



CHORUS

This is the accepted manuscript made available via CHORUS. The article has been published as:

Two-center close-coupling calculations of positron-molecular-hydrogen scattering

R. Utamuratov, A. S. Kadyrov, D. V. Fursa, M. C. Zammit, and I. Bray

Phys. Rev. A **92**, 032707 — Published 11 September 2015

DOI: [10.1103/PhysRevA.92.032707](https://doi.org/10.1103/PhysRevA.92.032707)

Two-centre close-coupling calculations of positron-molecular hydrogen scattering

R. Utamuratov, A. S. Kadyrov, D. V. Fursa, M. Zammit, and I. Bray

*Curtin Institute for Computation and Department of Physics, Astronomy and Medical Radiation Sciences,
Curtin University, GPO Box U1987, Perth, WA 6845, Australia*

A two-centre close-coupling method that includes positronium (Ps) formation channels has been developed for positron scattering on molecular hydrogen. Calculations are performed within the fixed-nuclei approximation. Results for the grand total, Ps-formation and direct ionization cross sections are presented. In general, good agreement with experiment is seen in all the calculated cross sections.

PACS numbers: 34.10.+x, 34.80.-i, 34.80.Lx, 34.80.Uv

I. INTRODUCTION

Molecular hydrogen is a natural starting point for both theoretical and experimental studies of collisions with molecular targets. Positron collisions with this target have been studied extensively by various experimental groups over the last 30 years [1–14]. Theoretical studies of this scattering system are challenging because of the complexities associated with the molecular structure and its non-spherical nature. Rearrangement processes add another degree of complexity to the problem. Until recently theoretical studies [15–27] have been focused only at certain energy regions. In addition, there are few theoretical studies which include the Ps-formation channels explicitly. The first calculations of Ps-formation cross section [15–17, 20] were obtained with the use of the first Born approximation. Biswas *et al.* [21] used a coupled-static model, which only included the ground states of H₂ and Ps. This simple model is the only coupled-channel calculation available to date. Comprehensive review of the positron interactions with atoms and molecules has been given by Surko *et al.* [28].

Effect of using realistic target wave functions and channel coupling on the Ps-formation cross section has not yet been studied, and is our goal here using the convergent close-coupling (CCC) method [29, 30]. The CCC method has been successfully applied to electron-atom (see Bray *et al.* [31] and references therein) and two-centre positron-atom [30, 32–34] scattering problems. It has also been applied to calculate antihydrogen formation [35, 36] in low-energy collisions of positronium (Ps) and antiprotons. For positron scattering, the internal consistency of the two-center method is a powerful mechanism for validating the computational results [37]. The method has been extended to antiproton-atom collisions as well [38, 39].

The recent single-centre CCC calculations of positron scattering on molecular hydrogen by Zammit *et al.* [40] and antiproton collisions with H₂ by Abdurakhmanov *et al.* [41, 42] have shown that the CCC formalism can also be successfully applied to molecular targets. A limitation of the single-center approach to positron scattering, however, is that Ps formation is not included explicitly, but rather via positive-energy atomic pseudostates

with large angular momenta. This works well at energies below the Ps-formation threshold, and at energies above the ionization threshold with the limitation that the direct ionization and Ps-formation channels are inseparable. Furthermore, over the small energy range between the two thresholds it is formally invalid due to no allowance for positron flux into Ps-formation channels. The two-center approach, on the other hand, does explicitly include Ps-formation channels, and hence yields Ps-formation as well as direct-ionization cross sections, and is valid at all energies.

II. METHOD

In Figure 1 we present the coordinate system we use for positron-H₂ scattering, with the origin being at the center of mass, i.e. at the midpoint between the two protons. Vectors \mathbf{r}_0 , \mathbf{r}_1 , and \mathbf{r}_2 denote the positions of the positron, electron 1 and electron 2, respectively. To describe Ps-formation channels it is convenient to use Jacobi coordinates $(\mathbf{R}, \boldsymbol{\rho})$, where $\mathbf{R} = (\mathbf{r}_0 + \mathbf{r}_1)/2$ is the position of the Ps center of mass (c.m.) relative to the H₂ origin, and $\boldsymbol{\rho} = \mathbf{r}_0 - \mathbf{r}_1$ is the relative coordinate of the positron and electron. We emphasize that since there are two electrons which can form positronium, there are two corresponding sets of Jacobi coordinates. When necessary we will refer to them explicitly as $(\mathbf{R}_1, \boldsymbol{\rho}_1, \mathbf{r}_2)$ and $(\mathbf{R}_2, \boldsymbol{\rho}_2, \mathbf{r}_1)$. Fig. 1 shows one of them, where Ps is formed by electron 1. We consider H₂ within the Born-Oppenheimer approximation where the two protons are considered to be at a fixed internuclear distance denoted as d .

We are interested in relatively low-energy positron collisions, where Ps formation is significant, and therefore we can neglect the relativistic and spin-orbit interactions. For this case the scattering wave function Ψ must satisfy the Schrödinger equation

$$(H - E)\Psi(\mathbf{r}_0, \mathbf{r}_1, \mathbf{r}_2, \mathbf{d}) = 0, \quad (1)$$

where E is the total energy and H is the total Hamiltonian of the system. The Hamiltonian of the e⁺-H₂ system

can be written as

$$H = H_0 + V_e(\mathbf{r}_1, \mathbf{d}) + V_e(\mathbf{r}_2, \mathbf{d}) + 1/d + V_p(\mathbf{r}_0, \mathbf{d}) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{1}{|\mathbf{r}_0 - \mathbf{r}_1|} - \frac{1}{|\mathbf{r}_0 - \mathbf{r}_2|}, \quad (2)$$

where

$$H_0 = -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2$$

is the free Hamiltonian of the three particles, while V_e and V_p are the electron-nucleus and positron-nucleus potentials, respectively.

In this work, following the CCC approach [30], we explicitly include Ps-formation channels with the use of a two-centre expansion technique. This is done by expanding the total scattering wavefunction Ψ of the collision system in terms of the target (H_2) and positronium (Ps) states in the following way [30]:

$$\begin{aligned} \Psi \approx & \sum_{\alpha=1}^{N_\alpha} F_\alpha(\mathbf{r}_0) \psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \mathbf{d}) \\ & + \sum_{\beta=1}^{N_\beta} \{G_\beta(\mathbf{R}_1) \psi_\beta(\boldsymbol{\rho}_1) \phi_{\text{ion}}(\mathbf{r}_2, \mathbf{d}) \\ & + G_\beta(\mathbf{R}_2) \psi_\beta(\boldsymbol{\rho}_2) \phi_{\text{ion}}(\mathbf{r}_1, \mathbf{d})\}, \end{aligned} \quad (3)$$

where the first term corresponds to expansion in terms of the target wavefunctions ψ_α with expansion coefficients being F_α , while the second term corresponds to expansion in terms of the positronium states ψ_β with coefficients G_β . N_α and N_β are the number of target states and Ps states, respectively. Indices α and β are used to denote a full set of quantum numbers for the target and Ps, respectively. Basis states may contain both eigen- and pseudo-states of both the target and Ps depending on the choice. The second term allows for both active electrons to form positronium. The residual ion of H_2^+ is described by ϕ_{ion} , and we consider it to be only in its ground state.

Substituting expansion (3) into Eq. (1) we obtain a set of momentum-space coupled-channel equations for the transition matrix elements [30] (for brevity we make the \mathbf{d} -dependence implicit)

$$\begin{aligned} T_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_\gamma) = & V_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_\gamma) + \sum_{\gamma''}^{N_\alpha + N_\beta} \int \frac{d\mathbf{k}_{\gamma''}}{(2\pi)^3} \\ & \times V_{\gamma'\gamma''}(\mathbf{k}_{\gamma'}, \mathbf{k}_{\gamma''}) G_{\gamma''}(k_{\gamma''}^2) T_{\gamma''\gamma}(\mathbf{k}_{\gamma''}, \mathbf{k}_\gamma), \end{aligned} \quad (4)$$

where $\gamma = \{\alpha, \beta\}$ and \mathbf{k}_γ is the momentum of the free particle relative to the c.m. of the bound subsystem in channel γ . The effective two-body free Green's functions $G_{\gamma''}(k_{\gamma''}^2)$ are defined as:

$$G_\alpha(k_\alpha^2) = (E + i0 - k_\alpha^2/2 - \epsilon_\alpha)^{-1}, \quad (5)$$

$$G_\beta(k_\beta^2) = (E + \epsilon_{\text{ion}} + i0 - k_\beta^2/4 - \epsilon_\beta)^{-1}, \quad (6)$$

for the target and Ps channels, respectively. It describes the free relative motion of particle γ'' and bound pair γ'' with binding energy $\epsilon_{\gamma''}$. Where ϵ_{ion} is the binding energy of the H_2^+ residual ion.

The transition matrix elements $V_{\gamma'\gamma''}(\mathbf{k}_{\gamma'}, \mathbf{k}_{\gamma''})$ are defined as:

$$\begin{aligned} V_{\alpha'\alpha}(\mathbf{k}_{\alpha'}, \mathbf{k}_\alpha) &= \langle \mathbf{k}_{\alpha'} | \langle \psi_{\alpha'} | U_{\alpha'\alpha} | \psi_\alpha \rangle | \mathbf{k}_\alpha \rangle, \\ V_{\beta'\beta}(\mathbf{k}_{\beta'}, \mathbf{k}_\beta) &= \langle \mathbf{k}_{\beta'} | \langle \psi_{\beta'} \phi_{\text{ion}} | U_{\beta'\beta} | \psi_\beta \phi_{\text{ion}} \rangle | \mathbf{k}_\beta \rangle, \\ V_{\beta\alpha}(\mathbf{k}_\beta, \mathbf{k}_\alpha) &= \langle \mathbf{k}_\beta | \langle \psi_\beta \phi_{\text{ion}} | U_{\beta\alpha} | \psi_\alpha \rangle | \mathbf{k}_\alpha \rangle, \end{aligned} \quad (7)$$

where

$$\begin{aligned} U_{\alpha'\alpha} &= V_p(\mathbf{r}_0, \mathbf{d}) - \frac{1}{|\mathbf{r}_0 - \mathbf{r}_1|} - \frac{1}{|\mathbf{r}_0 - \mathbf{r}_2|}, \\ U_{\beta'\beta} &= V_p(\mathbf{r}_0, \mathbf{d}) + V_e(\mathbf{r}_1, \mathbf{d}) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{1}{|\mathbf{r}_0 - \mathbf{r}_2|}, \\ U_{\beta\alpha} &= U_{\alpha\beta} = H - E \end{aligned} \quad (8)$$

are the corresponding channel potential operators.

After performing a partial-wave expansion of the incoming and outgoing particles' plane waves $|\mathbf{k}_\gamma\rangle$, Eq. (4) is solved for each total angular-momentum projection K , spin S , and parity Π . The partial-wave expansion is performed for $V_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_\gamma)$ (and for $T_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_\gamma)$) according to

$$\begin{aligned} V_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_\gamma) &= \sum_{L', M', L, M, K} Y_{L' M'}(\hat{\mathbf{k}}_{\gamma'}) \\ &\times \mathcal{V}_{\gamma' L' M', \gamma L M}^{K S \Pi}(k_{\gamma'}, k_\gamma) Y_{L M}^*(\hat{\mathbf{k}}_\gamma), \end{aligned} \quad (9)$$

where $Y_{LM}(\hat{\mathbf{k}}_\gamma)$ are the spherical harmonics of unit vector $\hat{\mathbf{k}}_\gamma$. Quantum numbers L and L' are the angular momenta of the free particles in channels γ and γ' , and M and M' are their projections, respectively. Note that the total angular momentum projection is $K = M + m = M' + m'$ (we set \mathbf{d} to be the axis of quantization in all channels). Here m and m' are the angular momentum

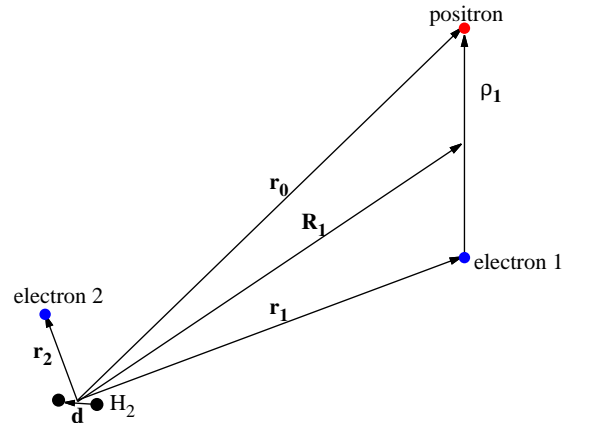


FIG. 1. (Color online) Coordinate system for e^+ - H_2 collision.

projections of the target molecule or Ps in channels γ and γ' . The effective potentials in partial waves are given by

$$\begin{aligned} \mathcal{V}_{\gamma'L'M',\gamma LM}^{K\Sigma\Pi}(k_{\gamma'}, k_{\gamma}) &= \delta_{K,M+m} \iint d\hat{\mathbf{k}}_{\gamma'} d\hat{\mathbf{k}}_{\gamma} Y_{L'M'}^*(\hat{\mathbf{k}}_{\gamma'}) \\ &\quad \times V_{\gamma'\gamma}(\mathbf{k}_{\gamma'}, \mathbf{k}_{\gamma}) Y_{LM}(\hat{\mathbf{k}}_{\gamma}). \end{aligned} \quad (10)$$

Expansion (9) transforms equation (4) into

$$\begin{aligned} \mathcal{T}_{\gamma'L'M',\gamma LM}^{K\Sigma\Pi}(k_{\gamma'}, k_{\gamma}) &= \mathcal{V}_{\gamma'L'M',\gamma LM}^{K\Sigma\Pi}(k_{\gamma'}, k_{\gamma}) \\ &\quad + \sum_{\gamma''}^{N_{\alpha}+N_{\beta}} \sum_{L''} \int \frac{dk_{\gamma''}}{(2\pi)^3} k_{\gamma''}^2 \\ &\quad \times \mathcal{V}_{\gamma'L'M',\gamma L''M''}^{K\Sigma\Pi}(k_{\gamma'}, k_{\gamma''}) \\ &\quad \times G_{\gamma''}(k_{\gamma''}^2) \\ &\quad \times \mathcal{T}_{\gamma''L''M'',\gamma LM}^{K\Sigma\Pi}(k_{\gamma''}, k_{\gamma}), \end{aligned} \quad (11)$$

where L'' is the angular momentum of the free particle in channel γ'' .

In the present work we only use a few Ps eigenstates so as to take advantage of their analytical form. The target states are obtained by diagonalizing the H_2 Hamiltonian in a set of antisymmetrized two-electron configurations, built from Laguerre one-electron orbitals, for each target symmetry characterized by the projection of orbital angular momentum m_T , parity π_T , and spin s_T . This results in a set of square-integrable negative and positive energy pseudostates. With increasing of the basis sizes, the negative-energy states converge towards the true eigenstates, while the positive energy pseudostates become increasingly dense in energy, and effectively represent the target continuum. To calculate H_2 states, we adopt the fixed-nuclei approximation and perform calculations at the ground-state equilibrium internuclei distance, which is $d = 1.4 a_0$. Note that when d is set to 0 one should obtain the He results. We used this test for both structure and scattering calculations. Details of H_2 structure calculations can be found in [40].

The derivation of the rearrangement matrix elements are similar to the He case. However, algebra is somewhat more difficult because of nuclear separation and target orientation dependency. Another difference is that partial wave expansion is done over the total angular momentum projection K . By choosing the z-axis to be along the \mathbf{d} (body-frame) we can write the electron interaction with the nuclei as

$$\begin{aligned} V_e(\mathbf{r}, \mathbf{d}) &= -\frac{1}{|\mathbf{r} - \mathbf{d}/2|} - \frac{1}{|\mathbf{r} + \mathbf{d}/2|} \\ &= \sqrt{4\pi} \sum_{\lambda=0}^{\infty} (1 + (-1)^{\lambda}) \sqrt{2\lambda+1} \frac{r_{>}^{\lambda}}{r_{>}^{\lambda+1}} Y_{\lambda 0}(\hat{r}), \end{aligned} \quad (12)$$

where $r_{>} = \max\{r, d/2\}$. It is possible to transform the obtained results with this choice of z-axis to any given orientation of the molecule.

For simplicity, we consider only the spherical part of the nuclear potential when calculating the rearrangement matrix elements:

$$V_p(\mathbf{r}_0, \mathbf{d}) = \frac{1}{|\mathbf{r}_0 - \mathbf{d}/2|} + \frac{1}{|\mathbf{r}_0 + \mathbf{d}/2|} \approx \frac{2}{r_{>}} \quad (13)$$

where now $r_{>} = \max\{r_0, d/2\}$. Then the momentum space representation of the above positron-nucleus potential can be shown to be

$$\bar{V}_p(p) = \frac{4\pi^2 \sin(dp)}{dp^3}. \quad (14)$$

With these we further follow the procedure used for positron-He calculations [33].

For positron scattering from the ground state of H_2 only states with zero total spin are required and so $S = 1/2$. T -matrix elements are used to obtain body-frame scattering amplitudes $f_{fi}^{(B)}$, which are then transformed to lab-frame scattering amplitudes $f_{fi}^{(L)}$ via rotation by Euler angles. Orientationally-independent cross sections are calculated by averaging over all rotations of the molecule [43]. An orientationally averaged analytic Born subtraction method [43] is employed for H_2 direct transition channels to reduce the number of partial waves requiring explicit solution.

III. RESULTS

In the present work we calculate various cross sections for $e^+ - \text{H}_2$ scattering using the two-center CCC method. The direct ionization cross section is obtained by simply summing the individual cross sections for excitation to the positive-energy pseudostates of the target. The direct ionization combined with Ps-formation cross sections give the total electron-loss cross sections, which can also be calculated by the single centre CCC approach, but only above the ionization threshold. Combination of the total electron-loss, excitation and elastic scattering cross sections give the grand total cross section.

Generally, resulting cross sections should be checked for the convergence by increasing the basis sizes for both target and Ps centres. However, calculation of rearrangement matrix elements for positron- H_2 scattering are computationally very expensive. Therefore in this work we use a complete set of states only in the target space and restrict Ps to a few low-lying eigenstates. This type of calculation is an initial test of the method, which should still give reasonably accurate Ps-formation cross sections. This is because in the low energy region, where most of the experimental data is available, the main contribution to Ps formation comes from the ground and the lowest lying excited states of Ps. In addition, we don't consider the elastic scattering region below the Ps-formation threshold which was very accurately calculated by the single-centre CCC method [40].

To simplify scattering calculations we make three approximations. First, we assume that the H_2^+ ion remains

in its ground state in the Ps-formation channels. Second, we neglect electron exchange between Ps and the residual H_2^+ ion. These two approximations have previously been used in calculations of positron scattering on helium [33] and magnesium [32], yielding good results. Lastly, we consider only the spherical part of the nuclear potential when calculating the rearrangement matrix elements. However, it is difficult to estimate the quality of this approximation and we have to rely on agreement of the final result with experiment.

To test convergence of the results we performed calculations with three different basis sizes. The corresponding results are denoted as $CCC(N_{l_{\max}}, N_{Ps})$, where for $l \leq l_{\max}$, $N - l$ one-electron orbitals will be used in generating the H_2 target structure, and N_{Ps} is the number of Ps-eigenstates. For example, the $CCC(14_2,3)$ calculation utilizes 14 s , 13 p and 12 d -orbitals, which generates 139 H_2 states. It also includes the three $1s$, $2s$, and $2p$ Ps-states.

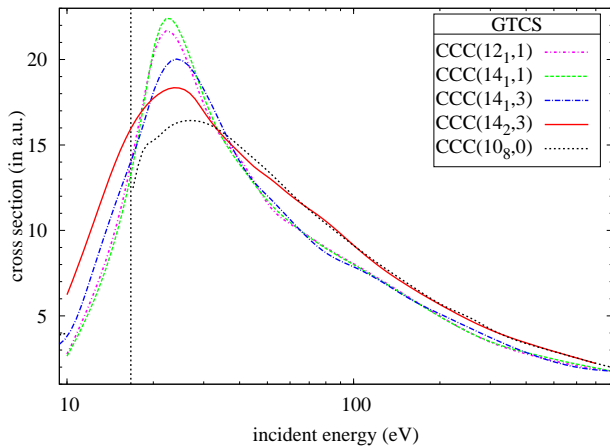


FIG. 2. (Color online) The grand total cross section (GTCS) for $e^+ - H_2$ scattering calculated with different basis sizes. The single centre $CCC(10_8,0)$ results of Zammit *et al.* [40] are only valid above the direct ionization threshold indicated by the vertical line.

Fig. 2 shows the grand total cross section (GTCS) for $e^+ - H_2$ scattering calculated with different bases. We have also presented the single-centre CCC results [40]. Comparison between the $CCC(12_1,1)$ and the $CCC(14_1,1)$ calculations shows the level of convergence with regards to N_{\max} . In the remaining figures we concentrate on effects of including more Ps-states and H_2 states with larger angular momentum and keep N_{\max} fixed at 14. It can be seen that the results $CCC(14_1,1)$ and $CCC(14_1,3)$ are close to each other indicating that having three Ps states is sufficient to take into account Ps-formation channels within reasonable accuracy, however, both results are below the single centre CCC results at higher energies. With additional 12 d -orbitals included in H_2 we obtained cross sections converging to the single-centre CCC results above the ionization threshold. This shows that $CCC(14_2,3)$ contains enough target and

Ps states to give convergent GTCS. It is worth noting that the two-centre method can achieve convergence at a much faster rate compared to the single centre method. The single centre calculations of Zammit *et al.* [40] contain 556 target states with orbital angular momenta up to eight. In this work, the two centre $CCC(14_2,3)$ contains only three Ps eigenstates and 139 target states with maximum orbital angular momenta equal to 2. As has been discussed before [30, 33], the reason for the slow convergence in the single-centre method is the absence of explicit boundary conditions for Ps-formation channels. By including higher angular momenta orbitals, a single-centre method can indirectly take into account Ps-formation channels via excitations to positive energy pseudostates with high angular momenta. However, at energies just above the ionization threshold convergence requires large $N_{l_{\max}}$. Outside this region the agreement between the single- and two-center approaches is excellent.

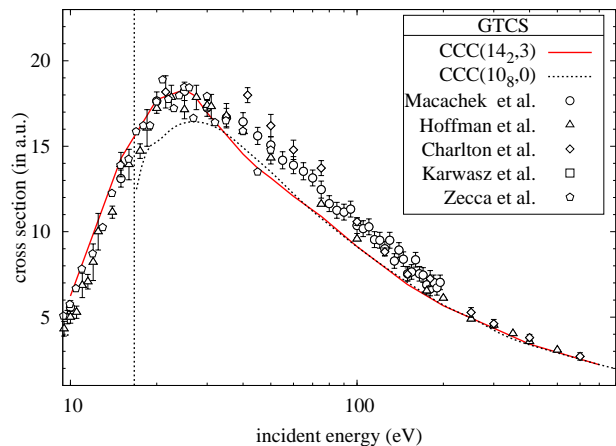


FIG. 3. (Color online) The grand total cross section for (GTCS) $e^+ - H_2$. Experimental data are due to Machacek *et al.* [14], Hoffman *et al.* [1], Charlton *et al.* [2], Karwasz *et al.* [12] and Zecca *et al.* [13]). The single centre results are due to Zammit *et al.* [40]. The present calculations are described in the text.

In Fig. 3 we compare our results with the available experimental data for GTCS. As was mentioned earlier we are concentrating only on the energy range above the Ps-formation threshold. Starting from the threshold the two-centre results agree very well with the experimental data. Above 30 eV the single-centre and two-centre results are almost indistinguishable. This is an important demonstration of internal consistency of the CCC approach to such collisions. It is far from trivial because the explicit Ps-formation component can be quite large.

Fig. 4 presents the Ps-formation cross sections, which in the region near the maximum are as much as 50% of the GTCS. Our results obtained with different bases are compared with the experimental data of Zhou *et al.* [10], Fromme *et al.* [6] and Machacek *et al.* [14]. $CCC(14_1,1)$ underestimates experimental measurements. Adding two

more Ps states brings the Ps-formation cross section up to agree better with the experimental data. When d -orbitals are added to the H_2 basis the maximum of the Ps-formation cross section drops by about 10%. There is generally good agreement between different sets of experimental data. However, our results underestimate ex-

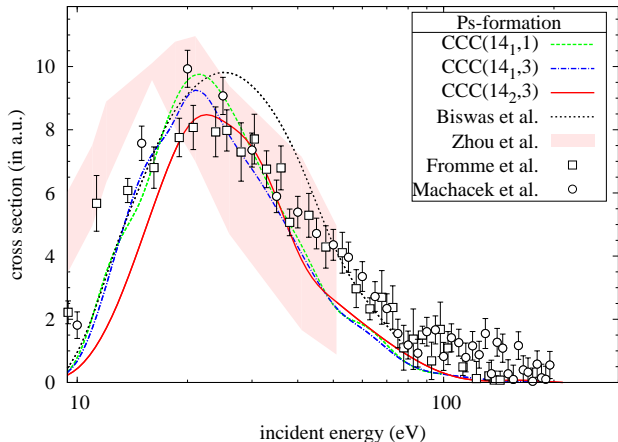


FIG. 4. (Color online) The Ps-formation cross section in $e^+ - H_2$ collisions. Experimental data are due to Zhou *et al.* [10], Fromme *et al.* [6] and Machacek *et al.* [14]. The present calculations are described in the text. Coupled static model calculations of Biswas *et al.* [20] are also shown.

perimental cross sections above 50 eV. We suspect that at these energies there will be a substantial contribution from Ps-formation in higher excited states, which is missing from the present calculations.

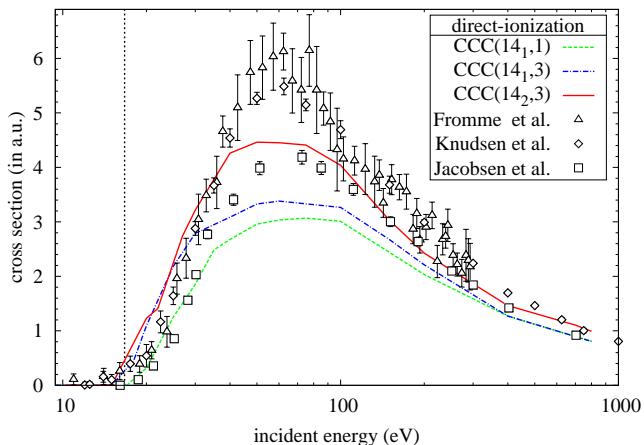


FIG. 5. (Color online) The total direct ionization cross sections for $e^+ - H_2$ collisions. Experimental data are due to Fromme *et al.* [6], Knudsen *et al.* [7] and Jacobsen *et al.* [9]. The theoretical results are described in the text.

In Fig. 5 we compare our results for the direct total ionization cross section (TICS) with the available experimental data. The experimental data of Fromme *et al.* [6] and Knudsen *et al.* [7] are in agreement with each other

but differ from measurements of Jacobsen *et al.* [9] between 30 and 100 eV. CCC(14_{2,3}) is in better agreement with the measurements of Jacobsen *et al.* [9]. CCC(14_{1,1}) and CCC(14_{1,3}) underestimate both sets of experimental data. As far as we are aware the present results are the first theoretical calculations for this process.

The total electron-loss cross section is given in Fig. 6. In the two-centre method they are calculated as a sum of TICS and Ps-formation cross sections. In the single-centre formalism it is just a sum of all cross sections for excitations to positive-energy pseudo-states. Perfect internal consistency would require agreement here between the two methods above the ionization threshold. In practice this is impossible near the threshold because we would require a massive basis expansion in the single center approach which should behave like a step-function: zero below threshold and all of Ps-formation immediately after. Also, at energies above 30 eV the lack of higher Ps states in the two-center approach explains the visible discrepancy. CCC(14_{2,3}) results are in reasonable agreement with experimental data up to 30 eV. Above 30 eV they underestimate both the experimental data and the single-centre results.

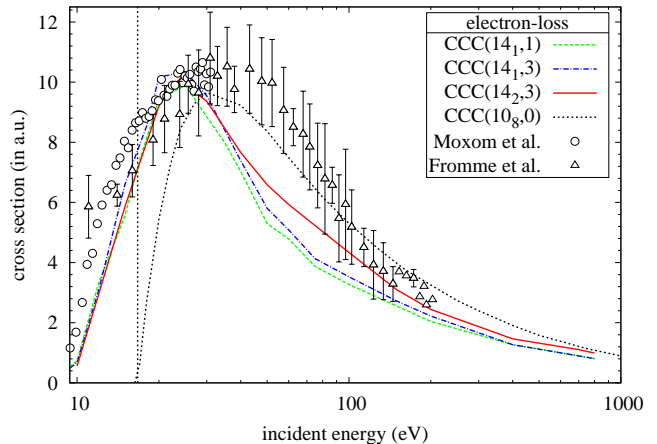


FIG. 6. (Color online) The total electron-loss cross section for $e^+ - H_2$ collisions. Experimental data are due to Moxom *et al.* [8] and Fromme *et al.* [6]. The theoretical calculations are described in the text.

IV. CONCLUSION

In conclusion, we have developed a two-centre close-coupling approach to $e^+ - H_2$ scattering including Ps-formation channels and presented orientation-averaged results for the grand total, Ps-formation, direct ionization and total electron loss cross sections. All channels have been treated within the fixed-nuclei approximation. In addition, three approximations have been used to facilitate the calculations of the Ps-formation channels. We assumed that the residual H_2^+ ion remained in its ground

state in the Ps-formation channels and neglected electron exchange between Ps and the residual H_2^+ ion. We also considered only the spherical part of the nuclear potential when calculating the rearrangement matrix elements. While the first 2 approximations are believed to be reliable, it is difficult to estimate the impact of the third one. However, the obtained results are generally in good agreement with experimental data, indicating that, in particular, the spherical part is the main contributor to the nuclear potential. In the future, we plan to remove some of the aforementioned approximations. Due to time-consuming calculations of the rearrangement amplitudes we have included only a few low-lying eigenstates

for the Ps centre. We plan to investigate more efficient ways of calculating Ps-formation matrix elements in order to be able to include Ps pseudostates as well. We also aim to apply the method to other diatomic molecules.

ACKNOWLEDGMENTS

The authors acknowledge the support of the Australian Research Council, the National Computing Infrastructure, and The Pawsey Supercomputer Center. A.S.K. acknowledges partial support from the US National Science Foundation under Award No. PHY-1415656.

-
- [1] K. R. Hoffman, M. S. Dababneh, Y. F. Hsieh, W. E. Kauppila, V. Pol, J. H. Smart, and T. S. Stein, *Phys. Rev. A* **25**, 1393 (1982).
- [2] M. Charlton, T. C. Griffith, G. R. Heyland, and G. L. Wright, *J. Phys. B* **16**, 323 (1983).
- [3] L. S. Fornari, L. M. Diana, and P. G. Coleman, *Phys. Rev. Lett.* **51**, 2276 (1983).
- [4] T. G. Griffith, in *Positron scattering in gases*, edited by J. W. Humberston and M. R. C. McDowell (Plenum Press, New York, 1984) pp. 53–63.
- [5] L. M. Diana, P. G. Coleman, D. L. Brooks, and P. K. Pendleton, *Phys. Rev. A* **34**, 2731 (1986).
- [6] D. Fromme, G. Kruse, W. Raith, and G. Sinapius, *J. Phys. B* **21**, L261 (1988).
- [7] H. Knudsen, L. Brun-Nielsen, M. Charlton, and M. R. Poulsen, *J. Phys. B* **23**, 3955 (1990).
- [8] J. Moxom, G. Laricchia, and M. Charlton, *J. Phys. B* **26**, L367 (1993).
- [9] F. M. Jacobsen, N. P. Frandsen, H. Knudsen, and U. Mikkelsen, *J. Phys. B* **28**, 4675 (1995).
- [10] S. Zhou, H. Li, W. E. Kauppila, C. K. Kwan, and T. S. Stein, *Phys. Rev. A* **55**, 361 (1997).
- [11] J. P. Sullivan, S. J. Gilbert, J. P. Marler, L. D. Barnes, S. J. Buckman, and C. M. Surko, *Nucl. Instr. and Meth. B* **192**, 3 (2002).
- [12] G. P. Karwasz, D. Pliszka, and R. S. Brusa, *Nucl. Instr. and Meth. B* **68**, 68 (2006).
- [13] A. Zecca, L. Chiari, A. Sarkar, K. L. Nixon, and M. J. Brunger, *Phys. Rev. A* **80**, 032702 (2009).
- [14] J. R. Machacek, E. K. Anderson, C. Makochekanwa, S. J. Buckman, and J. P. Sullivan, *Phys. Rev. A* **88**, 042715 (2013).
- [15] D. P. Sural and S. C. Mukherjee, *Physica* **49**, 249 (1991).
- [16] R. R. Bussard R W and D. R. J, *Astrophysical Journal* **228**, 928 (1979).
- [17] A. Ray, P. P. Ray, and B. C. Saha, *Journal of Physics B: Atomic and Molecular Physics* **13**, 4509 (1980).
- [18] G. Danby and J. Tennyson, *J. Phys. B* **23**, 1005 (1990).
- [19] E. A. G. Armour and J. W. Humberston, *Phys. Rep.* **204**, 165 (1991).
- [20] P. K. Biswas, T. Mukherjee, and A. S. Ghosh, *J. Phys. B* **24**, 2601 (1991).
- [21] P. K. Biswas, M. Basu, A. S. Ghosh, and J. W. Darewych, *J. Phys. B* **24**, 3507 (1991).
- [22] D. D. Reid, W. B. Klann, and J. M. Wadehra, *Phys. Rev. A* **70**, 062714 (2004).
- [23] F. Arretche, R. da Costa, S. d’A. Sanchez, A. Hisi, E. de Oliveira, M. do N. Varella, and M. Lima, *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **247**, 13 (2006), proceedings of the XIII International Workshop on Low-Energy Positron and Positronium Physics.
- [24] S. d. A. Sanchez and M. A. P. Lima, *Nucl. Instr. and Meth. B* **266**, 447 (2008).
- [25] T. Mukherjee and N. K. Sarkar, *J. Phys. B* **41**, 125201 (2008).
- [26] R. Zhang, K. L. Baluja, J. Franz, and J. Tennyson, *J. Phys. B* **44**, 035203 (2011).
- [27] W. Tenfen, K. T. Mazon, S. E. Michelin, and F. Arretche, *Phys. Rev. A* **86**, 042706 (2012).
- [28] C. M. Surko, G. F. Gribakin, and S. J. Buckman, *J. Phys. B* **38**, R57 (2005).
- [29] I. Bray and A. T. Stelbovics, *Phys. Rev. A* **46**, 6995 (1992).
- [30] A. S. Kadyrov and I. Bray, *Phys. Rev. A* **66**, 012710 (2002).
- [31] I. Bray, D. V. Fursa, A. S. Kadyrov, A. T. Stelbovics, A. S. Kheifets, and A. M. Mukhamedzhanov, *Phys. Rep.* **520**, 135 (2012).
- [32] R. Utamuratov, D. V. Fursa, A. S. Kadyrov, A. V. Lugovskoy, J. S. Savage, and I. Bray, *Phys. Rev. A* **86**, 062702 (2012).
- [33] R. Utamuratov, A. S. Kadyrov, D. V. Fursa, I. Bray, and A. T. Stelbovics, *J. Phys. B* **43**, 125203 (2010).
- [34] A. V. Lugovskoy, A. S. Kadyrov, I. Bray, and A. T. Stelbovics, *Phys. Rev. A* **85**, 034701 (2012).
- [35] A. S. Kadyrov, A. V. Lugovskoy, R. Utamuratov, and I. Bray, *Phys. Rev. A* **87**, 060701 (2013).
- [36] A. S. Kadyrov, C. M. Rawlins, A. T. Stelbovics, I. Bray, and M. Charlton, *Phys. Rev. Lett.* **114**, 183201 (2015).
- [37] J. J. Bailey, A. S. Kadyrov, and I. Bray, *Phys. Rev. A* **91**, 012712 (2015).
- [38] I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, I. Bray, and A. T. Stelbovics, *Phys. Rev. A* **84**, 062708 (2011).
- [39] I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, S. K. Avazbaev, J. J. Bailey, and I. Bray, *Phys. Rev. A* **91**, 022712 (2015).

- [40] M. C. Zammit, D. V. Fursa, and I. Bray, Phys. Rev. A **87**, 020701 (2013).
- [41] I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray, Phys. Rev. Lett. **111**, 173201 (2013).
- [42] I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, S. K. Avazbaev, and I. Bray, Phys. Rev. A **89**, 042706 (2014).
- [43] W. A. Isaacs and M. A. Morrison, Phys. Rev. A **53**, 4215 (1996).