LETTER TO THE EDITOR

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LETTER TO THE EDITOR

Continuum effects on positron scattering of atomic hydrogen at intermediate energies

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Abstract. An optical potential method to study the positron–hydrogen atom scattering system within the close-coupling framework that includes both the positron–hydrogen and positronium–proton channels has been implemented. Ionization, positronium formation and total cross sections are reported and are compared to other available theoretical and experimental data.

In this decade, we have seen a number of major advances in the theoretical studies of positron scattering by atomic hydrogen. These theoretical studies (Hewitt et al 1990, Mitroy 1993, Higgins and Burke 1993, McAlinden et al 1994) have explicitly coupled the positronium (Ps) channels together with the hydrogen atom channels in their theoretical calculations. These new-generation scattering methods provide the most realistic investigations for positron scattering by atomic systems and have been used to study positron scattering from atomic hydrogen and alkali metal atoms. Intense work by a number of theoretical groups has culminated in a series of accurate total cross sections for transitions studied at low energies (Kernoghan et al 1995, Mitroy 1995, Gien 1997). Theoretical studies of positron–hydrogen scattering in the intermediate-energy regime is a challenging endeavour as it would imply a lot of discrete states and the continuum must be incorporated in a practical manner. Ratnavelu et al (1996) had used a simple six-state close-coupling calculation that used three H states (1s, 2s, 2p) and three Ps states (1s, 2s, 2p) to study positron scattering from atomic hydrogen at intermediate energies of 4–100 Ryd. It provided a comprehensive and realistic study of the scattering process but nevertheless incomplete, as higher discrete states and the continuum were neglected. Recently, Kernoghan et al (1996) and Mitroy (1996) have used a large $L^2$ basis of hydrogen states (30 and 28 states, respectively) together with the Ps(1s), Ps(2s) and Ps(2p) states to study positron scattering by atomic H at intermediate energies. Although they have been performed in momentum space (Mitroy 1996) and in coordinate space (Kernoghan et al 1996), both methods should be equivalent. Their results may suggest a useful benchmark for theoretical calculations in the intermediate energy region. However, there are noticeable differences between these two studies in the calculation of various cross sections, especially in the calculation of the ionization cross sections. A complete theoretical method among other virtues must be able to predict accurate cross sections for the ionization process.

In figure 1 we depict the ionization cross sections that show some of the qualitative and quantitative differences between these calculations at 20–100 eV. We also show recent...
measurements of Weber et al (1994) and Jones et al (1993). These measurements show conflicting trends at $E < 100$ eV. The 33-state $R$-matrix (CC(30,3)) cross sections of Kernoghan et al seem to favour the UCL (University College London) data of Jones et al rather than that of Weber et al. The CC(28,3) cross sections of Mitroy (1996) show better agreement with the UCL data over the whole energy range. Nevertheless, there are some disconcerting differences between the CC(30, 3) and CC(28, 3) models for the energy range between 35 and 80 eV. This raises the question of convergence of the large $L^2$ basis. It is highly probable that the inclusion of the f-pseudostates in the work of Kernoghan et al may explain these differences. We also depict the ionization cross sections of Ratnavelu (1991) which show good agreement with the UCL data for $E > 30$ eV. Ratnavelu (1991) had used the continuum optical potential method of McCarthy and Stelbovics (1983a) to calculate these ionization cross sections.

The scarcity of theoretical studies, and the differences that exist between the theoretical predictions of the ionization cross sections, motivated the present work to study positron scattering by atomic hydrogen at intermediate energies. In the 1980s, McCarthy and Stelbovics (1983b) proposed the coupled-channels optical method (CCOM) for electron–atom scattering. Their treatment of the optical potentials has achieved much success as in the study of $e^–$–H, $e^–$–He, $e^–$–Na, $e^–$–K and $e^–$–Mg (Lower et al 1987, Ratnavelu and McCarthy 1990, Brunger et al 1990, McCarthy et al 1989, 1991) scattering systems. The CCOM has provided an interesting and unique way of treating the continuum effects and recently has provided some interesting results for electron impact excitation of $2^3S$ He (Zhou et al 1998) and $n = 3$ excitation of ground-state hydrogen (Ratnavelu and Zhou 1998).

In this work we have successfully implemented the optical potential method of McCarthy and Stelbovics (1983b) for positron–hydrogen atom scattering processes. Previously, Bransden et al (1985) and McCarthy et al (1993) have also applied the CCOM to $e^+–H$ and $e^+–$–alkali

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**Figure 1.** The ionization cross sections (in $\pi a_0^2$) for positron–hydrogen scattering: —····, the continuum optical potential of Ratnavelu (1991); ▼, CC(30, 3); ▲, CC(28, 3); •, the UCL data; and ■, Bielefeld data.
atoms, respectively. However, Bransden et al had not allowed for the explicit inclusion of Ps formation in the close-coupling expansion of the total wavefunction of the system. The later work of McCarthy et al used an optical potential to allow for virtual Ps formation that showed some significant results for positron scattering from Na and K.

Here, we have incorporated the continuum optical potential model within the close-coupling method of Mitroy (1993) which allows both manifolds of positron–hydrogen and positronium–proton channels. Following the notational details in Mitroy (1993), Schrödinger’s equation for the e+–H system can be written as

\[ \left( -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{|r_1 - r_2|} - E \right) \Psi(r_1, r_2) = 0 \]  

or alternatively as

\[ \left( -\frac{1}{4} \nabla_R^2 - \frac{1}{|R - \frac{1}{2} \rho|} - \frac{1}{|R + \frac{1}{2} \rho|} - \frac{1}{\rho} - E \right) \Psi(\rho, R) = 0. \]

The total wavefunction of the system can be written as

\[ \Psi(r_1, r_2) = \sum_\alpha \psi_\alpha(r_1) F_\alpha(r_2) + \sum_\beta \phi_\beta(\rho) G_\beta(R) \]  

where \( \psi_\alpha(r_1) \) are the hydrogenic target states and \( \phi_\beta(\rho) \) are the positronium states.

In implementing the CCOM method, we partition the target space by using the projection operators \( P \) and \( Q \) where

\[ P = \sum_{i \in P} |\psi_i\rangle \langle \psi_i| \]  

and

\[ Q = 1 - P. \]

Thus, the optical potential \( V^{(Q)} \) can be formulated, with the \( Q \)-space eliminated for the positron–hydrogen channels as

\[ V^{(Q)} = V + VQ \frac{1}{Q(E^{(*)} - K - K)} QV \]  

where \( V = v_1 + v_2 + v_3 \) with \( v_1 \) the electron–nucleus potential, \( v_2 \) is the positron–nucleus potential and \( v_3 \) the positron-electron Coulomb potential. The last term in (6) is the complex polarization potential.

Following McCarthy and Stelbovics (1983b), the complex polarization term of equation (6) can be calculated. In the present work the \( Q \)-space considered only includes the continuum channels. The details of calculating the complex polarization potential for the continuum can be found in McCarthy and Stelbovics (1983b) and Ratnavelu (1991) and will not be described here.

We can write the momentum space Lippmann–Schwinger equations (Mitroy 1993) for a positron with momentum \( k \) incident on hydrogen atom in state \( \Psi_\alpha \) (atomic units are assumed throughout) are written as

\[
\langle k' \Psi_{\alpha'} | T | k \Psi_\alpha \rangle = \langle k' \Psi_{\alpha'} | V^{(Q)} | k \Psi_\alpha \rangle + \sum_{\alpha''} \int d^3k'' \frac{\langle k' \Psi_{\alpha'} | V^{(Q)} | k'' \Psi_{\alpha''} \rangle \langle k'' \Psi_{\alpha''} | T | k \Psi_\alpha \rangle}{(E^{(*)} - \epsilon_{\beta''} - \frac{1}{2} k''^2)} \\
+ \sum_\beta \int d^3k'' \frac{\langle k' \Phi_\beta' | V | k'' \Phi_\beta'' \rangle \langle k'' \Phi_\beta'' | T | k \Psi_\alpha \rangle}{(E^{(*)} - \epsilon_{\beta''} - \frac{1}{2} k''^2)}
\]  

(7)
\[ \langle k'\Phi_{\beta'}|T|k\Psi_u \rangle = \langle k'\Phi_{\beta'}|V|k\Psi_u \rangle + \sum_{\alpha'} \int d^3k'' \frac{\langle k'\Phi_{\beta'}|V|k''\Psi_{\alpha''}\rangle \langle k''\Psi_{\alpha''}|T|k\Psi_u \rangle}{(E^{(v)} - \epsilon_{\beta''} - \frac{1}{2}k''^2)} + \sum_{\beta'} \int d^3k'' \frac{\langle k'\Phi_{\beta'}|V|k''\Phi_{\beta''}\rangle \langle k''\Phi_{\beta''}|T|k\Psi_u \rangle}{(E^* - \epsilon_{\beta''} - \frac{1}{2}k''^2)} \] (8)

We have performed the following calculations:

CC(3, 3): In this calculation, the simplest model of three hydrogen states H(1s), H(2s) and H(2p) and the three positronium states Ps(1s), Ps(2s) and Ps(2p) were used.
CCO(3, 3): Besides the six physical states incorporated in the above close-coupling expansion, optical potentials for the continuum were used in the 1s–1s, 1s–2s, 2s–2s, 1s–2p, 2p–2p and 2s–2p couplings.
CC(6, 3): In this model, the six hydrogen states 1s, 2s, 2p, 3s, 3p and 3d have been included together with Ps 1s, 2s, 2p, 3s, 3p and 3d.
CCO(6, 3): This calculation allows for the continuum optical potential in the 1s–1s, 1s–2s, 1s–2p, 2s–2s, 2p–2p and 2s–2p couplings in the nine-state calculation.

The numerical details of solving the coupled Lippmann–Schwinger equations for positron–hydrogen scattering has been well detailed by Mitroy and co-workers (Mitroy 1993, 1996, Ratnavelu et al 1996). In general, the coupled equations are solved to a maximum angular momentum of \( J = 24 \) at 50 eV and \( J = 36 \) at 100 eV. The rearrangement kernel was included to a maximum of \( J = 16 \). A quadrature mesh of 48 points were used to discretize the integral equations. In all cases, the cross sections calculated did not reveal irregular features.

In figure 2, we show the ionization cross sections calculated with the CCO(3, 3) and CCO(6, 3) together with the CC(28, 3) and CC(30, 3) models. We also depict the ionization

![Figure 2](image-url)
cross section of Ratnavelu (1991). The present CCO(3, 3) and CCO(6, 3) confirm the qualitative and quantitative features of the continuum optical potential of Ratnavelu. This provides an indirect test that the continuum optical potential has been incorporated accurately in the present work. The present models also show excellent agreement with the UCL data from 30 eV onwards. Below 30 eV, the present methods predict cross sections that are above the UCL data. It may be plausible that the approximations used in the continuum optical potential method may fail at lower intermediate energies. The good agreement between the CC(28, 3) and CC(30, 3) in the lower region may substantiate this argument. However, the lack of convergence of the $L^2$ calculations also suggests that further convergence studies must be done to explain the quantitative differences that exist between these two calculations at other intermediate energies. Our calculations demonstrate that the CCO(3, 3) and CCO(6, 3) have converged over most of the energies. The inevitable question is now to reduce the experimental errors so as to provide a more discriminating test for theories.

In figure 3, the Ps formation cross sections calculated in the various theoretical methods are depicted with the experimental data of the Bielefeld–Brookhaven collaboration (Weber et al 1994) and the Detroit group (Zhou et al 1997). We only depict the ‘best’ measurements of Zhou et al and not their lower limit values. The new measurements show similar qualitative features of the previous experiments but differ in magnitude for $E < 40$ eV. In the present calculations, as in the CC(28, 3) and CC(30, 3), only three Ps states were used in the close-coupling expansion. Thus we are only able to calculate the Ps formation in the Ps(1s), Ps(2s) and Ps(2p) states. We follow Mitroy’s (1996) procedure to assume a $1/n^3$ scaling for Ps formation in the $n \geq 3$ states. This leads to the total Ps formation formula

$$\sigma_{Ps} = \sigma_{Ps(1s)} + 1.6(\sigma_{Ps(2s)} + \sigma_{Ps(2p)}).$$

(9)

Figure 3. The Ps formation cross sections (in $\pi a_0^2$) for positron–hydrogen scattering. The legend for the theoretical models are the same as in figure 2 except for the CC(3, 3) (+) and CC(6, 3) (×). The experimental data are from Detroit (▼) and Bielefeld–Brookhaven (■).
The present CCO(6, 3) and CCO(3, 3) cross sections lie above the CC(28, 3) calculation. The qualitative shape of the total Ps cross sections are also reproduced quite well by all the theories. The present data are within the experimental error bars of Weber et al but are slightly above the latest measurements for \( E < 50 \) eV. The CC(30, 3) data is much lower than the other calculations and in good agreement with Zhou et al. The effects of the continuum optical potential are clearly seen by comparing the CCO(3, 3) and the CCO(6, 3) data with the corresponding CC(3, 3) and CC(6, 3). The inclusion of the continuum optical potential reduces the cross sections by as much as 10–18\% for \( 30 < E < 90 \) eV. Some effects are still noticed at higher energies.

![Figure 4. The total reaction cross section (in \( \pi a_0^2 \)) for positron–hydrogen scattering. The legend is the same as in figure 3.](image)

The total cross section for the present models is shown together with the CC(28, 3) and CC(30, 3) in figure 4. The latest measurements of Zhou et al (1997) are also shown. The CC(28, 3) and CC(30, 3) cross sections lie within the experimental error bars and do not show any disagreement with the experiments. The present models lie below the lower bounds of the experimental data for \( E < 60 \) eV. We observe that incorporating the \( n = 3 \) discrete states of H in the CCO(6, 3) model enhances the cross sections from the CCO(3, 3) model. It is gratifying to see that the present CCO(6, 3) cross sections are within 10–15\% with experiment and other theories for \( E > 60 \) eV. We are certain that a larger basis set in the present method such as allowing \( n = 4 \) states and the same continuum optical potentials will improve the agreement.

In conclusion, we have shown here a small basis calculation using six- and nine-states together with the continuum optical potential that provides an alternative method of studying positron–hydrogen atom scattering at intermediate energies. It has shown some interesting results for most of the significant physical phenomena such as the ionization and Ps formation cross sections.
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