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Application of exterior complex scaling to positron-hydrogen collisions including rearrangement

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The first application of an exterior complex scaling method to an atomic scattering problem with distinct rearrangement channels is reported. Calculations are performed for positron-hydrogen collisions in an s-wave model employing an electron-positron potential of $V_{12} = -(8+(r_1-r_2)^2)^{1/2}$, using the time-independent propagating exterior complex scaling (PECS) method. This potential has the correct long-range Coulomb tail 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.

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I. INTRODUCTION

By the mid 1990's electron-atom scattering calculations based on solving the time-independent Schrödinger equation had improved in quality and sophistication to the degree that for the fundamental problem of electron-hydrogen scattering most scattering cross sections were reliably calculated to an accuracy of a few percent. The ionization process, especially angular- and energy-differential cross sections, were less well established. The exterior complex scaling (ECS) method was proposed as an alternative method for electron-atom ionization problems by Rescigno, McCurdy and coworkers [1], 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 [2]. More recently, Bartlett and Stelbovics [3] adapted the numerical implementation of this method using a propagation and iterative coupling technique, and presented benchmark calculations for a complete range of electron-hydrogen collisions [4], including the notoriously difficult energy region near the ionization threshold [5, 6]. However, the interaction of positrons with atoms is not as well quantified as their electron-atom counterparts and continue to be the subject of significant experimental and theoretical research [7, 8].

One of the simplest collision systems that features both positronium formation (rearrangement) and ionization (breakup) is the collision of a positron with atomic hydrogen. Measurements of the positronium formation, breakup and total cross sections of this collision include Jones et al. [9] and Zhou et al. [10, 11], while calculations that consider both the positronium and breakup channels include: the R-matrix method [12], the close-coupling method [13, 14], Kohn variation method [15], TDCC/distorted-wave hybrid method [16] and convergent close-coupling [17, 18]. Generally, there is reasonably good agreement between measurement and theory, but the collision is yet to be completely described. The angular cross sections for positronium formation have not been measured and have only been calculated using the close-coupling optical (CCO) method [19] that is typically only accurate at higher energies, and the angular differential cross sections of the breakup channel are yet to be described by any state-of-the art theory.

The principal difficulty presented to theorists by positron-atom collisions, that is not encountered in electron-atom collisions, is the presence of a rearrangement channel, namely positronium formation. Whereas the scattering and breakup amplitudes are naturally formulated with respect to the center of mass of the system, in Cartesian coordinates centered on the proton, the positronium channel is best represented in Jacobi coordinates centered on the center of mass of the outgoing positron and electron. All state-of-the-art methods thus far applied to the positron scattering problem have had difficulty accommodating these two coordinate systems; close-coupling methods require expansions on both centers, and convergent calculations are computationally intensive. By contrast, although electron exchange is also a rearrangement in electron-atom collisions, it does not affect the convergence of an expansion about the center of mass and is easily formulated in a single coordinate system.

The purpose of this paper is to explore the positron-hydrogen collision system using exterior complex scaling, a method which has not previously been applied to a rearrangement collision. To do so we focus here on a simple two-dimensional model for which we can unambiguously

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converge numerical tests of the method. Instead of using a collinear model we have chosen to use an *s*-wave model for the positron-hydrogen collision with a modified electron-positron interaction potential that allows the description of all the channels in this problem, including positronium formation. With this model we investigate the ability of ECS-based methods to evaluate all collision dynamics open to the system.

In the next section we describe the ECS approach to positron scattering together with the model problem that we use here to test that approach. In Section III we discuss the procedures that are required to compute the amplitudes for all of the possible channels in positron-hydrogen scattering and present computational results obtained using this approach. We make some concluding remarks about the general applicability of the method to the complete problem in Section IV.

II. EXTERIOR COMPLEX SCALING APPROACH TO POSITRON SCATTERING

The scattered wave functions for positron-hydrogen collisions are calculated using a simple extension of the propagating exterior complex scaling (PECS) method used previously for electron-hydrogen collisions [3, 4], and independently verified using the finite-element discrete variable representation (FEM-DVR) ECS method [2]. In these methods the total wave function is separated into the sum of the incident wave function and the final-state scattered wave function

$$\mathbf{\Psi} = \mathbf{\Psi}_0 + \mathbf{\Psi}_{\rm sc}, \tag{1}$$

which allows the Schrödinger equation to be rearranged to the form

$$(E - \mathbf{H})\,\mathbf{\Psi}_{\rm sc} = (\mathbf{H} - E)\,\mathbf{\Psi}_0, \tag{2}$$

where the right hand side (r.h.s.) is known analytically.

In this paper we consider an *s*-wave model where only the first term of the partial wave expansion of Eq. (2) is retained, limiting the angular momentum of the electron, positron and the system to zero. In atomic units (a.u.) this gives the partial differential equation

$$\left(E + \frac{1}{2}\frac{\partial^2}{\partial r_1^2} + \frac{1}{2}\frac{\partial^2}{\partial r_2^2} - \frac{1}{r_1} + \frac{1}{r_2} - V_{12}\right)\psi_{\rm sc} = \\ \frac{2\sqrt{\pi}}{k_0}\left\{\left(\frac{1}{r_1} + V_{12}\right)\sin\left(k_0 r_1\right)\phi_{1\rm s}(r_2)\right\}, \tag{3}$$

where the radial coordinates r_1 and r_2 are assigned to the positron and electron, respectively, V_{12} is the electron-positron potential, E is the total energy and ϕ_{1s} is the radial wave function of the ground-state hydrogen target. This equation is solved numerically on a discretized grid in a finite region of coordinate space extending to R_0, where the outer boundary conditions are obviated

by transforming the radial coordinates beyond this point with an exterior complex scaling transformation

$$r \mapsto \begin{cases} r, & r < R_0 \\ R_0 + (r - R_0)e^{\mathrm{i}\theta}, & r \geq R_0 \end{cases}. \tag{4}$$

The electron-hydrogen calculations using the PECS method [3] were able to utilize the symmetry properties of the wave function under exchange of radial coordinates and solve a triangular grid where $r_2 \leq r_1 \leq R_0$. However, for the positron-hydrogen collisions considered here, the positron and electron are distinguishable particles that do not have exchange symmetry, thus the numerical grids were solved for all $r_1, r_2 \leq R_0$. In all other respects the numerical methods used for these calculations were the same as given in previous papers on the methods.

One way of choosing an *s*-wave model would be to approximate the electron-positron potential by $V_{12} = -1/\max{(r_1, r_2)}$, which has the the same form as the interelectronic interaction in the Temkin-Poet model for electron-hydrogen scattering [20, 21], but with the opposite sign. However, in the asymptotic region where positronium is expected to form ($r_1 \approx r_2 >> 1$), this form of the V_{12} potential approaches zero and there is no potential well to allow positronium to form. To overcome this problem and provide a complete test of the ECS approach to positron scattering, we make use here of a model potential

$$V_{12} = -\frac{1}{\sqrt{8 + (r_1 - r_2)^2}} \tag{5}$$

that behaves asymptotically like the electron-positron potential of the problem in full dimensionality, but provides a potential well for positronium to form in this model. This potential has the unique property of giving a positronium binding energy of -0.25 a.u. (-6.8 eV), the same as real positronium and has an infinite number of bound positronium states. While the novelty of this model potential precludes comparison of our results with other two-dimensional model positron-hydrogen calculations, it is eminently suitable for testing our ECS-based methods.

III. CALCULATION OF AMPLITUDES FOR POSITRON SCATTERING, POSITRON IMPACT IONIZATION AND POSITRONIUM FORMATION

The essential physics of positron-hydrogen collisions is immediately visible in the wave function $\psi_{\rm sc}$ itself. In Fig. 1 we present the real part of the scattered wave functions of this model collision at several energies that demonstrate the emergence of the final-state channels. Our calculations extended to $R_0 = 400$a.u., though for clarity only the first 80 a.u. are presented. At 6 eV, below the positronium formation and ionization thresholds, the scattered wave function exhibits a single elastic collision channel in the region where the electron is bound to
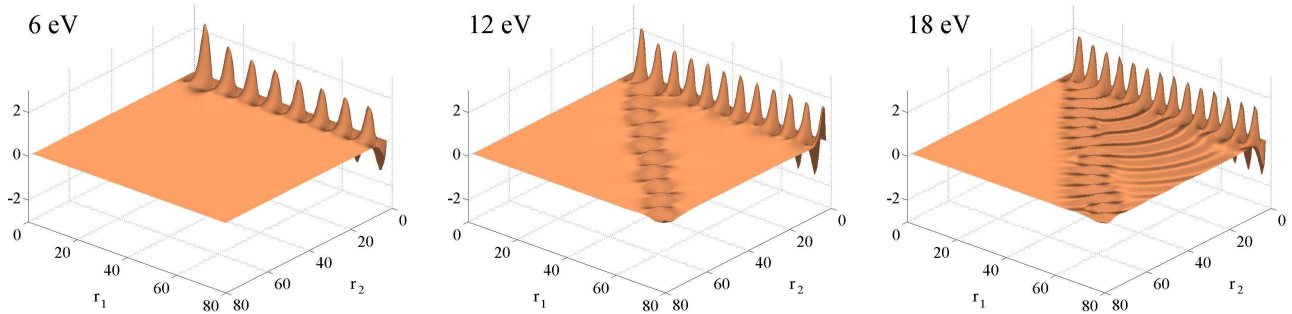
FIG. 1: (Color online) Real part of the positron-hydrogen s-wave model scattered wave functions in coordinate space (positron coordinate is r_1, electron coordinate is r_2) with incident positron energies of 6 eV (below Ps formation threshold), 12 eV (above Ps threshold), and 18 eV (above ionization threshold). Distances are in atomic units (Bohr).

the nucleus $r_2 \approx 1$. At 12 eV, above the positronium formation threshold but below the ionization threshold, the emergence of the continuum wave along $r_1 \approx r_2$ in the scattered wave function is confirmation that positronium does indeed form in this model when using the model potential given in Eq. (5). At this energy, the 1s, 2s and 3s channels for (model) positronium formation are open and each has a different wave number (momentum) for the outgoing positronium. The superposition of these channels gives the "snaking" effect visible in this wave function along $r_1 \approx r_2$. Finally, above the ionization threshold (13.6 eV), the 18 eV scattered wave function clearly shows the hydrogen and positronium final-state channels mixed with an outgoing wave for complete breakup (ionization). It is also evident from these wave functions that there is little probability of finding the positron in the region $r_1 < r_2$, which supports the classical interpretation that the positron will leave the nucleus with more momentum than the electron due to repulsion between the positron and nucleus.

In the ECS-based methods [2, 4] the scattering and ionization amplitudes are evaluated from the scattered wave functions using a formally exact integral expression [2],

$$f_n = N\langle\phi_n|E - H_d|\psi_{\rm sc}\rangle. \qquad (6)$$

In Eq. (6) H_d is the channel Hamiltonian for the arrangement in question, and ϕ_n is an eigenstate of H_d and is thus a distorted wave corresponding to a particular final state, n, in that arrangement. The normalization constant N varies depending on the normalization chosen for ϕ_n and $\psi_{\rm sc}$. In this two-dimensional model, the volume integral in Eq. (6) can be converted using Green's theorem to a surface integral that is particularly convenient for numerical calculations:

$$f_n = N\frac{\rho}{2}\int_0^{\pi/2} d\alpha \left(\psi_{\rm sc}\frac{\partial}{\partial\rho}\phi_n - \phi_n\frac{\partial}{\partial\rho}\psi_{\rm sc}\right), \qquad (7)$$

where $\rho = \sqrt{r_1^2 + r_2^2}$ is the hyperradius and $\alpha = \arctan r_2/r_1$ is the hyperangle in hyperspherical coordinates.

The principal purpose of this paper is to test whether this approach for calculating scattering and ionization amplitudes, which to date has not been tested for non-trivial rearrangement scattering, can be extended to give accurate results for the positron-hydrogen collision system in the presence of the positronium channel.

A. Elastic and inelastic scattering

The expression for the scattering amplitude in this formulation, for collisions containing a ground- or excited-state hydrogen atom in the final channel, is the same as it would be electron-hydrogen collisions,

$$f_n^{\rm H} = \rho \int_0^{\pi/2} d\alpha \left(\psi_{\rm sc}\frac{\partial}{\partial\rho}\phi_n^H - \phi_n^H\frac{\partial}{\partial\rho}\psi_{\rm sc}\right). \qquad (8)$$

The final state function for these channels is given by

$$\phi_n^{\rm H} = \frac{1}{k_n}\sin(k_n r_1)\varphi_n^{\rm H}(r_2), \qquad (9)$$

where $\varphi_n^{\rm H}(r)$ is the hydrogen radial wave function and k_n is the momentum of the scattered positron. The corresponding scattering cross section is given in terms of this amplitude by

$$\sigma_n^{\rm H} = \frac{k_n}{k_0}|f_n^{\rm H}|^2. \qquad (10)$$

As a cross-check for the surface-integral calculations, the total cross section (TCS) was calculated using the optical theorem

$$\sigma_T = -\frac{2}{k_0}\Im\left(\langle\psi_0|\overleftarrow{H} - E|\psi_{\rm sc}\rangle\right). \qquad (11)$$

We note that $\langle\psi_0|\overleftarrow{H} - E|$ in this formulation reduces to the driving term (r.h.s.) of Eq. (2) and is thus known analytically.

The TCS and scattering cross sections for the final-state hydrogen channels H(ns) with $n \leq 4$ are shown
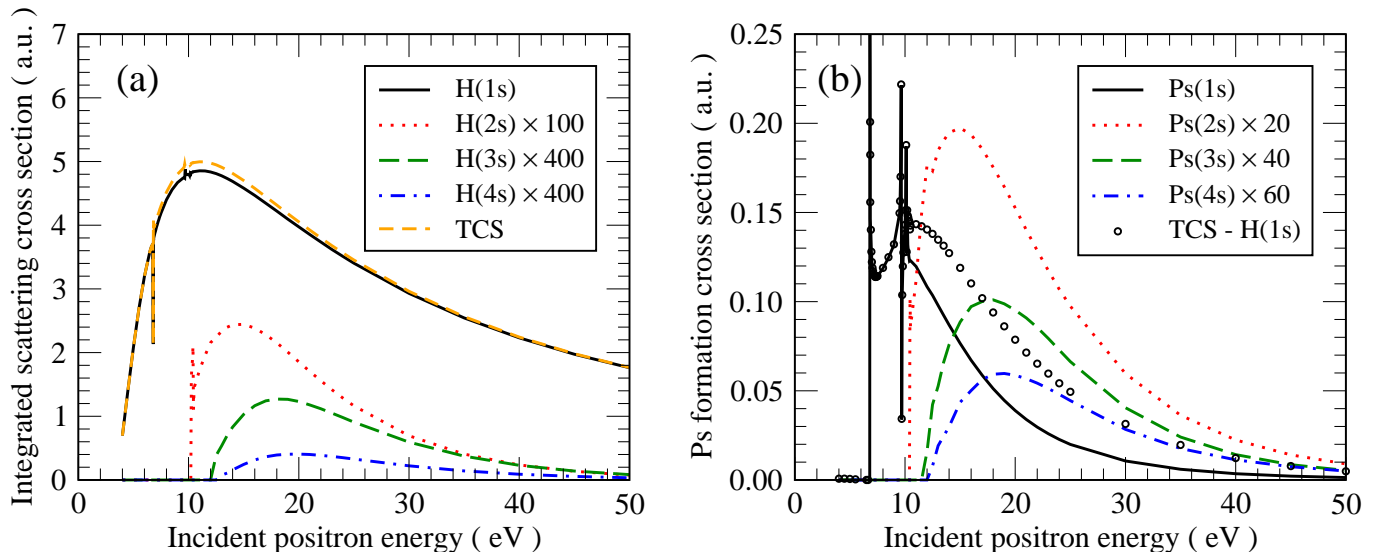
FIG. 2: (Color online) Positron-hydrogen s-wave model (a) integrated scattering cross sections for final-state hydrogen states H(ns), and (b) integrated positronium formation (rearrangement) cross sections for final-state positronium states Ps(ns). Total cross sections (TCS) are calculated using the Optical Theorem.

in Fig. 2(a) for incident positron energies of 4-50 eV. Below the positronium formation threshold at 6.8 eV the TCS and H(1s) results are in agreement to high accuracy, and resonance structures are evident near the opening of positronium and hydrogen channels. It is also evident that the elastic H(1s) channel overwhelmingly dominates the TCS, so contributions from ionization, positronium formation and inelastic collisions will be significantly smaller than the elastic channel. This is in marked contrast to the full positron-hydrogen collision, where positronium formation is dominant at 20 eV and the peak scattering, rearrangement and ionization cross sections are of the same order of magnitude [17]. The much smaller rearrangement and ionization cross sections of the present model, therefore, provide a rigorous test of the proposed surface integral techniques for calculating cross sections.

B. Positronium formation

The method for calculating positronium formation cross sections using Eqs (6) and (7) is similar to that for the hydrogen channel but with an asymptotic final-state wave function formulated in Jacobi coordinates, where $R = (r_1 + r_2)/2$ and $r = r_1 - r_2$, centered on the positronium atom, giving

$$f_n^{\mathrm{Ps}} = 2\rho \int_0^{\pi/2} d\alpha \left(\psi_{\mathrm{sc}} \frac{\partial}{\partial \rho} \phi_n^{\mathrm{Ps}} - \phi_n^{\mathrm{Ps}} \frac{\partial}{\partial \rho} \psi_{\mathrm{sc}} \right) \quad (12)$$

$$\phi_n^{\mathrm{Ps}} = \frac{1}{k_n} \sin(k_n R) \varphi_n^{\mathrm{Ps}}(r) \quad (13)$$

$$\sigma_n^{\mathrm{Ps}} = \frac{1}{2} \frac{k_n}{k_0} |f_n^{\mathrm{Ps}}|^2, \quad (14)$$

where $\varphi_n^{\mathrm{Ps}}(r)$ is the radial wave function for the model positronium atom with an electron-positron potential given by Eq. (5), and k_n is the momentum of the positronium atom.

Figure 2(b) gives the positronium formation cross sections from threshold to 50 eV for Ps(ns) final states with $n \leq 4$. In the Ore gap, between the Ps(1s) threshold at 6.8 eV and the H(2s) threshold at 10.2 eV, only the H(1s) and Ps(1s) channels are open and our calculations for TCS minus H(1s) are in agreement with the Ps(1s) calculations in this region to high accuracy, including the resonance structures. This comparison confirms the efficacy of the surface integral method in Eq. (12) for calculating the positronium cross sections using a different coordinate system than that used for calculating the scattered wave function. The success of this test is a central result of this work. The positronium formation cross sections of this model are nearly two orders of magnitude smaller than the elastic cross sections and both converge very quickly with respect to increasing ρ in Eqs (8) and (12).

C. Positron-impact ionization

A formal requirement of the surface integral technique for calculating scattering amplitudes from the scattered wave function in Eqs (6) and (7) is that ϕ_n must be asymptotically orthogonal to all other open channels contained in the scattered wave function. In the case of electron-impact ionization of hydrogen-like atoms, the final state distorted waves can be chosen to be a product of Coulomb functions for each electron in the field of the bare nucleus, and they are automatically orthog-
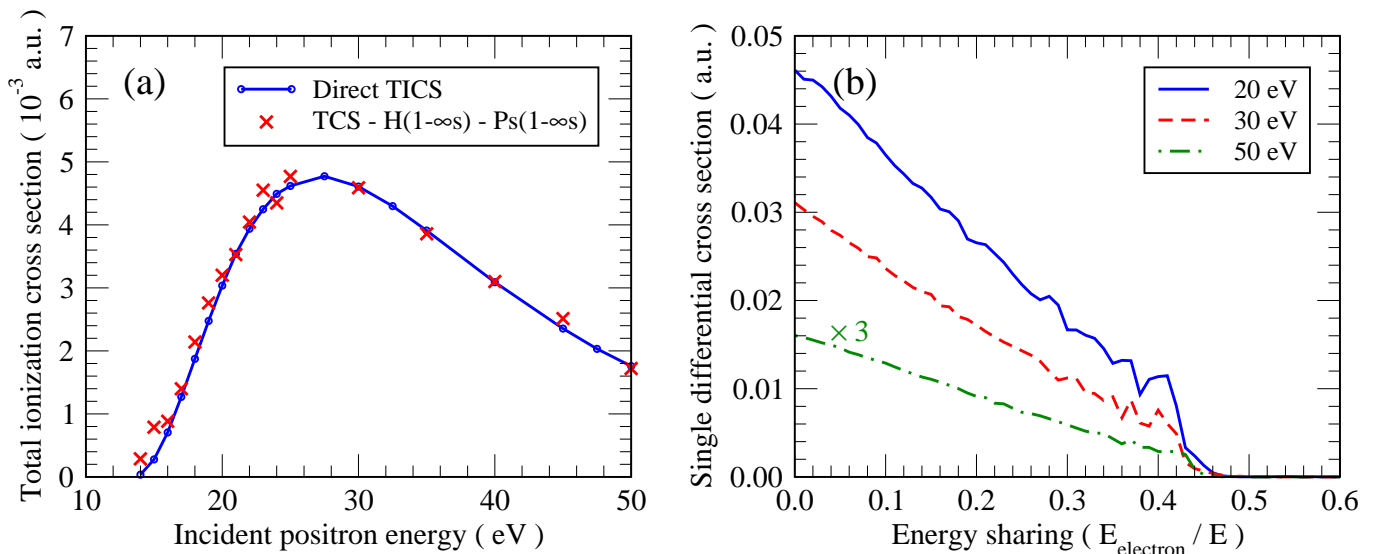
FIG. 3: (Color online) Positron-hydrogen s-wave model (a) total ionization cross sections from direct surface integral calculation and subtraction of extrapolated H(ns) and Ps(ns) cross sections from the TCS, and (b) energy-differential ionization cross sections at 20, 30, and 50 eV incident positron energy.

onal to all of the two-body channels that are open at the same total energy. That is the approach with which essentially exact calculations have been performed for breakup problems involving two continuum electrons in both atoms [2, 4] and (using molecular ion states) in molecules [22].

For positron-impact ionization, however, there is no known asymptotic representation of the final-state continuum waves (represented as a product of single-coordinate functions) that is orthogonal to both the positronium channels *and* the hydrogen channels, which correspond to different two-body arrangement channels. This problem is similar to that encountered with the four-body s-wave calculations for electron-helium collisions undertaken with the ECS method [23] where final-state continuum waves for single ionization that were orthogonal to all of the two-electron bound states of helium were not known. Fortunately, we can treat the present case with an "asymptotic subtraction" technique developed in that paper [23]. Given that we are able to accurately calculate amplitudes for the positronium channels, $f_n^{\rm Ps}$, we can asymptotically subtract these channels from the scattered wave function using the relation

$$\overline{\psi}_{\rm sc} = \psi_{\rm sc} - \sum_n f_n^{\rm Ps} \varphi_n^{\rm Ps}(r) e^{ik_n R}, \qquad (15)$$

The ionization amplitude can then be calculated in a sim-

ilar way to electron-hydrogen ionization using

$$f^{\rm ion} = \sqrt{\frac{2}{\pi}}\rho \int_0^{\pi/2} d\alpha \left(\overline{\psi}_{\rm sc} \frac{\partial}{\partial\rho} \phi^{\rm ion} - \phi^{\rm ion} \frac{\partial}{\partial\rho} \overline{\psi}_{\rm sc} \right) (16)$$

$$\phi^{\rm ion} = \frac{1}{k_1 k_2} \varphi_{k_1}^{Z=-1}(r_1) \varphi_{k_2}^{Z=+1}(r_2) \qquad (17)$$

$$\sigma^{\rm ion} = \frac{k_1 k_2}{k_0} \int_0^E d\epsilon_2 |f^{\rm ion}|^2, \qquad (18)$$

where $\varphi_{k_i}^{Z=\pm1}(r_i)$ are hydrogenic Coulomb waves with charge $Z = \pm1$ and normalized to $\sin(k_i r_i)$ for $Z = 0$. The asymptotic subtraction of Eq. (15) renders $\overline{\psi}_{\rm sc}$ effectively orthogonal to the positronium two-body channels, and the choice of the Coulomb function, $\varphi_{k_1}^{Z=-1}(r_1)$, as the distorted wave for the electron automatically ensures orthogonality of $\phi^{\rm ion}$ to the two-body hydrogen channels.

The total ionization cross sections (TICS) for our model problem, calculated using the method outlined above, for energies from threshold to 50 eV are shown in Fig. 3(a) and labeled as "Direct TICS". The peak TICS is three orders of magnitude smaller than the TCS, so in order to validate these results through subtraction of the H(ns) and Ps(ns) cross sections from the TCS, the TCS and H(1s) calculations required convergence to a precision of better than 0.01%. This extremely high level of precision was achieved using very fine spacing of the numerical grids. The cross sections for H(ns) and Ps(ns) were calculated directly for $n \leq 8$ and, given their significant contribution, the cross sections for $n > 8$ were estimated from an extrapolation using the $1/n^3$ scaling law for high Rydberg states (the direct cross sections showed reasonable convergence to this law with large n). Given the large computational challenge presented by this validation procedure, its agreement with the direct TICS

results is extremely good and verifies the correctness of the asymptotic subtraction for computing the ionization amplitudes.

In Fig. 3(b) we present the single-differential ionization cross section (SDCS), with respect to the energy of the outgoing electron, at incident positron energies of 20, 30 and 50 eV. The minor instabilities in these results, which increase near equal energy sharing, are an artifact of subtracting an *asymptotic* approximation of the positron channels from the scattered wave function at *finite* distances and the reduced accuracy of the high-n positronium cross sections used for the subtraction. However, the SDCSs become smoother with increasing hyperradius ρ and increasing incident positron energy; these calculations were undertaken at 1200-2000 bohr.

As a check of the independence of the TICS and SDCS results on the choice of coordinate systems, we also calculated the ionization cross sections using a final state testing function expressed in Jacobi coordinates:

$$\phi^{\text{ion}} = \frac{1}{k_1 k_2} \sin(k_R R) \varphi_\infty^{\text{Ps}}(k_r, r), \qquad (19)$$

where the momenta are given by $k_R = k_1 + k_2$ and $k_r = (k_1 - k_2)/2$, and $\varphi_\infty^{\text{Ps}}(k_r, r)$ is a (model) positronium continuum wave in Jacobi coordinates centered on the positronium atom with momentum k_r. Since there is now strong orthogonality between the final-state testing function ϕ^{ion} and the bound two-body positronium channels, but not the hydrogenic channels, we carry out asymptotic subtraction, in analogy with Eq. (15), using the calculated hydrogenic two-body amplitudes before computing the ionization amplitude. The results (not shown) were consistent, to good accuracy, with those presented in Figs 3(a) and (b).

IV. CONCLUSION

In this paper we have formulated and tested methods for extracting amplitudes for all positronium formation, scattering and ionization channels open to this *s*-wave model for positron-hydrogen collisions. The precision and self-consistency of the results confirms the efficacy of these techniques. An important outcome of this investigation is that it not only has verified that ECS-based methods can be applied to rearrangement collision problems; it has also confirmed that the cross sections, both differential and integrated, can be extracted using their most natural coordinate system, irrespective of the coordinate system chosen to undertake the calculation of the scattered wave function. The next phase in this project will be to extend these methods to positron-hydrogen collisions in their full dimensionality, which will include an investigation into the most appropriate coordinate system to calculate the scattered wave functions that minimizes the computational overhead.

Acknowledgements

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