculations based on the CC method are available [31], which if properly parameterized may provide very accurate results but in general are not constrained to provide a unique physical solution.

In figure 1 the calculated cross sections of electron scattering on the ground state of positronium (Ps(n = 1)) are presented. These calculations cover a broad energy region, starting with a purely elastic case and spreading well above the positronium ionization threshold. Below the positronium excitation threshold results of this work are compared with the most accurate values from the literature, summarized in table 1 of [28].

The present calculations have been performed by considering free e+Ps(n = 1) waves to represent the incoming wave function in equations (7) and (8). The inhomogeneous term arising from the incoming wave has been screened in equation (11) for e+Ps(n = 1) separations exceeding \( \chi_{ps} = 35 \) a.u. Partial wave expansion has been limited to max \((l_i, l_j) \leq 9\) and proved to be sufficient to get well converged results. Calculations were also limited to total angular momentum states \( L \leq 5\).

As can be seen in figure 1, a basis of \( 35 \times 35 \) Lagrange–Laguerre mesh functions is sufficient to discretize radial dependence of FM amplitudes and to get converged results in a broad energy region. Only well beyond the positontronium ionization threshold a basis of \( 35 \times 35 \) functions turns out to be insufficient in describing the inelastic cross section, nevertheless convergence is reached by increasing the basis to \( 40 \times 40 \) functions.

Table 1. Relative error \( (E_{ex} - E_{calc}) / E_{exact} \) of the calculated binding energies \( (E_{calc}) \) of the S-wave \( n = 1 \) and \( n = 5 \) positronium states. Values are tabulated as a function of number \( (N_x) \) of the Lagrange–Laguerre quadrature points used in the calculation. Two sets of calculations respectively for complex scaling angle \( \theta = 6^\circ \) and \( \theta = 8^\circ \) are compared. The notation \( x[y] \) means \( x10^y\).

| \( N_x \) | \( \theta = 6^\circ \) | \( \theta = 8^\circ \) |
|---|---|---|
| \( n = 1 \) | \( n = 5 \) | \( n = 1 \) | \( n = 5 \) |
| 15 | \(-9.6[-17] - 4.0[-15]i\) | \(1.0[-2] - 1.4[-2]i\) | \(1.7[-16] + 8.0[-16]i\) | \(5.7[-3] - 1.8[-2]i\) |
| 20 | \(1.6[-16] + 4.0[-15]i\) | \(-1.4[-5] - 7.5[-4]i\) | \(7.8[-16] + 4.0[-15]i\) | \(-1.3[-3] - 3.2[-3]i\) |
| 30 | \(-1.0[-15] - 2.0[-13]i\) | \(-3.5[-6] - 9.6[-7]i\) | \(-3.4[-16] - 1.9[-13]i\) | \(-6.6[-6] + 4.8[-6]i\) |
| 40 | \(-1.9[-15] - 1.5[-13]i\) | \(-3.3[-10] + 7.1[-10]i\) | \(-2.7[-15] - 1.5[-13]i\) | \(-1.1[-9] + 8.1[-10]i\) |

As discussed in our previous works employing complex scaling [2, 32], large complex scaling angles are not suited to perform scattering calculations in A > 2 particle systems. This work confirmed this. In this work the complex scaling parameter has been limited to \( \theta < 10^\circ \), with \( \theta = 7 - 8^\circ \) representing an optimal choice. Regardless of the simplicity of the employed approach the calculations turn out to be very accurate and in line with most accurate published values. The phase shifts calculated below the Ps(n = 2) threshold differ from those reported in [26, 28] by less than 0.5%. This proves that elastic differential cross sections, which are usually determined from the calculated phase shifts, are also well reproduced.

As it is well known, the complex scaling operation breaks the Hermiticity of the Hamiltonian. Consequently the unitarity of the S-matrix is not provided by the symmetry properties of the complex scaling equations. This is the reason why using complex scaling it is more difficult to attain numerically the unitarity of the S-matrix than to get highly accurate phase shifts. Regardless of this fact the unitarity of S-matrix in the presented e+Ps(n = 1) calculations is assured with three-digit accuracy once the electron impact energy exceeds 0.03 a.u. This is clearly demonstrated by analyzing the inelastic e+Ps(n = 1) cross section, extracted relying on the unitarity property of the S-matrix. In particular, inelastic cross sections are consistent with a zero value in the purely elastic region, below the Ps(n = 2) threshold. An accurate description of the near-threshold collisions is naturally the most problematic case for the complex scaling method. After the complex scaling operation outgoing waves converge with an exponential factor \(-krsin\theta\), where k is the relative momenta of the scattered clusters and r is a target-projectile separation distance. This exponent vanishes for low impact energies and therefore approximation of the outgoing waves by using square-integrable basis functions becomes inefficient.

3.3. e− + H scattering

Electron collisions with atomic hydrogen is a well studied problem, presenting probably the most popular benchmark for the three-body Coulombic scattering problem. This system has been considered by several different techniques, finally giving rise to public access databases [9, 35], as well as public access codes [36].
In the figure 2 calculations of electron scattering on the ground state of the hydrogen atom are presented. The present calculations have been performed using the same setup as for the \( e^+Ps(n = 1) \) case, described in the last section. A free \( e^+H(n = 1) \) wave is considered when separating the inhomogeneous term in equations (7) and (8). Thirty-five to 40 Lagrange-mesh functions were employed for discretizing the radial dependence of FM amplitudes in the \( x \) and \( y \) directions and proved to be enough to get converged results. The calculated values agree perfectly with those found in the literature [34, 37] as well as with the experimental data of Zhou et al [33]. Below the \( H(n = 2) \) excitation threshold calculated total cross sections are compared with those compiled from the literature [26, 28] and represented by full black squares.

The phase shifts calculated below the \( H(n = 2) \) threshold agree perfectly well with the most accurate calculations found in the literature. All the phase shifts fall within the limits defined by the values compiled in references [34, 37]. The calculated total elastic cross sections, see figure 3, both below as well as above the ionization threshold perfectly agree with the published values in the Aladdin database, based on the computation by Bray and Stelbovics [35] using the converged close coupling method.

As pointed out in the previous section, presenting the \( e^-H(n = 1) \) scattering, the complex scaling technique turns out to be the most difficult to apply at very low energies, close to the threshold. By reducing the energy it becomes increasingly difficult to preserve the unitarity of the calculated S-matrix. This feat is best demonstrated by the deviation from the zero value of the inelastic \( e^-H(n = 1) \) cross section close to \( H(n = 1) \) threshold (see two lowest energy points,
situated at $E_{cm} = 0.0624$ and 0.08 a.u., respectively. Naturally the unitarity of the calculated S-matrix improves once the number of basis functions is increased; nevertheless at very low energies this convergence turns to be rather slow.

3.4. $e^+ + H(n = 1) \rightarrow p^+ + Ps(n = 1)$ scattering

There is increased interest in studying (anti)proton–positronium collisions in view of the possible production of antihydrogen atoms. This system has mostly been explored using different variations of the close coupling method [15, 38]; there also exist calculations based on hyperspherical-harmonics [39], the variational method [40, 41] as well as FM equations [19, 42–44] but these are limited to the energy region of a few lowest energy excitations of either a hydrogen or positronium atom.

Elastic $e^+ + H(n = 1)$ collisions below the positronium excitation threshold does not present any new features compared to the $e^+ + H(n = 1)$ or $e^+ + Ps(n = 1)$ elastic scattering, discussed in the two previous subsections. Therefore I will concentrate on the energy region above the $p^+ + Ps(n = 1)$ production threshold. In figure 4 the calculations were performed by considering only free $e^+ + H(n = 1)$ (left panel) or $p^+ + Ps(n = 1)$ (right panel) waves to separate the inhomogeneous term in equations (7) and (8).

Calculations considering the $e^+ + H(n = 1)$ entrance channel are well converged for a moderate basis of $30 \times 30$ Lagrange-mesh functions and does not depend on the variation of a complex scaling parameter in the range $\theta = 5^\circ$–$10^\circ$. The results of the present work agree perfectly with other theoretical calculations as well as with the experimental data of Zhou et al [33]. The experimental total cross section is only underestimated for the highest energy point, which still has a non-negligible contribution from the large total angular momentum states not included in the present calculation. For this point contribution of the $L = 7$ state, the largest total angular momentum state considered in this calculation, still accounts for $\approx 10\%$ of the total cross section, whereas this state has a negligible contribution at lower energies. The unitarity of the S-matrix is well preserved, which is demonstrated by the fact that below the $H(\alpha = 2)$ excitation threshold the inelastic cross section agrees with a $Ps(n = 1)$ production one (at these energies $Ps(n = 1)$ production represents the only inelastic channel).

Calculations considering the $p^+ + Ps(n = 1)$ entrance channel turns out to be less accurate. Particularly problematic are the calculations performed in the Ore gap region$^2$ and dominated by relatively low proton (positronium) impact energies. In this region the inelastic $p^+ + Ps(n = 1)$ cross section, extracted using the unitarity property of S-matrix, is visibly not converged and improves moderately when increasing the Lagrange-mesh basis size. On the other hand, the hydrogen production cross sections calculated from the non-diagonal S-matrix element coupling $e^+ + H(n = 1)$ and $p^+ + Ps(n = 1)$ channels turns out to be accurate and well converged even at very low energies.

Even though the low energy region is not the most relevant region to use the complex scaling method—it is still worthy to pay more attention to the Ore gap region, where $p^+ + Ps(n = 1)$ cross sections converge slowly. In order to improve convergence I have constructed an inhomogeneous term in equations (7) and (8) based on distorted waves instead of the simple free waves used before. The effect of the choice of an inhomogeneous term is studied in figure 5 by comparing inelastic $p^+ + Ps(n = 1)$ cross sections in the problematic Ore gap region. These calculations were performed using a basis of $30 \times 30$ Lagrange-mesh functions, with the complex scaling parameter set to $\theta = 5^\circ$ and the total angular momentum expansion limited to $L = 3$.$^3$ Four types of distorted waves, based on the choice of long-range potential in equation (9), have been used:

- distorted wave by considering long-range dipole coupling of $Ps(n \leq 2)$ states, with $\lambda_{ab}(X_n) = -C_{ab}(\phi_{b,p}^+(X_n) | \phi_{a,p}^+|_2^2$;
- considering long-range dipole coupling of $Ps(n \leq 2)$ states together with a residual $p^+ + Ps(n = 1)$ polarization potential;
- dipole coupling of $Ps(n \leq 3)$ states together with a residual $p^+ + Ps(n = 1)$ polarization potential;
- inhomogeneous term based on free wave.

In figure 5 the calculated $p^+ + Ps(n = 1) \rightarrow e^+ + H(n = 1)$ reaction cross section is presented as a range, obtained by comparing three different values: cross sections calculated from non-diagonal S-matrix elements ($S_{p^+ + H(n = 1), p^+ + Ps(n = 1)}$ and $S_{p^+ + Ps(n = 1), e^+ + H(n = 1)}$) as well as the cross section extracted from the diagonal S-matrix element $S_{p^+ + Ps(n = 1), p^+ + Ps(n = 1)}$ via the unitarity condition.$^7$ It is clear that the distorted waves improve considerably accuracy of the calculated cross

$^2$ Ore gap is the energy region between the positronium formation threshold and the first excitation of the target atom (in this case hydrogen).

$^3$ This limitation have been used in order to compare the results with those from [42].

$^4$ The expression $\sum_{\alpha n x} x_{n a} + a_n \times n_x \times n_x + n_x \times n_x$ has been used to regularize the former potential at the origin. Coefficient $C_{\alpha}$ is a result of the presence of mass scaling factors, present in a definition of Jacobi coordinates $x_{\alpha}, e_{\alpha}, x_{\alpha}^2$.

$^5$ In the Ore gap region the relation $|S_{p^+ + Ps(n = 1), e^+ + H(n = 1)}|^2 = 1 - |S_{p^+ + Ps(n = 1), p^+ + Ps(n = 1)}|^2$ should hold.
sections even at very low energies. Inclusion of the dipole coupling of the $\text{Ps}(n \leq 2)$ states is already enough to get rather accurate results, in agreement with those in [42], obtained employing the conventional boundary condition approach. By considering a more complete residual $p+\text{Ps}$ ($n = 1$) interaction to determine the distorted incoming wave allows one to improve the accuracy of the results even further.

4. Conclusion and perspectives

The Coulombic three-body scattering problem has been addressed since the inception of quantum mechanics, however, it has yet to have been fully resolved by mathematically rigorous methods. In this work it has been demonstrated that the conventional smooth complex scaling method can be adapted to solve Coulombic three-body problems. A novel method has been developed, which combines complex scaling, distorted wave and FM equation formalisms. This formalism has been tested in studying three realistic Coulombic problems: electron scattering on ground states of hydrogen and positronium atoms as well as an $e^+ + \text{H}(n = 1) \rightarrow p + \text{Ps}(n = 1)$ reaction. Accurate results were obtained in a wide energy region, also extending beyond the atom ionization threshold. Calculations for high projectile impact energies turned out to be very accurate and reliable. They agree perfectly with the available experimental data and the most accurate theoretical calculations. On the other hand the complex scaling technique has a natural deficiency in describing very low energy scattering. Still, it is demonstrated that by using distorted incoming waves the description of the scattering process even at very low energies can be significantly improved.

This work presents a pioneering application of the smooth complex scaling method in solving Coulombic three-body problems. There remains some important aspects of three-body scattering to be explored. In particular, the differential break-up (atom ionization) cross sections should be extracted from the calculated wave functions. The efficiency of the smooth complex scaling method in describing differential break-up amplitudes has been already demonstrated in [32] for nuclear problems, dominated by the short-ranged interactions. Coulombic break-up presents additional challenges due to lack of the knowledge of the scattered wave for three-charged particles. An appropriate formulation of how to handle this problem was proposed some 50 years ago by Peterkop [45]. The original prescription of Peterkop has been further refined in a work by Kadyrov et al [46], resolving the problematic case of two-charged particles leaving close to each other. The last formalism has been successfully implemented in [47].

Another challenge is to consider charged particle scattering on the excited states of the hydrogen-type atoms.
Additional complications may arise due to the presence of long-range dipole coupling between the energy degenerate excited target states. It is not obvious if in such a system an inhomogeneous term can be straightforwardly screened as has been done for the scattering on ground state targets in this work. Distorted wave formalism might be very useful in achieving this goal.

As quoted in the introduction one of the great assets of the smooth complex scaling technique is the simplicity and ease with which it can be adapted to any numerical technique. Therefore this method can be easily incorporated to treat scattering problems in $N \geq 3$ systems. The smooth complex scaling method has been already been successfully implemented to describe the break-up process including scattering in four-nucleon systems [2, 48], dominated by the short-ranged interactions. Recently the last study has been successfully extended to include repulsive Coulomb interaction [49]. The solution of the realistic Coulombic four-particle problems requires the generalization of the existing codes, used to handle the four-nucleon scattering problem, to a case where particles have different masses. This development is envisaged in the near future, and it is expected to be a fully surmountable challenge both from the formal as well as computational points of view.

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