Electron- and positron-impact atomic scattering calculations using propagating exterior complex scaling

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Abstract. Calculations are reported for four-body electron-helium collisions and positron-hydrogen collisions, in the $S$-wave model, using the time-independent propagating exterior complex scaling (PECS) method. The PECS $S$-wave calculations for three-body processes in electron-helium collisions compare favourably with previous convergent close-coupling (CCC) and time-dependent exterior complex scaling (ECS) calculations, and exhibit smooth cross section profiles. The PECS four-body double-excitation cross sections are significantly different from CCC calculations and highlight the need for an accurate representation of the resonant helium final-state wave functions when undertaking these calculations. Results are also presented for positron-hydrogen collisions in an $S$-wave model using an electron-positron potential of $V_{12} = -(8 + (r_1 - r_2)^2)^{-1/2}$. This model is representative of the full problem, and the results demonstrate that ECS-based methods can accurately calculate scattering, ionization and positronium formation cross sections in this three-body rearrangement collision.

1. Introduction
The exterior complex scaling (ECS) method was first applied to electron-atom ionization problems by Rescigno, McCurdy and coworkers [1] (Berkeley group), and was demonstrated to provide highly accurate ab initio solutions for electron-hydrogen collisions through direct solution of the time-independent Schrödinger equation in coordinate space. An extension of this method, propagating exterior complex scaling (PECS) was later developed by Bartlett and Stelbovics [2] (Perth group) in an effort to reach the computationally demanding region near the ionization threshold [3, 4] and high energies where accurate calculations require a large number of partial waves. This method provides computationally efficient and highly accurate ab initio calculations of electron-impact scattering and ionization cross sections of hydrogen for all kinematic arrangements over a large range of energies below, above and near the ionization threshold, including excited and charged hydrogenic targets [5].

The Berkeley group have since applied the ECS method to other three-body collision systems [6] and more recently to the four-body electron-helium system in an $S$-wave model [7, 8], where
only a single partial wave with all angular momenta equal to zero is considered. These ECS calculations used a time-dependent technique and the results were generally in accord with time-independent convergent close-coupling (CCC) calculations [9, 10]. In this paper we report progress by the Perth group in extending the PECS method to calculate four-body electron-helium collisions in the S-wave model using a time-independent approach, and compare the results with ECS and CCC calculations.

In an effort to extend the range of collision systems accessible to the ECS-based techniques, the Berkeley and Perth groups have initiated a collaboration to investigate positron-hydrogen collisions. Whilst it is a three-body system, further complexities are encountered, compared with electron-atom collisions, due to the probability of forming positronium (a bound electron-positron "atom") in the final state. Rearrangement collisions have not previously been investigated with ECS-based methods. Using a model potential we report PECS positron-hydrogen collision cross sections in the S-wave model for scattering, rearrangement (positronium formation) and breakup (ionization) collisions.

2. Electron-helium collisions
The PECS method for electron-helium collisions, developed by the Perth group, is a four-body extension to the three-body approach used for electron-hydrogen collisions [2]. The wave function is separated into an incident wave function and an outgoing scattering wave function $\psi_{sc}$, which is calculated numerically using the differential equation

$$
(E - \hat{H}) \psi_{sc}(r_0, r_1, r_2) = A \left( \hat{H} - E \right) \sin(k_0 r_0) \phi_n(r_1, r_2).
$$

(1)

Here the Hamiltonian is given by

$$
\hat{H} = -\frac{1}{2} \frac{\partial^2}{\partial r_0^2} - \frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} - \frac{2}{r_0} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{\max(r_0, r_1)} + \frac{1}{\max(r_0, r_2)} + \frac{1}{\max(r_1, r_2)},
$$

(2)

$\phi_n$ is the target helium S-wave wave function and the $A$ operator makes the right-hand-side of (1) antisymmetric with respect to exchange of any two radial coordinates. Exterior complex scaling is applied to the radial coordinates using the transformation

$$
z(r) \mapsto \begin{cases} 
r, & r < R_0 \\
R_0 + (r - R_0)e^{i\theta}, & r \geq R_0,
\end{cases}
$$

(3)

where the start of the scaling region, $R_0$, is made sufficiently large so as to provide convergent cross sections. Outgoing waves diminish exponentially under this transformation and explicit knowledge of the boundary conditions is not required. These equations were solved on a three-dimensional triangular-pyramidal numerical grid with varying grid spacing using an extension of the propagation algorithm outlined in [5]. A five-point Numerov-like finite-difference algorithm was used in the calculations, and provides improved accuracy relative to the three-point algorithm used in the previous PECS implementation. This method allows larger grid spacing to be used and thus greatly increases computational efficiency. The cross sections are then extracted from the scattering wave function using a hyperspherical surface integral similar to that used in electron-hydrogen calculations.

The PECS cross sections for elastic collisions and excitation to the first two excited states of helium are shown in Figure 1, and show good general agreement with the four-body CCC and ECS calculations. These calculations were undertaken with a grid extending to 50 a.u. and in all cases the PECS calculations exhibit relatively smooth energy-dependence.

The real “acid test” for a full four-body treatment of electron-helium collisions is an investigation of four-body processes that cannot be calculated using methods that rely upon
Figure 1. Electron-helium S-wave integrated scattering cross sections for elastic and single-excitation collisions from a ground-state (1\(^1\)S) target at incident electron energies between 20 and 60 eV. The present PECS results are compared with CCC [9] and time-dependent ECS [8] calculations.

Figure 2. (a) Electron-helium S-wave integrated scattering cross sections for double-excitation collision from a ground-state (1\(^1\)S) target to the first doubly-excited state (2s2\(^1\)S) at incident electron energies between 60 and 200 eV. The present PECS results are compared with CCC [10] calculations. (b) Real part of helium S-wave 2s2\(^1\)S wave function calculated using exterior complex scaling.
a three-body frozen-core approximation. The excitation of ground-state helium to the doubly-excited autoionizing $2s^2s^1S$ state was the first such collision that we investigated with the PECS method. We present our PECS cross sections for this collision in Figure 2a and compare them with CCC calculations \[10\]. While the overall magnitude of the calculations are similar, the shape of the energy dependence of the two sets of results are markedly different, with the CCC results showing a sharp resonance-like feature at 80 eV and the PECS results exhibiting a smooth energy-dependence in this region. The resonance-like feature of the CCC results is above the double-ionization threshold and is unexpected. Whilst it is stated that these double-excitation calculations were undertaken with the ECS method \[8\] the results were not included in the publication.

In Figure 2b we plot the real part of the $2s^2s^1S$ helium wave function that was used in our calculations, which we calculated to have a complex energy of $-0.722834 - 0.0012003 i$ a.u. where, according to scattering theory, the imaginary part of the energy is proportional to the resonance width, and hence inversely to the lifetime of the state. The energy and widths of resonant states are commonly calculated using a complex rotation of the Hamiltonian, however our calculations were made by diagonalizing the real target Hamiltonian on a 70 a.u. numerical grid and using exterior complex scaling, which allows the unrotated wave function to be calculated and the complex energies to be resolved. The outgoing wave along each coordinate axis diverges very slowly, which is consistent with the formal theory for resonant states in the time-independent representation. The energy of our calculation is in agreement (to 5 significant digits) with \[8\]. The CCC calculations, on the other hand, were undertaken using a real Laguerre basis that is not able to model the resonant states as accurately, which we believe may account for the significant discrepancy between the shape of the $2s^2s^1S$ cross sections.

Our PECS results for single-ionization of a ground-state target ($1s1s^1S \rightarrow 1sk_s$) are shown in Figure 3. The shape of the total ionization cross sections is in agreement with CCC and ECS calculations, but is about 5% lower. The single differential cross section (SDCS) results at 53.9 eV are shown in Figure 3b. The shape of the single differential cross sections is in agreement with CCC and ECS calculations, but is about 5% lower.

Figure 3. Electron-helium $S$-wave (a) total single-ionization cross sections ($1s1s^1S \rightarrow 1sk_s$) between 24 and 60 eV, and (b) single-ionization single-differential cross section calculations at 53.9 eV (30 eV above threshold) from a ground-state ($1^1S$) target using $R_0=100$ a.u. The present PECS results are compared with CCC \[9\] and time-dependent ECS \[8\] calculations.
Figure 4. PECS positron-impact S-wave scattering calculations using a model $V_{12}$ potential for a ground-state hydrogen target at incident positron energies between 4 and 35 eV. (a) Cross sections for elastic collisions and excitation to the 2s final-state are compared with the total cross section (TCS) calculated using the optical theorem. (b) Rearrangement collision cross sections for ground and 2s excited final-state positronium channels.

E.V. using a 100 a.u. grid are compared with ECS calculations in Figure 3b. The PECS method subtracts an asymptotic approximation of the bound-state scattering wave functions from the total scattering wave function, as used in the ECS calculations [7], to overcome interference associated with the non-orthogonality of the bound states of helium with the continuum functions used to approximate the asymptotic single-ionization final-state. After this subtraction, the PECS SDCS becomes smooth and the shape is reminiscent of the SDCS in the S-wave model of electron-hydrogen collisions [11] extracted at the same hyperradius, which becomes increasingly convex at very large distances.

3. Positron-hydrogen collisions

In the “standard” S-wave model for positron-hydrogen collisions in Cartesian coordinates (centred on the nucleus), the positron-electron interaction potential would be given by $V_{12} = -1/\max(r_1, r_2)$, where $r_1$ and $r_2$ are the radial coordinates of the positron and electron, respectively. Asymptotically, in the region of positronium formation where $r_1 \approx r_2$ this potential approaches zero and positronium does not form. To circumvent this problem we have used the model electron-positron potential

$$V_{12} = \frac{-1}{\sqrt{8 + (r_1 - r_2)^2}}, \quad (4)$$

which results in positronium forming a ground state with a binding energy of $-0.25$ a.u. (the same as real positronium) and a series of bound excited states (with energies differing from real positronium).

The PECS method for calculating the scattering wave function is the same as used for electron-hydrogen collisions in the S-wave model [11], with the appropriate change of charge
Figure 5. PECS positron-impact S-wave ionization calculations using a model $V_{12}$ potential for a ground-state hydrogen target. (a) Total ionization cross section at incident positron energies between 14 and 35 eV compared with the remainder of the optical theorem TCS after all hydrogen and positronium final-state channels are subtracted. (b) Ionization single-differential cross section for an incident 30 eV positron.

of the projectile and an extension from a triangular grid to a square grid to account for the lack of symmetry (and exchange) in the positron-hydrogen collision. The cross sections are extracted from the scattering wave function using the usual surface integral method [5, 6]. However, in a similar fashion to electron-helium ionization [7], the positronium channels are subtracted from the scattering wave function to resolve the interference due to non-orthogonality of the positronium channels and the hydrogenic continuum waves used to calculate the ionization amplitudes.

Our PECS integrated scattering cross section results for elastic collisions and 2s excited final-state collisions are shown in Figure 4 and exhibit clear resonance structures near the threshold energy for positronium formation (6.80 eV). The total cross section (TCS), calculated using the optical theorem, is shown for comparison. From this we note that the model potential used in our S-wave calculations gives cross sections that are overwhelmingly dominated by elastic collisions. All the positron-hydrogen results presented here have been independently verified using the finite-element discrete-variable representation (FEM-DVR) ECS method of the Berkeley group.

Figure 4b shows cross sections for positronium formation in the ground and first excited state. Clear resonance structure is evident when the first excited positronium state, Ps(2s), and first excited hydrogen state, H(2s), become energetically allowed near 10 eV. Between 7 and 10 eV, where only the H(1s) and Ps(1s) channels are open, the positronium cross section matches the TCS after the H(1s) cross section is subtracted. This provides a rigorous test of the positronium cross section and resonance structure in this region.

The TICS calculations shown in Figure 5a are three orders of magnitude smaller than the elastic scattering cross sections. Once again, to verify the accuracy of these results, they are compared with the remainder of the TCS after all hydrogen and positronium formation cross sections are subtracted (using the calculated cross sections of the first six excited states of each and then extrapolated to an infinite number of channels with an $n^{-3}$ scaling law approximation). Due to the very small ionization cross sections, this close agreement required the TCS and H(1s) cross sections to be calculated to a precision of better then 0.01% on a grid extending to 400
a.u. with very fine grid spacing.

The SDCS calculations at 30 eV are plotted in Figure 5b, and show a negligible probability that the electron escapes with greater energy than the positron. Minor fluctuations in the cross section, especially near equal energy sharing, are thought to be an artifact of subtracting the asymptotic positronium final-state wave functions from our scattering wave function at a finite hyperradius.

4. Conclusion

We have presented results for three-body and four-body processes in the $S$-wave model of electron-helium collisions using the time-independent PECS method. The three-body processes are in good general agreement with previous CCC and ECS calculations while exhibiting smooth cross-sections with respect to energy and energy-sharing. However, there is significant disagreement in the shape and peak energy of the cross section for the double excitation of ground state helium to the first autoionizing $2s^2 1S$ state, which is thought to be due to the poorer description of the resonant wave functions in the CCC calculations. These results give us confidence that the PECS method can give accurate \textit{ab initio} calculations for the full four-body treatment of electron-helium collisions.

The $S$-wave results for positron-hydrogen collisions, using a model potential, presented here confirm that ECS-based methods are able to accurately calculate all collision processes, including positronium formation, in this two-centred rearrangement collision. We expect the techniques used in these calculations can be applied to the full positron-hydrogen system, and based on our experience with developing the ECS-based methods for electron-hydrogen collisions, we expect that we will achieve accurate \textit{ab initio} calculations for all integrated and differential cross sections over a wide range of energies.

Whilst this paper details solutions to the electron-helium and positron-hydrogen collisions in the $S$-wave model using model potentials that cannot be compared with measurements, it has provided important verification of the efficacy of the PECS time-independent method in extracting cross sections for all channels open to these collision systems. Our efforts will now be directed towards applying these methods to the full problems.

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