Convergence study of the close-coupling approach to positron-helium collisions

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Abstract. Positron-helium collisions have been studied using a two-center close-coupling method. Convergent, pseudoresonance-free cross sections have been obtained by using complete expansions on both the helium and positronium centers. The low energy elastic cross sections, phase-shifts and total cross sections are compared with experimental data and results of other theories.

1. Introduction
The convergent close-coupling (CCC) method with a two center expansion has very successfully described positron-hydrogen collisions [1]. It has been shown that a two-center expansion with sufficient number of states from both the atom and positronium (Ps) centers yields smooth and convergent results [2].

Although the CCC method using only a single center expansion was successful in describing elastic, total and total break-up positron-helium cross sections at some energies [3, 4], it was unable to get convergent results in the Ore gap, or estimate the Ps-formation cross section. Two-center methods using only eigenstates for at least one of the centers can, in general, give good estimates. However, they often produce pseudo-resonances in the cross sections. For example, close-coupling results of Hewitt et al [5] and Campbell et al [6] have suffered from pseudo-resonances below 30 eV incident energies.

Studies of positron-hydrogen collisions using the two-center CCC approach have shown that pseudo-resonances will be eliminated if full pseudostate expansions are used on both centers. Consequently, we expect that complete two-center expansions will be required to get pseudo-resonance-free cross sections for calculating positron-helium collisions as well.

The positronium (Ps) formation channels have now been added to the CCC method for positron-helium scattering. Convergent results have been obtained for elastic scattering phase-shifts, ground and excited state Ps-formation and He excitation cross sections. We present the results for the elastic cross sections and low energy phase-shifts in order to make comparison with the benchmark results of the variational calculations of Van Reeth and Humberston [7]. Cross sections for Ps-formation, helium excitation and ionization processes will be presented elsewhere.

2. Method
The basic idea of the two-center convergent close-coupling approach is to expand the total scattering wavefunction in terms of the full set of target and positronium states. Using the
expanded $e^+$-He total wavefunction the Schrödinger equation is reduced to a set of momentum-space coupled integral equations for the transition amplitudes, which are solved in partial-wave reduced form.

The helium and positronium states are obtained by independently diagonalizing their Hamiltonians using Laguerre bases, which will ensure square integrability of the resulting wavefunctions. By increasing the basis sizes, the negative energy states converge towards the true eigenstates, while the positive energy pseudostates yield an increasingly dense discretization of the continuum.

Convergence in the cross sections is obtained by increasing the basis sizes of both the He and Ps centers. Ps-formation processes are calculated explicitly as transitions to negative-energy Ps-states. The ionization is also calculated simply as electron capture into positive-energy pseudostates of Ps and He.

We made the following two approximations in order to simplify the calculations. Firstly, the frozen-core treatment of helium, which assumes that one of the electrons is always in the $\text{He}^+(1s)$ state [8]. Such an approximation gives a reasonably accurate ground state of He with ionization energy of 23.74 eV instead of the actual 24.58 eV, and more accurate excited states. Secondly, we neglected the electron exchange between positronium and $\text{He}^+$ ion. This approach is supported by Van Reeth and Humberston [9], who stated that the $\text{He}^+$ ion behaves similarly to a proton because of tightly bound electron in the ion and also mean kinetic energies of the two electrons are different by a factor of eight, which makes electrons effectively distinguishable.

3. Results

In our present method we can include as many eigen- or pseudo-states from both centers as computing resources allow. In this work we present results of three kinds of calculations. The first one, denoted by CC($24,3$), is with 24 ($9s,8p,7d$) helium pseudostates and three ($1s,2s,2p$) Ps eigenstates, is similar to the calculation of Campbell et al [6]. The second and third ones have 27 ($10s,9p,8d$) and 33 ($12s,11p,10d$) pseudostates for both centers, denoted as CCC($27,27$) and CCC($33,33$), respectively. These two demonstrate that results the level of convergence. The CCC($33,33$) calculations are more time consuming than the CCC($27,27$) ones and therefore done at fewer energy points.

Figs. 1 and 2 presents phase-shifts below Ps-formation threshold. Our results compare well with the variational calculations [7], which are believed to be highly accurate and benchmarks. Convergence of the CCC calculations is excellent, and so by comparison with the multi-configuration single-center calculations [3], we can conclude that variance from the variational results is due to the present frozen-core treatment of helium.

Fig. 3 presents elastic cross sections below the Ps-formation threshold. Our results agree well with the experimental data and the results of variational calculations [7], except at the very low energies, due to the frozen-core approximation. The apparent good agreement of our CC($24,3$) calculations at the lower energies with experiment is coincidental as convergence has not yet been achieved.

We note that very similar results were obtained by one center CCC calculations using very high orbitals ($l_{\text{max}} = 8$) [3]. At low and medium incident energies it is very important to properly consider strong electron-positron correlations. Therefore in one-center expansions it was required to use very high angular momenta to get convergent results. In the two center method positron-electron correlation is explicitly included as Ps-formation channels, therefore there was no need to use high angular momenta states. Although not shown, we have checked (at a few partial wave and energy points) if it is the case by including f-states, and it has insignificant effect on the results. This was seen in positron-hydrogen case as well.

Fig. 4 displays total cross section from Ps-threshold up to energies where effect of Ps-formation diminishes. CCC results agree well with the experimental data [12, 11] up to 30 eV. At the
higher energies the CCC total cross section overestimates the experimental data. This is due to primarily the frozen-core treatment of He. The better agreement of CC(24,3) results and experimental data is coincidental as these results are not yet convergent. One remarkable feature of the CCC results is that they are smooth over the whole energy range, while our CC(24,3) and the results of Campbell et al [6] have resonance structure around 22 eV.

4. Conclusion
The two center CCC method has been applied to positron-helium scattering. Convergent cross sections were obtained by using an equal number of pseudostates for both helium and Ps centers. Low energy elastic cross sections and phase-shifts have been obtained by using only s-, p-, and d-orbitals, and the results agree well with experiments and benchmark calculations of Van Reeth and Humberston [7].

The present total cross sections are slightly higher than the experimental ones at incident energies above 30 eV. We believe that this overestimation is due to the frozen-core treatment...
of helium. We expect that relaxation of the frozen-core approximation will lead to a slight reduction of the corresponding cross sections, as was found in the single-center calculations of Wu et al. [4], and so will result in even better agreement with experiment.

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