Potential splitting approach to e–H and e–He\(^+\) scattering

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Abstract

An approach based on splitting the reaction potential into a finite range part and a long range tail part to describe few-body scattering in the case of a Coulombic interaction is proposed. The solution to the Schrödinger equation for the long range tail of the reaction potential is used as an incoming wave. This reformulation of the scattering problem into an inhomogeneous Schrödinger equation with asymptotic outgoing waves makes it suitable for solving with the exterior complex scaling technique. The validity of the approach is analyzed from a formal point of view and demonstrated numerically, where the calculations are performed with the finite element method. The method of splitting the potential in this way is illustrated with calculations of the electron scattering on the hydrogen atom and the positive helium ion in energy regions where resonances appear.

Keywords: three-body scattering theory, Coulomb interaction, complex scaling

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

1. Introduction

Difficult fundamental problems should, if possible, be addressed to few-body physics which offers detailed, numerically almost exact, solutions. Electron scattering off the hydrogen atom and the helium cation are just such problems, and being of fundamental importance to atomic physics, any developed approach is worth testing with these problems. By comparing very detailed theoretical and computational results on the one hand to experimental results on the other, one can obtain guidelines to the development of an understanding of more complicated systems. The simplest many-body electron-scattering problem is no doubt electron scattering on the hydrogen atom or a hydrogen like ion. These problems can be treated by few-body techniques as well as, for example, advanced many-body methods.

The implementation of the complicated boundary conditions at large distances is a major difficulty for the present kind of problems, especially when the long-range Coulomb interaction is present [1]. To date, several methods have been developed for constructing solutions to the three-body scattering problem (see [2] and references therein). Considerable efforts to avoid using the explicit form of the asymptotic nature of the wave function have been made, where several of these are based on complex scaling theory [3]. Since the original approach of [4] is valid only for sufficiently fast decaying potentials, a modification [5], which uses a cut-off of the reaction potential at some distance \( R \), was proposed for long-range, non-Coulomb, potentials together with the exterior complex scaling (ECS) [6, 7]. Although this modification works well for those potentials, its extension to the Coulomb case is problematic since the cut-off Coulomb potential cannot generate correct asymptotic dynamics of the system [1]. Other ways of employing complex scaling to scattering problems have appeared in [8, 9] where complex rotation of the basis functions rather than of the system Hamiltonian has been proposed and studied.

In several recent studies, we have reported a method which is capable to treat correctly the Coulomb scattering problem using ECS [10–12]. The key point of this method is splitting the long-range Coulomb potential into the core and tail parts. The tail part is then used to construct the distorted incident wave, which is responsible for the asymptotic Coulomb dynamics. The core part of the potential in its turn...
generates the inhomogeneous term in the Schrödinger equation providing the sound platform for the application of the ECS technique for solving the equation. The present study is the next step in the development of a theory and the necessary computational tools to be able to calculate three-body many-channel scattering for systems which are described with numerical potentials having a known asymptotic analytical form. For example, the reaction \( \text{H}^+ + \text{H}_2 \rightarrow \text{H}_3 \rightarrow \text{H} + \text{H}_2 \) is just such a reaction. The method is an extension of our previously presented resonance theory and code [13]. This implies that we can compute the resonant eigenstates [14] responsible for the resonance peaks using the same finite element basis as used in the cross section calculations.

The paper is organized as follows. In section 2, the formalism of the potential splitting approach is developed, while in section 3 our computational method and the results for the electron–hydrogen and electron–He\(^+\) scattering processes are discussed. Atomic units are used throughout the paper.

2. Theoretical approach

For the electron scattering off a hydrogen-like atom, the Hamiltonian for the full problem is written in terms of the electron-nucleus radius-vectors \( \mathbf{r}_1 \), \( \mathbf{r}_2 \) as

\[
H = -\frac{1}{2} \Delta r_1 - \frac{1}{2} \Delta r_2 - \frac{Z}{|\mathbf{r}_1|} - \frac{Z}{|\mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|},
\]

where \( Z \) is the nuclear charge, and the nucleus mass is assumed to be infinite. As the total angular momentum is conserved, processes with different angular momenta can be studied independently. In the present paper, we only consider the scattering process with a zero total angular momentum. The reason for that at this stage of the work is our desire to avoid unnecessary technical complications. It allows us to focus on the approach and its validity. The straightforward extension of the approach on the case of arbitrary total angular momenta is ongoing but remains as our next step in the development process.

Due to the conservation of the total angular momentum the Hamiltonian (1) commutes with the total angular momentum operator and subsequently with the projection \( P_{L=0} \) onto the subspace of the zero total angular momentum

\[
HP_{L=0} = P_{L=0}H.
\]

Using this property in the Schrödinger equation for the total wave function \( \Psi_{\text{tot}} \),

\[
H \Psi_{\text{tot}} = E \Psi_{\text{tot}},
\]

we arrive at the actual Schrödinger equation in the subspace of the zero angular momentum

\[
H_0 \Psi = E \Psi.
\]

Here \( H_0 \) and \( \Psi \) are defined as respective projections

\[
H_0 = P_{L=0}HP_{L=0}, \quad \Psi = P_{L=0} \Psi_{\text{tot}}.
\]

The projection \( H_0 \) of the full Hamiltonian (1) on the subspace of zero total angular momentum reads

\[
H_0 = H^K + V(r_1, r_2, \theta),
\]

where the kinetic energy is given by

\[
H^K = \frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}_1^2} - \left( \frac{1}{2r_1^2} + \frac{1}{2r_2^2} \right) \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} \right) = \frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}_2^2}
\]

for the electron

\[
V(r_1, r_2, \theta) = -\frac{Z}{r_1} - \frac{Z}{r_2} + V_{12}(r_1, r_2, \theta),
\]

where the electron-electron interaction is given by

\[
V_{12}(r_1, r_2, \theta) = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1r_2 \cos \theta}}.
\]

The wave function \( \Psi = \psi(r_1, r_2, \theta) \) is the function of three variables and, as the scattering solution to the Schrödinger equation (2), must have the appropriate asymptotic behavior at large separations between particles. The latter requirement will be discussed below. We would like to emphasize that no approximations have been made in our formalism so far and the solution of the equation (2) provides the complete description of the problem with the zero value of the total angular momentum.

The symmetrization of the wave function with respect to interchange of electrons can be performed by standard procedure by using the symmetrization operator \( P^S \),

\[
P^S = \frac{1}{\sqrt{2}} (1 + (-1)^S P_{12}),
\]

where the permutation operator \( P_{12} \) interchanges the electrons 1 and 2, and \( S = 0, 1 \) for the singlet or triplet case, respectively. The properly symmetrized wave function \( \Psi^S = P^S \Psi \) is then the solution to the same Schrödinger equation (2) as the nonsymmetrized \( \Psi \). This fact allows us working with \( \Psi \) in our subsequent derivations making the symmetrization only at the final stage of the formalism.

2.1. Potential splitting approach

The scattering problem consists in solving the Schrödinger equation (2) supplied with the proper boundary conditions [1]. In the three-body case these conditions are complicated especially when the Coulomb interaction is present in the asymptotic configuration. The complex scaling originally was introduced in the solution process in order to make the boundary conditions trivial. The Schrödinger equation should be recast in the form of the properly organized inhomogeneous equation [10–12]. The splitting procedure which is given here is designed to transform the original Schrödinger equation (2) into the driven equation which then can be solved by ECS with trivial boundary conditions at large separations between particles. For definiteness we imply that
electron 1 collides with the bounded complex of electron 2 and the nucleus.

Let \( \chi^R(r) \) be the indicator of the domain \( r \geq R \), i.e.

\[
\chi^R(r) = \begin{cases}
0, & r < R, \\
1, & r \geq R,
\end{cases}
\]

and \( \chi_R = 1 - \chi^R \) be its complementary partner.

The reaction potential \( V^\text{reac}(r_1, r_2, \theta) \)

\[
V^\text{reac}(r_1, r_2, \theta) = V(r_1, r_2, \theta) - \left( -\frac{Z}{r_2} \right)
\]

is split into the sum of the core \( V_R \) and the tail \( V^R \) components

\[
V^\text{reac}(r_1, r_2, \theta) = V_R(r_1, r_2, \theta) + V^R(r_1, r_2, \theta),
\]

where

\[
V_R = V^\text{reac}\chi^R(r_1), \quad V^R = V^\text{reac}\chi^R(r_1).
\]

The distorted incident wave \( \Psi^R(r_1, r_2, \theta) \) is the solution to the scattering problem with the sum of the bound potential \( -\frac{Z}{r_2} \) and the tail potential \( V^R(r_1, r_2, \theta) \):

\[
\left( \hat{H} - \frac{Z}{r_2} + V^R(r_1, r_2, \theta) - E \right) \Psi^R(r_1, r_2, \theta) = 0.
\]

The scattered part of the wave function \( \Phi(r_1, r_2, \theta) \) is now defined as \( \Phi = \Psi - \Psi^R \), and therefore it satisfies the driven Schrödinger equation

\[
(\hat{H}_0 - E)\Phi = -V_R\Psi^R.
\]

This constitutes the main equation of the potential splitting approach, which satisfies two critical requirements which are necessary for ECS application: the right hand side (rhs) is of finite range with respect to the variable \( r_1 \) and \( \Phi \) behaves as a superposition of pure outgoing waves in all asymptotic regions. Therefore, the equation (13) can be solved by ECS [6, 7] with the exterior scaling radius \( Q \geq R \). Indeed, as the ECS consists in the transformation \( r = \rho(r) \) for \( r > Q \) with \( \text{Im}z(r) > 0 \) then after ECS, the function \( \Phi \) becomes an exponentially decreasing function, implying that boundary conditions equal to zero can be used in order to solve the ECS-transformed equation (13).

As we see from (13), the distorted incident wave \( \Psi^R \) is the essential part of the formalism. Although this is the three-body quantity we will see that under certain conditions it can be represented by its leading term which is constructed from the two-body ingredients. Let us now turn to the construction of \( \Psi^R \).

First, we determine the asymptotic initial state by introducing the function \( \Psi^R_0(r_1, r_2, \theta) \) as the solution to (12), where the potential \( V^R(r_1, r_2, \theta) \) is replaced by its leading term in the incident configuration

\[
V^R_0(r_1) = -\frac{Z - 1}{r_1} \chi^R(r_1).
\]

The variables in this case can be separated and the solution, in the case of zero total angular momentum, can be explicitly derived [11, 15] as

\[
\Psi^R_0 = \frac{j^i}{p_1 r_1} \phi_{\alpha, \beta}(r_2) Y_{\ell_0, \theta}(0, 0)
\]

and

\[
= \frac{a_{\ell_0, \ell_1}^R (r_1, r_1)}{r_1 < R,}
\]

\[
= e^{i\theta} F_{\ell_1}(r_1, r_1) + A_{\ell_0, \ell_1}^R (r_1, r_1), \quad r_1 \geq R.
\]

Here the direction of the z-axis is chosen to coincide with the direction of the incident momentum \( \mathbf{p} \). The function \( \phi_{\alpha, \beta}(r_2) \) is the target bound state wave function for the two-body system with the energy \( \varepsilon_{r_2} \) and quantum numbers \( n_r, \ell_r \). The value of the incident momentum \( p_1 \) is related to the total scattering energy, \( E \), as

\[
E = p_1^2/2 + \varepsilon_r + j_f, \quad j_f \text{ is the Riccati-Bessel function, the Sommerfeld parameter is given by } n_f = -(Z - 1)/\|p_f \|.
\]

The Coulomb outgoing wave function

\[
u^R_i(n_r, p_r r_1) = e^{-i\omega}(G_r(n_r, p_r r_1) + i F_r(n_r, p_r r_1))
\]

is expressed in terms of the regular \( F_r \) and irregular \( G_r \) Coulomb wave functions [16] and the Coulomb phase shift \( \gamma_r \). The coefficients \( a_i^R, A_i^R \) are defined as [15]

\[
a_i^R = e^{i\omega} W_r(F_r, u_i^+)/W_r(j_f, u_i^+),
\]

\[
A_i^R = e^{i\omega} W_r(F_r, j_f)/W_r(j_f, j_f),
\]

where the Wronskian, \( W_r(f, g) = f g' - f' g \), is calculated at \( r = R \).

At the second stage of constructing \( \Psi^R \) we represent it as

\[
\Psi^R = \Psi^R_0 + \Psi^R_1
\]

and obtain for the function \( \Psi^R_1 \) the inhomogeneous equation

\[
\left( \hat{H}_0 - \frac{Z}{r_2} + V^R - E \right) \Psi^R_1 = -(V^R_0 - V^R)\Psi^R_0.
\]

All incoming waves in \( \Psi^R_0 \) are included in the function \( \Psi^R_0 \), implying \( \Psi^R_1 \) contains outgoing waves only. Therefore, \( \Psi^R_1 \) remains bounded after the ECS transformation and approaches zero at large distances. Equation (18) is thus of the type which can be solved by the ECS approach. Indeed, in the region where \( \phi_{\alpha, \beta}(r_2) \) is not negligible (i.e. \( r_2 \leq \text{const} \)), one obtains

\[
V^R(r_1, r_2, \theta) - V^R_0(r_2) \sim O(r_1^{-2})
\]

as \( r_1 \to \infty \). The non-Coulomb asymptotic tail of such a potential can be truncated at some \( r_1 = R', R' > R \), and the ECS approach with the exterior scaling radius \( Q' \geq R' \) can be applied as shown in [17]. We have described the formalism of computing the distorted wave \( \Psi^R \), which is valid for arbitrary value of the splitting radius \( R \). In the case when \( R \) is large, the second stage of defining \( \Psi^R \) by (18) results in a negligible correction. Indeed, for large \( R \) the rhs of (18) is as small as \( R^{-2} \) so one gets the same order \( O(R^{-2}) \) for the solution \( \Psi^R_1 \). As a result the incident distorted wave is given in the leading order by \( \Psi^R_0 \).

Now we proceed with the solution of the full problem (13). In the same way as in (17), the solution \( \Phi \) of the full problem (13) can be represented as

\[
\Phi = \Phi_0 + \Phi_1,
\]

\[
\Phi_0 = \sum_{\ell_i} \sum_{j_i} \chi_\ell \psi_{\ell, j} (r_1) Y_{\ell, j}(0, 0)
\]

by the ECS approach with the exterior scaling radius \( Q' \geq R' \) can be solved by ECS. Indeed, in the region where \( \phi_{\alpha, \beta}(r_2) \) is not negligible (i.e. \( r_2 \leq \text{const} \)), one obtains

\[
V^R(r_1, r_2, \theta) - V^R_0(r_2) \sim O(r_1^{-2})
\]

as \( r_1 \to \infty \). The non-Coulomb asymptotic tail of such a potential can be truncated at some \( r_1 = R', R' > R \), and the ECS approach with the exterior scaling radius \( Q' \geq R' \) can be applied as shown in [17]. We have described the formalism of computing the distorted wave \( \Psi^R \), which is valid for arbitrary value of the splitting radius \( R \). In the case when \( R \) is large, the second stage of defining \( \Psi^R \) by (18) results in a negligible correction. Indeed, for large \( R \) the rhs of (18) is as small as \( R^{-2} \) so one gets the same order \( O(R^{-2}) \) for the solution \( \Psi^R_1 \). As a result the incident distorted wave is given in the leading order by \( \Psi^R_0 \).

Now we proceed with the solution of the full problem (13). In the same way as in (17), the solution \( \Phi \) of the full problem (13) can be represented as

\[
\Phi = \Phi_0 + \Phi_1,
\]
where the functions \( \Phi_0, \Phi_1 \) are the solutions to the equations
\[
(H_0 - E)\Phi_i = (H_0 - E)\Phi_i = -V_{\text{coul}} \Psi_i^R, \quad i = 0, 1.
\]
Thus the total wave function \( \Psi \) is given by
\[
\Psi = \Psi_i^R + \Phi_0 + \Psi_i^R + \Phi_1.
\]
As discussed above, the two last terms in this equation vanish when \( R \to \infty \). However, for moderate values of \( R \), their contributions might not be negligible. We discuss their influence in the next section and show numerically the decreasing character of the contributions of \( \Psi_i^R \) and \( \Phi_1 \) for increasing values of \( R \).

In order to completely restore the function \( \Psi \), we should first solve (18) for \( \Psi_i^R \). Here, there exist two possibilities. We can construct \( \Psi_i^R = \Psi_{i,0}^R + \Psi_{i,1}^R \), and solve (13) for \( \Phi_1 \). Alternatively, we can solve the two equations (21) for \( \Phi_0, \Phi_1, \) and determine the function \( \Psi \) with (22). The second approach demands more computational effort. On the other hand, it allows each of the four contributions in (22) to be determined independently, so one can analyze and compare corresponding amplitudes. It is for this reason why we adopt the second method in the present paper.

As mentioned earlier, the wave function for the system should be properly symmetrized with respect to the permutation of electrons. After applying the symmetrization operator \( P^S \) to (21), the symmetrized solutions \( \Psi_i^S = P^S\Psi_i \) are given by:
\[
(H_0 - E)\Psi_i^S = -P^S V_{\text{coul}} \Psi_i^R, \quad i = 0, 1.
\]

### 2.2. Asymptotic behavior of the scattering wave function

In order of solving the problem by ECS the wave function \( \Phi_1 \) is obtained in the region \( r_1, r_2 < Q \), where the coordinates are real. The amplitudes and cross sections corresponding to the various scattering processes occurring in the system can then be calculated from the wave function in that region provided \( Q \) is sufficiently large. The total state-to-state \((n, \ell) \to (n, \ell)\) scattering amplitude \( A_{n,\ell}^S \) is split into a few terms according to the representation (22) of the total wave function \( \Psi \),
\[
A_{n,\ell}^S = |A_{n,\ell}^R| + |A_{n,\ell}^S| + \tilde{A}_{n,\ell}^S.
\]
The term \( |A_{n,\ell}^R| \) corresponds to the function \( \Psi_i^R \) and is calculated explicitly using the representation (15) of \( \Psi_i^R \) for \( r_1 > R \):
\[
|A_{n,\ell}^R| = \delta_{n,0} \delta_{\ell,0} (A_\ell^R + \tilde{A}_\ell^R).
\]
Here \( A_\ell^R \) is defined in (16), and the partial Coulomb scattering amplitude is given by
\[
A_\ell^C = \exp(2i\sigma_\ell) - 1.
\]
The terms \( |A_{n,\ell}^S| \) and \( \tilde{A}_{n,\ell}^S \) correspond to the functions \( \Psi_i^S \) and \( \Phi_1 \), respectively. The method used to calculate the amplitudes is derived from the asymptotic form of the scattered wave function at large distances [1],
\[
\Phi^S(r_1, r_2, \theta) \sim \sum_{n,\ell} \tilde{A}_{n,\ell}^S \frac{1}{\sqrt{2}} (1 + (-1)^S \rho_{r_2}) \varphi_{n,\ell}^0(r_2)
\]
\[
\times u_{n,\ell}(\eta_p, p_{r_1}) Y_{\ell,0}(\theta, 0) + B(r_1, r_2, \theta),
\]
where the function \( B(r_1, r_2, \theta) \) represents the three-body ionization term. For large hyperradius \( \rho = \sqrt{r_1^2 + r_2^2} \), it decreases as \( B(r_1, r_2, \theta) \sim \rho^{-1/2} \). Projecting the representation (26) on the two body wave functions and taking into account the orthogonality of the two and three-body states, we obtain the local representation for the partial amplitudes \( \tilde{A}_{n,\ell}^S \) for large \( r_1 \):
\[
\tilde{A}_{n,\ell}^S \approx \sqrt{2} \left( u_{n,\ell}(\eta_p, p_{r_1}) \right)^{-1} \int_0^\infty dr_2 \int_0^\infty \sin \theta d\theta
\]
\[
\times r_2 \varphi_{n,\ell}^0(r_2) \phi_{r_1, r_2, \theta} Y_{\ell,0}(\theta, 0).
\]
The symmetrized term is neglected as the discrete state wave function decreases exponentially with \( r_1 \). This representation is also used in order to calculate \( |A_{n,\ell}^S| \), where the function \( \Phi^S(r_1, r_2, \theta) \) is replaced with the function \( \Psi_i^S(r_1, r_2, \theta) \). In the calculations, we use the maximum value of \( r_1 \) available, i.e. \( r_1 = Q \). The spin weighted cross section is then given in terms of the amplitudes by
\[
\sigma_{n,\ell}^S = \frac{2}{4} \frac{\pi}{p_1} |A_{n,\ell}^S|^2.
\]

With this approach, the solution of the scattering problem becomes a two-stage process. First, the ECS method with \( Q \gg R \) is applied to the driven equations (18), (21) as discussed in [14]. In this method, each of the spatial coordinates is replaced with the complex one \( r \to s_\phi(r) \), where \( \phi \) is the asymptotic rotation angle. Any function \( u(r) \) is then transformed as \( (W^{\phi})u(r) = \sqrt{J(\phi)}u(s_\phi(r)) \), where \( J(\phi) \) is the Jacobian \( J(r) = ds_\phi(r)/dr \). The rotated Hamiltonian takes the form \( H(\phi) = W^{\phi} H W^{\phi}^{-1} \). The rotated equations (18), (21) can be written as
\[
(H(\phi) - E)W^{\phi}F = -W^{\phi}(\text{rhs}).
\]

Both the solutions and the rhs decrease at infinity, so these equations need to be solved with the boundary conditions equal to zero at infinity.

Furthermore, the scattering amplitudes are calculated from the non-rotated spatial part of the solutions, i.e. \( r_1, r_2 \leq Q \), with representations (25), (27). This means that the asymptotic behavior (26) is used so \( Q \) should be chosen large enough for this behavior to be valid.

The calculation of the differential ionization cross section has been extensively discussed in the literature (see, e.g. [2, 17, 19] and references therein). In our paper [12] we have already demonstrated for the electron–hydrogen scattering within the Temkin-Poet model that our approach equally well
calculates the cross sections for both the binary processes and the ionization. The calculation of the breakup cross section from the wave function requires more complicated procedures and represents a meaningful task by its own [2]. In this paper, however, we focus on the accurate calculation of the wave function for energies below as well as above the ionization threshold. The binary elastic and excitation cross sections are then calculated from the wave function for these energies. The calculation of the ionization cross section from the same wave function requires extra work with the same data. We leave this task for forthcoming paper considering the differential ionization cross section outside the scope of this paper. It is worth noting that our calculated results of the two-body excitation cross sections above the ionization threshold are as accurate as the results below the threshold (see the next section).

3. Numerical method and results

Here we apply the formalism developed in the preceding section for solving the scattering problem in the electron–H and electron–He\(^+\) systems. Being of fundamental importance in atomic physics these systems have been studied (see [18, 19] and references therein) by different methods and approximations. Therefore they are the perfect testbed for the formalism.

The numerical solution of the driven Schrödinger equation (29) is performed by the finite element method (FEM), which is described in details in [14]. The FEM grid used in the calculations resembles one of [12] for the coordinates \(r_1\) and \(r_2\), and coincides with the grid in [20]. As we need the solution of (18) with the ECS radius \(Q' > R\), we first discuss the results for the calculations of the cross sections with different splitting \(R\) and ECS \(Q\) radii. Our results for the singlet \(1s\to ns\) cross sections for the e–H and e–He\(^+\) scattering are presented in figures 1 and 2, respectively. We do not consider the corrections \(\Psi_f^n\) and \(\Phi_1\) in this discussion. We can see that, for a large ECS radius \(Q\), the cross sections have high accuracy already for relatively small values of \(R\). This means that the splitting procedure with discarded \(\Psi_f^n\) and \(\Phi_1\) terms does not introduce large inaccuracies in the amplitude calculations. On the other hand, in the case \(Q = R\), the cross sections are stabilized for large values of \(R\) only. As the amplitudes are calculated at the distance \(Q\) with the asymptotic representation (26), it means that the main contribution to the inaccuracy in the amplitude originates from the inaccuracy in this asymptotic representation. This inaccuracy can be reduced with the use of the integral representation for the amplitudes when available [2].

The size of the excited two body Coulomb state grows as the square of the quantum number, implying that the higher excited state the larger distance is necessary to reach a converged result. The size of a given helium ion state is smaller than that of the similar hydrogen state, implying that the cross sections for the He\(^+\) scattering stabilize for smaller distances. It is worth noting that results for both the hydrogen scattering excluding the asymptotic Coulomb interaction and the He\(^+\) scattering including this interaction converge equally well with respect to the splitting radius \(R\). This means that our splitting procedure completely takes into account the asymptotic Coulomb interaction.

The most important results for the justification of our approach are presented in figures 3 and 4. Here we show how the cross sections are influenced by the corrections \(\Psi_f^n\) and \(\Phi_1\). We compare the cross section \(\sigma\) calculated with the terms \(\Psi_0^n + \Phi_0\) only to the corrected cross section \(\sigma_{corr}\) calculated with the full wave function \(\Psi\) in (22) which includes all corrections. The relative differences \(|\sigma - \sigma_{corr}| / \sigma\) are shown in figures 3 and 4 for the e–H and e–He\(^+\) scattering, respectively. We present the corrections for three typical energy regimes: (1) at an energy with only one open channel,
momenta of the electrons are taken into account. One can see that the influence of the corrections is drastically smaller here and decreases very fast with the splitting radius \( R \). The reason for this is that the terms \( \psi_0^R \) and \( \psi_1^R \) decrease exponentially with \( R \) for the Temkin-Poet model while they behave as inverse powers (19) for the full scattering problem. So the multipole terms in the asymptotic electron-atom potential make the unwanted corrections bigger. Still they can be made as small as necessary with an appropriate choice of the splitting radius \( R \).

Our results for the singlet \( 1s \rightarrow ns \) cross sections for the e–H and e–He\(^+\) scattering are presented in figures 6 and 7. As we have seen in figures 3 and 4, the relative inaccuracy for the cross section is below \( 10^{-3} \). Therefore, the correction terms can be safely neglected. One can also see in figures 1, 2 that the best accuracy is achieved when the splitting and rotation radii are equal. Thus the results in figures 6, 7 are calculated with the values \( R = Q = 121 \) a.u. In both cases the calculated cross sections display complicated resonance behavior. The resonance structure of the e–He\(^+\) cross section is more reach due to the presence of the asymptotic Coulomb interaction.

The oscillation character of this cross section at small energies is also the Coulomb effect. We compared our calculated values with other results [19, 21, 22], and with the accurate data for electron–hydrogen elastic scattering in the vicinity of resonance states [23]. The relative difference is found to be less than \( 10^{-3} \).

4. Conclusions

Here we present a formalism for the application of the potential splitting method to solve a driven three-body zero total angular momentum Schrödinger equation, which includes the long-range Coulomb interaction, and realized using the ECS method. This has been applied to the e–H and e–He\(^+\) collision systems.
Generalization of the present formalism to a full total angular momentum method is now under development as is the subsequent extension to include several reaction channels. It is also planned to extend our theory and code such that we will be able to compute the influence of resonant collision complexes on the scattering cross sections as we have already presented for two-body problems [24].

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Figure 6. The singlet (spin weight included) 1s→1s, 2s, 3s, 4s cross sections (from above) for the e–H scattering as a function of the incident electron energy. The thresholds are 0, 0.375, 0.444 and 0.469 a.u., respectively.

Figure 7. The singlet (spin weight included) 1s→1s, 2s, 3s, 4s cross sections (from above) for the e–He+ scattering as a function of the incident electron energy. The thresholds are 0, 1.5, 1.778 and 1.875 a.u., respectively.

The total wave function is split into four components which pairwise describe the incoming and outgoing waves of the scattering process. The scattering amplitude is likewise split into four components. The theory as it is derived here is complete, in the sense that no components are neglected. The contributions are analyzed with respect to both the splitting $R$ and exterior scaling $Q$ radii.

We have numerically demonstrated that terms corresponding to non-factorisable part $\psi^n_R$ of the distorted incoming wave (17) decrease with increase in $R$. While these terms do not vanish as fast as for the Temkin-Poet model, they still can be neglected for moderate values of $R$ and $Q$. When comparing our numerical results with previously published results [19, 21–23] we find that the relative differences are less than $10^{-3}$. We can thus state that our potential splitting method allows us to obtain numerically exact solutions for the three-body scattering problem with a Coulomb interaction.