Positron scattering on atoms and molecules

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Abstract. An overview is given of recent progress in the calculation of positron scattering on atoms and molecules using the convergent close-coupling method. Particular emphasis is given to those cases where positronium formation is one of the reaction channels, as well as the importance of demonstrating convergence with increasing orbital angular momentum of the bases used. Targets considered are atomic hydrogen, lithium, and molecular hydrogen.

The last two decades have seen extraordinary progress in the field of electron, positron and photon scattering on atoms and ions. The problems of electron and photon scattering on atoms are very closely related. In the typical case of single photon absorption, the interaction proceeds by the resulting photo-electron scattering on the residual ion. For example, photon-helium scattering is essentially electron scattering on the singly charged helium ion.

Positron-atom scattering is a little more interesting due to the possibility of positronium (Ps) formation. This is a rearrangement collision that considerably increases the complexity of the problem. Though it has been often claimed that positron-atom scattering is simpler than the corresponding electron-scattering problem due to the absence of exchange, in practice the introduction of the Ps-formation channel creates considerably more significant challenges.

Historically, computational approaches to the problems have been subdivided into the low-, intermediate- and high-energy regimes. In addition, excitation and ionisation processes have also received different treatments. However, our interest in developing the convergent close-coupling (CCC) method has been to unify the approach to all such problems to be valid for the three projectiles across all energies and for the major excitation and ionisation processes.

In developing the CCC method for excitation we took note of the techniques used specifically in their regimes of validity. At low energies the R-matrix close-coupling approach [1] has yielded outstanding results. At the higher energies the perturbative approach [2] has been particularly successful. The CCC method [3] combines the two techniques because it formulates close-coupling as coupled Lippmann-Schwinger equations in momentum space, which may be readily expanded in a perturbative series. Furthermore, the coupled equations may be solved in a distorted-wave formalism [4]. However, unlike distorted-wave approximations the CCC results are independent of the choice of the distorting potential. In this sense the usage of such a potential is solely for numerical ease of solution.

Following the pioneering implementation of the close-coupling method to ionisation processes [5], we developed an even simpler CCC approach [6]. Rather than reconstructing the total wavefunction of the electron-atom system, we associated ionisation amplitudes with excitation of the positive-energy pseudostates. In other words, we extracted the required

ionisation amplitudes directly from the solution of the coupled equations. Along the way we found a resolution for the long-standing problem of potential double counting of ionisation processes from excitation of open pseudostates with energy $\epsilon_n > 0$ on either side of $E/2$, where $E > 0$ is the total energy. It turns out that convergence of the close-coupling formalism is such that the amplitudes for excitation of $\epsilon_n > E/2$ pseudostates go to zero with increasing basis size [7]. Thus, the outstanding agreement between the CCC theory and experiment for the e$^-$-H total ionisation cross section [8] has no double counting of ionisation problems. The successful implementation of the CCC method to electron scattering for excitation and ionisation processes was readily translated to single and double photoionisation processes [9, 10, 11, 12], which continues to be of current interest [13, 14].

Along the way we also considered formal scattering theory problems of breakup processes with long-ranged potentials, leading to a new surface-integral formalism for the underlying scattering theory that is valid for both short- and long-ranged potentials [15, 16]. The combination of formal theory and computational implementation for electron and photon scattering has been recently reviewed [17].

In our opinion e$^-$-H scattering is essentially a solved problem in the sense that accurate elastic, excitation and ionisation amplitudes can be computationally obtained at any energy of interest [18, 19]. However, this is not the case for the corresponding e$^+$-H problem. In the latter case we have a two-centre problem that requires two separate expansions, utilising atomic and Ps states [20, 21]. The CCC method is based on the complete Laguerre basis [3], and so having two non-orthogonal, but near complete expansions is fundamentally problematic. Nevertheless, the method works very well due to the fact that the two square-integrable expansions do not overlap at infinite separations where the excitation amplitudes are defined. Even so, we end up with another double-counting possibility for breakup processes from excitation of positive-energy atomic and Ps states. This does not appear to be a problem for integrated cross sections [22], but remains unresolved in the case of fully differential ones [23].

The two-centre CCC implementation of positron scattering on atomic hydrogen [21], alkali metals [24, 25], helium [26, 27] and alkaline earths [28] gives us an opportunity to test internal consistency of the approach by varying the treatment of the two centres. If we are not interested in explicit Ps-formation then a single centre approach is valid at energies below the Ps-formation threshold and above the ionisation threshold. This is because the positive-energy atomic states can be used to completely account for virtual or explicit effects of Ps-formation. In the latter case excitation of positive-energy atomic states represents both the ionisation and Ps-formation processes. This approach has been used in the single-centre implementations for noble gases [29] and molecular hydrogen [30]. Here, we give an overview of convergence considerations within the two centre CCC formalism.

We begin with the case of e$^+$-Li scattering at very low projectile energies. For the alkali metals Ps-formation is open at zero projectile energy, and so a two-centre formalism is required that has at least the Li(2S) and the Ps(1s) states. By Wigner [31], since Ps-formation is an exothermic reaction, at sufficiently low energies its cross section should behave as $1/k$ where k is the positron momentum. We investigate this in figure 1, where a series of CCC calculations are presented which vary the orbital angular momentum l of the Laguerre basis for the atom, and also the number of Ps s-states. Our starting point is the CCC(25_4,1), where $N_l = 25 - l$ for $l \leq l_{\max} = 4$, and only Ps(1s) state is included. One may expect this to be a reasonable starting point, however, adding just the Ps(2s) state reduces the Ps(1s) cross section by an excess of on order of magnitude, though with little effect on elastic scattering. Adding the Ps(3s) state has only a marginal effect. To further check the convergence of the results we keep only the Ps(1s) state, but set $l_{\max} = 8$, and indeed confirm the convergence. This indicates how the large-l atomic states can effectively take into account Ps states, even when they have such a large effect. A fit to the $1/k$ function confirms the predicted threshold behaviour for Ps-formation.
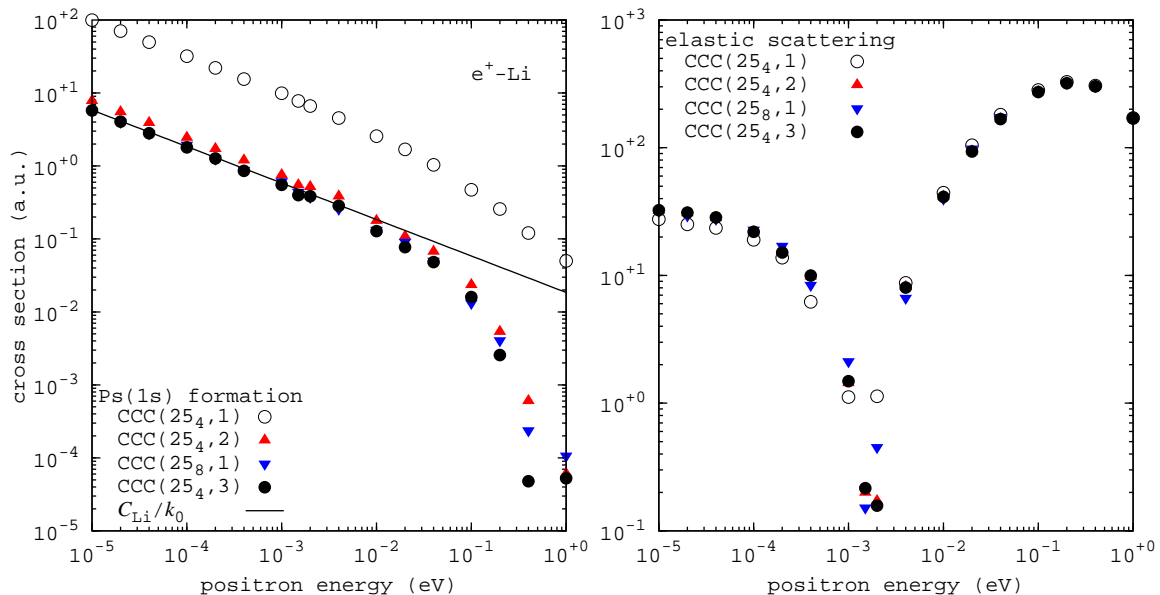
Figure 1. Positron-lithium scattering at low incident energies $k_0^2/2$. The CCC calculations are due to Lugovskoy *et al* [32]. They are labeled by $25_{l_{max}}$, where the Laguerre basis has $l \leq l_{max}$ and $N_l = 25 - l$, and also the number of Ps s-states used in the calculations.

We next turn to the consideration of (anti)hydrogen formation in (anti)proton-Ps scattering at low Ps energies. This is entirely equivalent to Ps-formation in positron-hydrogen (or electron-antihydrogen) scattering at energies just above the Ps-formation threshold. In this case (anti)hydrogen formation is an exothermic reaction and so its cross section should also behave as $1/k$, where k is Ps linear momentum. The results are presented in figure 2. Here we consider two approaches to convergence. One treats the two centres symmetrically, and the other has only the Ps(1s) state and atomic bases $N_l = 30 - l$ with $l_{max} = $ 5, 10 and 20. The CCC($4_2,4_2$) calculation has $N_l = 4 - l$ for $l_{max}=2$ on both centres, and is somewhat similar to the calculations of Mitroy [33, 34] with good agreement found. This represents an efficient approach to convergence because static dipole polarizability is accurately reproduced in both centres. However, the CCC(N,1) approach is particularly inefficient because it neglects the Ps static dipole poalrizability which is eight times bigger than that of atomic hydrogen. Accordingly, a steady increase in l_{max} is required to approach the convergent result.

The multiplication of the (anti)hydrogen cross section by k is done so that the threshold behaviour could be readily established. By doing a least squares fit at energies below 0.001 eV we found $k\sigma_H(k) \approx 0.13162 \pm 0.00005 - (13.2 \pm 0.2)k$. The smallness of the uncertainties, and the substantial second term indicates that the $1/k$ behaviour of $k\sigma_H(k)$ holds strictly only at threshold.

Another recent development is the implementation of the CCC method to molecular targets, with H_2^+ and H_2 as the starting points. This has been done in both spherical and spheroidal coordinate systems. In figure 3 the grand total cross sections are presented from single-centre e$^+$-H_2 calculations. The details of the calculations have been given by Zammit *et al* [30]. Briefly, a multiconfiguration treatment of H_2 in a two-electron basis constructed from the Laguerre functions yields a sufficiently accurate ground and excited states. By setting $l_{max} = 8$ we ensure that the contribution of Ps-formation channels is able to be treated to convergence, outside the small energy interval between Ps-formation threshold and ionisation, via the positive-energy
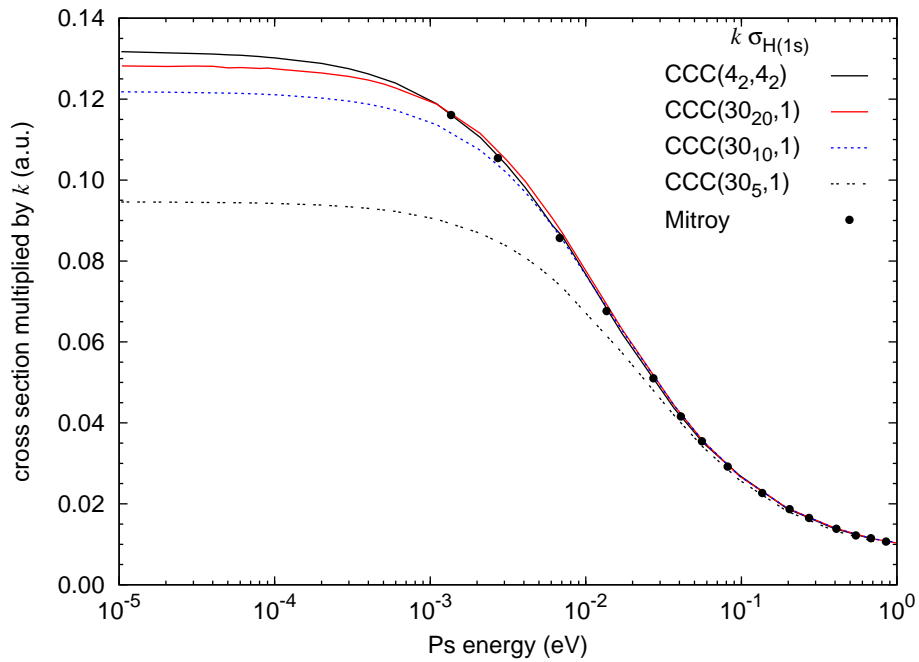
Figure 2. (Anti)hydrogen formation in positronium-(anti)hydrogen scattering at low Ps energies k^2. The CCC calculations, see text, are due to Kadyrov *et al* [35]. The calculations of Mitroy [33, 34] are also given. The cross sections have been multiplied by k to examine the threshold behaviour.
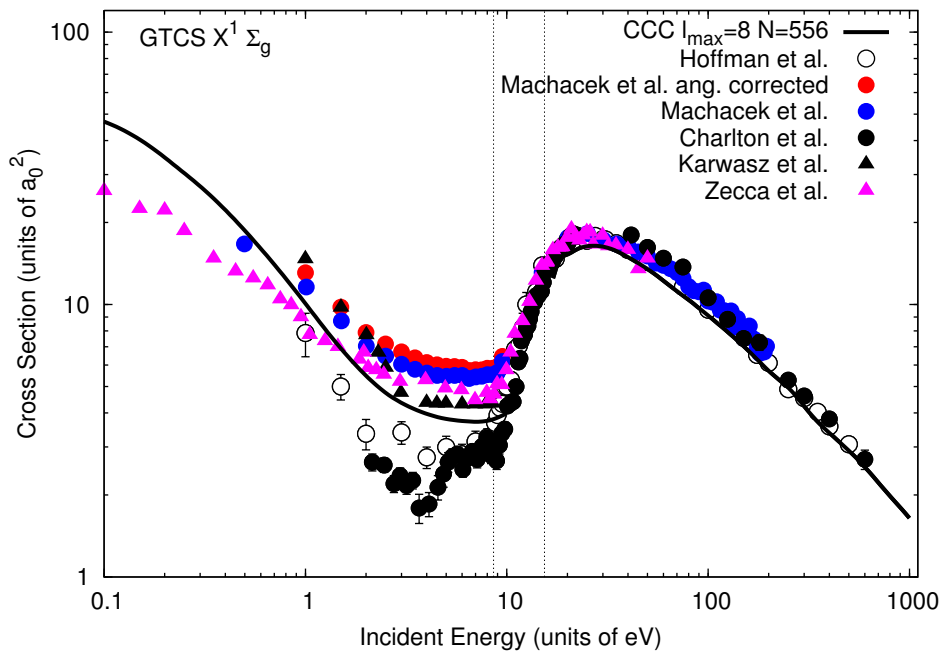

Figure 3. Grand total cross sections in positron-molecular hydrogen scattering. The calculations are due to Zammit *et al* [30]. The measurements are from Refs. [36, 37, 38, 39]. The data of Machacek *et al* are to be published.
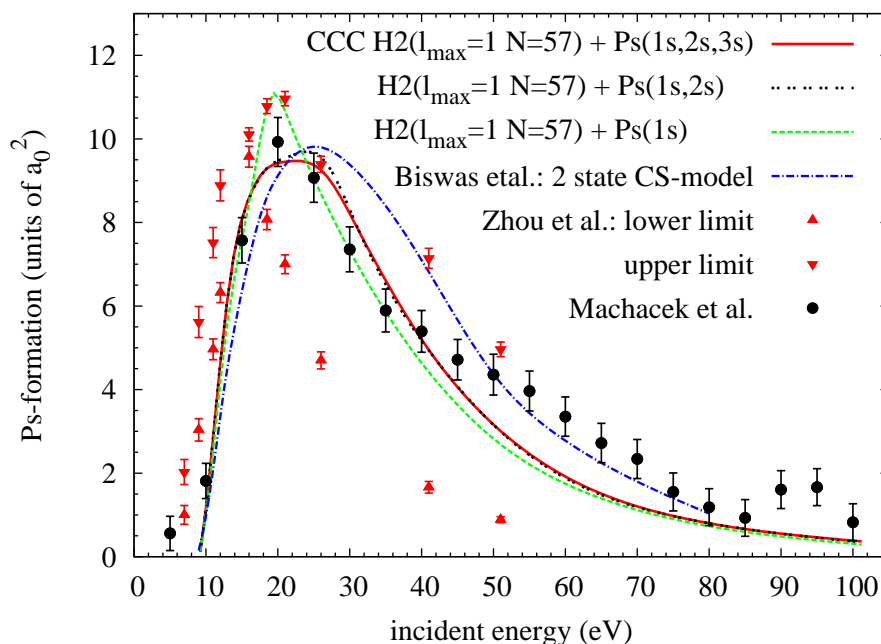
Figure 4. Total positronium-formations cross sections in positron-molecular hydrogen scattering. Present calculations are denoted by CCC. The two-state calculation is due to Biswas *et al* [40]. The measurements are due to Zhou *et al* [41]. The data of Machacek *et al* are to be published.

atomic pseudostates. We see some variation between experimental results, particularly at low energies, which makes comparison with experiment somewhat problematic. However, good agreement between all experiments and theory at the higher energies is very encouraging.

Most recently we have implemented a two-centre CCC approach to e^+-H_2 scattering. Figure 4 shows the preliminary results obtained. The two-centre calculations are very complicated and time consuming, particularly, when applied to complex targets such as molecules. Therefore, as a first step, we approached the problem with the use of the frozen-core model of H_2 (inner electron is the ground H_2^+ orbital but for the H_2 internuclear separation), and only s-states of Ps. Even with these approximations the results look very promising and compare well with the recent measurements of Machacek *et al* [to be published]. More work is under way to use more realistic wave functions and to include larger orbital angular momentum states of Ps.

Acknowledgments

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