Convergent close-coupling approach to positron and antiproton collisions with atoms

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Abstract.
Recent developments in application of the convergent close-coupling approach to antimatter-matter scattering are outlined. These include positron collisions with alkalis and helium, in the ground or metastable states, as well as extension of the method to heavy projectiles, such as antiprotons.

1. Introduction
Understanding of antimatter induced reactions with atoms (and molecules) remains a significant challenge, driven by the quest to advance fundamental knowledge of the underlying physical mechanisms, as well as the desire to control and to apply them. In this respect, ionization (or simply breakup) is particularly important. Theoretical treatment of antimatter-matter interactions may seem similar to those involving only matter. In the case of positron and electron scattering on atoms, the latter has the complexity of exchange arising from the indistinguishability of electrons, while the former has the complexity of rearrangement due to formation of positronium (Ps). Thus the positron-atom scattering system has two natural centres whereas the electron scattering system has only one. The two problems share similar complexity in the treatment of the target excitation and the three-body continuum.

The convergent close-coupling (CCC) method has been very successful in treating electron-atom scattering problems. The technique relies on a sufficiently large single centre expansion of the total wave function in order to correctly take into account all possible atomic excitation and ionisation processes. Convergence in transitions of interest is obtained by simply increasing the basis size. The same idea can be applied to positron scattering except now two-centre expansions are required. Such expansions incorporate the required atomic and Ps channels but make the calculations far more difficult and time-consuming.

Here we report on recent progress in applications of the CCC method to antimatter-matter interactions. In particular, we focus on developments in positron collisions with alkalis and metastable helium and extension of the CCC method to antiproton-atom scattering.

2. Positron scattering on metastable helium
For some targets, particularly excited ones, the Ps-formation channel is open starting from zero collision energy. Positron scattering on the $2^3S$ metastable state of helium is an example of such
a system where the Ps-formation threshold is negative (-2.06 eV). This system has not been yet studied neither theoretically nor experimentally. Recently, we have reported two-centre CCC results for positron scattering on the ground state of helium [1] where a good agreement between the theory and experimental data has been seen. Here we apply this formalism to positron scattering on metastable helium. The motivation for this study is twofold. First, we would like to check the applicability of the two-centre CCC approach to a system with a negative Ps-formation threshold. Second, the recent experimental achievements on electron scattering from metastable helium [2], in the group that also has a positron beam, suggests that in a not too distant future there might be experimental data to compare with our calculations. Moreover, there are still unresolved differences between theory and experiment on electron scattering from metastable states of He [3, 4]. Alternative studies using positrons instead of electrons may therefore shed more light on the situation.

Comparison of the total cross sections for positron scattering from He(2\(^3\)S) and He(1\(^1\)S) is given in Fig. 1. Relative magnitudes of cross sections vary substantially depending on the processes. The total scattering cross section for He(2\(^3\)S) is larger than that for He(1\(^1\)S) by more than two orders of magnitude. Though not shown, for Ps formation this ratio turns out to be around 50, while for breakup of He(2\(^3\)S) it is around 10. The large relative ratio of cross section for He(2\(^3\)S) and He(1\(^1\)S) shows the importance of scattering from excited states in understanding positron scattering from helium [5].

3. Positronium formation in positron-alkali collisions
The two-center CCC method has been implemented for the case of positron scattering with alkali atoms. This is another example of the case with the negative Ps-formation threshold. To calculate cross sections for positron-alkali scattering we employ the frozen-core approximation. The target is considered as a hydrogen-like atom with one active electron interacting with an inert ion core. This approach is valid for impact energies less than 60 eV where the inner-shell electrons do not participate directly in a collision event. The core electrons provide screening of the nucleus and take part in exchange with the active electron. Also, the virtual core excitation is accounted for phenomenologically by introducing a small polarization potential. The core wavefunctions are obtained by using the Hartree-Fock method. These functions are required to calculate effective potentials for positron and active-electron interactions with the core. We use the equivalent local approximation to take into consideration the exchange part of the electron-ion interaction. Target wavefunctions are computed by diagonalizing the target atom Hamiltonian in the basis of Laguerre functions. This provide a good representation of low lying discrete atomic states and also a square-integrable representation of the target continuum. Finally, we formulate a set of momentum-space coupled Lippmann-Swinger equations for the T-matrix and solve them.
The cross sections have been calculated for a broad range of energies of practical interest [9]. Convergence in the calculated cross sections has been acheived by increasing the basis sizes and orbital angular momentum of the included states for each of the centers. Figure 2 shows the positronium formation cross section. We compare our calculations with the experimental data [6] and other theoretical results [7, 8]. The red line was obtained with the full basis including ten s, nine p and eight d states for both target and Ps centres. To calculate the blue curve we used the truncated pseudostate basis with three eigenstates (1s, 2s and 2p) for positronium and twenty nine states (2s-9s, 2p-9p, 3d-9d and 4f-9f) for lithium. We see that all theoretical curves are in an overall qualitative agreement. As expected our truncated-basis calculations agree better with the results by McAlinden et al [7] than our convergent full-basis cross sections. The differences can be attributed to the fact that we take into account the exchange part of the electron-electron interaction and also use close but different representation of the positronium and lithium states. The exchange interaction was also taken into account in the hyper-spherical close-coupling calculations [8]. The authors obtained the resonance-free energy dependence for the positronium formation cross section. We see that our and their results (black solid line) are very close to each other and differ slightly in the peak magnitude.

4. Antiproton-impact ionization of hydrogen

In antiproton-hydrogen collisions at the keV energy region the protonium formation channel is negligible [10]. This greatly simplifies the problem as the scattering system essentially has only one natural centre. Consequently, a standard one-centre expansion of the total wave function using sufficiently large orthogonal Laguerre basis is used. Such a basis allows to correctly account for all the atomic excitation channels as well as ionization. In the case of light projectiles the three-dimensional CCC integral equations are reduced to one dimensional ones using the partial-wave expansion. However, for heavy projectiles like antiproton the partial-wave method becomes impractical. Instead, we use the transformation into the impact-parameter space. This results in one-dimensional integral equations for the scattering amplitudes in the impact parameter representation [11]. Cross sections for the elastic scattering, excitation and ionization are calculated from the scattering amplitudes in impact-parameter representation.

Fig. 3 shows our results for the total ionization cross section (TICS) for antiproton-impact ionization of hydrogen in comparison with the experimental data [12] and other calculations [13, 14, 15, 16]. The experimental data are available only above 31.2 keV, however a controversy seems to exist at lower energies where the close-coupling methods [13, 14, 15] predict the TICS several times larger than that predicted by the CDW-EIS [16] approach. As a test of our expansion basis, we also reproduce the exact first Born TICS obtained in the full wave treatment by Bates and Griffing [17]. An excellent agreement with the exact Born result indicates that the size of our pseudobasis is sufficiently high to reproduce the physics of the process. Our full results (solid black curve) are in an excellent agreement with the experiment.
throughout the energy range considered. They show maximum around 30 keV with rapid decline with decreasing energy, whereas the results of some other groups [13, 14, 15] predict much larger cross sections at low energies. Only the results of the high-energy CDW-EIS method show the same trend as our results. However, they are 50% smaller. New measurements of cross sections at low energies would clarify the situation at this region.

![Figure 3](image)

**Figure 3.** The total cross section for antiproton-impact ionization of hydrogen. The CCC calculations have been obtained using 1176 pseudostates with $n_{\text{max}} = 20$ and $l_{\text{max}} = 8$.

5. Conclusion

We have given a brief account of the latest convergent close-coupling calculations of antimatter-matter interactions. Positron scattering on metastable helium shows that presence of excited states in the experimental target gas chamber may significantly enhance the cross sections. The results for positron scattering on lithium are in an overall agreement with available theoretical calculations. Meanwhile, the cross section for hydrogen ionization by antiproton significantly differs from the others and reopens the discussion on its low-energy behaviour.

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