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Convergent calculations of positron scattering from molecular hydrogen

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Abstract. An overview is given of the recently developed adiabatic-nuclei convergent close-coupling method for positron-molecule scattering. Fixed-nuclei single-centre calculations of positron-H_2 scattering are presented. Particular emphasis is given to demonstrating convergence with increasing size of the basis and the projectile partial-wave expansion. Results are converged to within $\pm 5\%$.

1. Introduction

Theoretical formulations of electron and positron collisions with molecules are often based on techniques developed for electron-atom scattering. Molecules, however, have the complexity of multi-centre potentials which leads to absence of spherical symmetry. In addition the rotational and vibrational degrees of freedom add to the complexity of scattering processes. *Ab initio* theoretical treatments of positron scattering are even more difficult than electron scattering. This is due to the strong electron-positron correlations and the additional channel of positronium (Ps) formation.

Over the last two decades the *ab initio* convergent close-coupling (CCC) method has had considerable success describing electron, positron and photon collisions with atoms and ions [1, 2, 3]. The CCC method was first developed to study electron collisions with atomic hydrogen and helium [4, 5], and then subsequently many more complex heavy atoms and ions (e.g. Hg, Ba, Cd) [6, 7, 8]. It is a complete scattering theory in the sense that it yields accurate elastic, excitation and ionisation cross sections irrespective of projectile-energy [9, 10, 11]. The strength of the method is in its ability to account for coupling to ionisation channels [4], to treat large close-coupling expansions and to demonstrate convergent results (accurate to within numerical accuracy approximately less than 5%) by increasing the size of the close-coupling (target state) expansion. The CCC method solves the coupled Lippmann-Schwinger equations in momentum space for the T-matrix. Ionisation channels are included into the close-coupling expansion via positive-energy target pseudostates. Pseudostates are obtained from diagonalisation of the target Hamiltonian using a complete Sturmian Laguerre basis. Our long term goal is to develop a complete scattering method for molecules.

As a first step we have recently developed the adiabatic-nuclei CCC method for molecules [12] and performed calculations of electron scattering from H_2^+ [12, 13] and positron scattering from H_2 [14]. In general these results are in good agreement with experiment and the method carries the same fundamental strengths as the atomic CCC method.

Non-perturbative scattering methods are based on solving the Schrödinger equation using either grid based techniques or a close-coupling expansion. For molecules these methods include the Schwinger multichannel [15], Kohn variational [16], molecular R-matrix with pseudostates [17], time-dependent close-coupling [18] and molecular CCC [12] methods. In order to rigorously test a scattering calculation one has to demonstrate convergence of results. In general to demonstrate convergence of a calculation, one must check the size of the close-coupling (target state) expansion, the accuracy of the target structure model, the size of the projectile-partial wave expansion and the density and size of grids used. Convergence of results is also dependent on the projectile impact-energy and scattering process of interest. In general it is easier to achieve convergent results of major scattering processes (total, elastic and ionisation cross sections). Note that convergent results are only accurate to within numerical accuracy, which is approximately less than $\pm 5\%$. The first truly convergent results of positron-molecule scattering were obtained by Zhang *et al*. [19], who accurately calculated the scattering length and Z-effective of positron-H_2 at zero energy [19, 20]. A number of R-matrix with pseudostates studies [21, 22, 23, 24] have performed convergence studies for both electron- and positron-molecule scattering. However as far as we are aware convergence has not been demonstrated for electron- or positron-molecule scattering results over a wide range of energies, even for the major scattering processes.

Here we demonstrate convergence of our latest CCC results over a broad energy range for positron scattering from H_2 in the fixed-nuclei approximation. Note that our preliminary results [14] only demonstrated convergence in the maximum orbital angular momentum $l_{\max}$ of the basis.

2. Convergence studies using the convergent close-coupling method

We are interested in obtaining convergent fixed-nuclei integrated cross sections $\sigma^S_{f,i}(R)$ for a transition from an initial state i to some final state f

$$\sigma^S_{f,i}(R) = (2\pi)^4 \frac{q_f}{q_i} \int d\hat{q}_f \left| \langle \boldsymbol{q}_f^{(-)} \Phi_f^N | V | \Psi_i^{SN(+)} \rangle \right|^2, \tag{1}$$

where S is the total spin of the scattering system, R is the fixed internuclear distance, $\langle \boldsymbol{q}_f^{(-)} \Phi_f^N | V | \Psi_i^{SN(+)} \rangle \equiv \langle \boldsymbol{q}_f^{(-)} \Phi_f^N | T^{SN} | \Phi_i^N \boldsymbol{q}_i^{(+)} \rangle$ in the Lab-frame, q is the linear momentum of the projectile, $|\Phi^N\rangle$ are the target pseudostates and $|\boldsymbol{q}^{(\pm)}\rangle$ refers to the projectile wave function, either a Coulomb-wave for an ionic target or a plane-wave for a neutral target. In the CCC method we perform a Body-frame close-coupling expansion of the total scattering wave function $|\Psi_i^{SN(+)}\rangle$ and solve for the T-matrix $\langle \boldsymbol{q}_f^{(-)} \Phi_f^N | T^{SN} | \Phi_i^N \boldsymbol{q}_i^{(+)} \rangle$, which is subsequently transformed to the Lab-frame. Transformation from the Body-frame T-matrix to the Lab-frame is detailed by Lane [25].

2.1. Convergence with the number of states

Referring to Eq. (1) integrated cross sections are dependent upon $|\Psi_i^{SN(+)}\rangle$. CCC calculations obtain convergence in $|\Psi_i^{SN(+)}\rangle$ and hence $\sigma^S_{f,i}(R)$ by increasing the number of target pseudostates N in the Body-frame fixed-nuclei multichannel expansion

$$\Psi_i^{SN(+)}(\mathbf{x}_0, \mathbf{x}; R) = \mathcal{A} \sum_{n=1}^{N} f_{n,i}^{SN(+)}(\mathbf{x}_0; R) \Phi_n^N(\mathbf{x}; R), \tag{2}$$

where $\mathcal{A}$ is the antisymmetrisation operator (in the case of electron scattering), $\mathbf{x}_0$ is spatial and spin coordinates of the projectile and $\mathbf{x}$ is collectively all target electronic spatial and

spin coordinates. Convergence is possible because target pseudostates radial functions are constructed from a complete Laguerre basis such that

$$\lim_{N\to\infty} \Psi_i^{SN(+)}(\mathbf{x}_0, \mathbf{x}; R) = \Psi_i^{S(+)}(\mathbf{x}_0, \mathbf{x}; R). \tag{3}$$

Laguerre basis functions are square-integrable and have the form

$$\varphi_{kl}(r) \;=\; \sqrt{\frac{\alpha_l (k-1)!}{(k+l)(k+2l)!}} (2\alpha_l r)^{l+1} \exp\left(-\alpha_l r\right) L_{k-1}^{2l+1}(2\alpha_l r), \tag{4}$$

where α_l is the exponential fall-off parameter, L_{k-1}^{2l+1} are the associated Laguerre polynomials and k ranges from 1 to N_l. A converged calculation must have a sufficiently accurate structure model and be converged with respect to the Laguerre basis size: N_l Laguerre basis functions for each orbital angular momentum l up to the maximum orbital angular momentum $l_{\max}$. As an example for H_2^+, a Laguerre basis of size N_l, $l_{\max}$ generates $N = \sum_{l=0}^{l_{\max}} (2l+1) N_l$ pseudostates.

2.2. Convergence of the partial-wave expansion

In the CCC method a partial-wave expansion of the projectile wave function allows the three-dimensional Lippmann-Schwinger equation to be solved in effectively one-dimension. The partial-wave expansion of the Body-frame physical T-matrix for an incident electron with orbital angular momentum L_i and orbital angular projection M_i has the form

$$\begin{aligned}\langle \boldsymbol{q}_f^{(-)} \Phi_f^N | T^{SN} | \Phi_i^N \boldsymbol{q}_i^{(+)} \rangle = (q_f q_i)^{-1} \sum_{\substack{L_f, L_i \\ M_f, M_i}} i^{L_i - L_f} e^{i(\sigma_{L_i} + \sigma_{L_f})} \\ \times T^{M\Pi S}_{f L_f M_f, i L_i M_i}(q_f, q_i; R) Y_{L_f M_f}(\hat{\boldsymbol{q}}_f^{(\mathrm{B})}) Y^*_{L_i M_i}(\hat{\boldsymbol{q}}_i^{(\mathrm{B})}),\end{aligned} \tag{5}$$

where σ_L is the Coulomb phase shift (for Coulomb waves), $T^{M\Pi S}_{f L_f M_f, i L_i M_i}(q_f, q_i; R)$ are the partial-wave T-matrix elements with total orbital angular projection $M = M_f + m_f = m_i + M_i$, total parity $\Pi = \pi_f (-1)^{L_f} = \pi_i (-1)^{L_i}$ and $\hat{\boldsymbol{q}}^{(\mathrm{B})}$ refers to the electron momentum vector in the Body-frame. Note that target states of diatomic molecules are characterised by their orbital angular momentum projection m and parity π. Referring to Eq. (1) integrated cross sections are dependent upon the Lab-frame T-matrix and hence the size of partial-wave expansion used. CCC calculations can only be performed for a partial-wave expansion of limited size. The size of the projectile partial-wave expansion is set by its maximum orbital angular momentum $L_{\max}$ and maximum orbital angular projection $M_{\max}$.

To complete the expansion and save on computational resources an analytic Born subtraction method is utilised

$$\sigma_{f,i}^S = \sum_{M\Pi} (\sigma_{f,i}^{M\Pi S} - \tilde{\sigma}_{f,i}^{M\Pi}) + \sigma_{f,i}^{\mathrm{AB}}. \tag{6}$$

Here $\sigma_{f,i}^{M\Pi S}$ is the orientationally averaged fixed-nuclei partial-wave integrated cross section, $\tilde{\sigma}_{f,i}^{M\Pi}$ is the orientationally averaged partial-wave Born integrated cross section and $\sigma_{f,i}^{\mathrm{AB}}$ is the orientationally averaged analytic Born integrated cross section, see Ref. [12] for details. Because of the lack of spherical symmetry in the positron/electron-nuclear potential, all orbital angular momentum of the projectile partial waves are coupled and the number of channels and scattering calculation size increases dramatically with increasing $L_{\max}$. The value of $M_{\max}$ also determines the number of channels, where calculations are run independently for each value of total orbital angular projection M, which ranges from $-M_{\max} - |m_i| \le M \le M_{\max} + |m_i|$. Hence by utilising a projectile partial-wave expansion calculations need to be checked for convergence in $L_{\max}$ and $M_{\max}$.

2.3. Convergence of grids

The CCC calculations require a sufficiently large and dense radial grid to accurately calculate V-matrix elements and a momentum quadrature (k-grid) grid to accurately integrate the off-shell integral in the Lippmann-Schwinger equation. Radial grids are checked within the analytic and partial-wave first Born approximations. To check the momentum quadrature grid, several calculations with different momentum quadrature grids are tried until a stable result is obtained. The following identity can also be checked to determine the approximate number of momentum quadrature points required

$$1 = \int_0^\infty d^3q \langle \Phi_n | \boldsymbol{q} \rangle \langle \boldsymbol{q} | \Phi_n \rangle. \tag{7}$$

For more details on the momentum quadrature grid see Ref. [4].

3. Convergence studies of positron-H_2 scattering

Target states of H_2 are described via the configuration-interaction (CI) expansion, which allows for an expansion over the two electrons $(n_0 l_0 m_0, n' l' m')$. In the present model all configurations of $n_0 \leq 3$, $n' \leq 3$ and $|m_0 + m'| \leq 1$ are built into the structure model. All other configurations are of frozen-core type $(1s\sigma_g, n' l' m')$, which primarily model the target continuum. The structure model chosen here represents the "inner" electron $(n_0 l_0 m_0)$ and "outer" electron $(n' l' m')$ by one-electron orbitals. For $n_0 \leq 3$ and $n' \leq 3$ short-ranged one-electron orbitals are used. The $1s\sigma_g$ orbital ($n_0 = n' = 1$) is represented by a converged (at an internuclear distance of $R_0 = 1.4\ a_0$) molecular-orbital of H_2^+. For the largest structure model used here the one-electron orbitals were constructed from a Laguerre basis that had $N_l = 17 - l$ functions up to $l = 7$ and $N_{l=8} = 10$. Hence the maximum orbital angular momentum of the basis had $l_{\max} = 8$. Diagonalising the target Hamiltonian with two-electron configurations built from this model, $N = 1013$ singlet target states were included in the scattering calculations. The maximum angular projection of these pseudostates is $m_{\max} = l_{\max} = 8$. The lowest-lying target state electronic energies of this structure model are compared with accurate calculations in Table 1. This structure model is in good agreement with accurate calculations at the equilibrium internuclear distance $R_0 = 1.4\ a_0$. The static dipole polarisability of this model is $\alpha_\parallel = 6.3775\ a_0^3$ and $\alpha_\perp = 4.6346\ a_0^3$ for the ground state, which compares well with the accurate calculations of Kolos *et al.* [26] ($\alpha_\parallel = 6.3805\ a_0^3$ and $\alpha_\perp = 4.5777\ a_0^3$). Hence this model, referred to as the 1013-state calculation, is sufficient to perform accurate scattering calculations.

For CCC calculations of positron scattering from the ground state of H_2, the total spin $S = 1/2$, odd and even parity Π and all total orbital angular projection M channels were included, where $-M_{\max} \leq M \leq M_{\max}$. Unless stated otherwise the present calculations used a projectile partial-wave expansion with maximum orbital angular momentum $L_{\max} = 8$ and maximum orbital angular projection $M_{\max} = 8$. The analytic Born subtraction method described in Eq. (6) was used to top-up results.

3.1. Convergence with the number of states

To investigate convergence with respect to the number of states, results of the 1013-state model are compared with 694- and 884-state CCC calculations at the the mean internuclear distance $R_m = 1.448\ a_0$ of H_2 vibrational ground state [20]. The 694-state calculation was produced with the same 1013-state model described above, however the one-electron orbitals were constructed from Laguerre basis functions that had maximum orbital angular momentum $l_{\max} = 6$, which produced target states with maximum orbital angular projection $m_{\max} = 6$. The 884-state model was produced with the same 1013-state model described above, except the one-electron orbitals were constructed with $N_l = 15 - l$, $l_{\max} = 8$ Laguerre basis functions.

Table 1. 1013-state model two-electron energies of singlet electronic target states of H_2 at the internuclear distance of $R_0 = 1.4$ a_0. Comparisons are made with accurate calculations [27, 28, 29, 30]. All values are in atomic units.

State	Present	Reference Energy	Reference
$X^1\Sigma_g^+$	-1.1689	-1.1745	[27]
$B^1\Sigma_u^+$	-0.7019	-0.7057	[28]
$EF^1\Sigma_g^+$	-0.6891	-0.6920	[28]
$C^1\Pi_u$	-0.6861	-0.6887	[29]
$B'^1\Sigma_u^+$	-0.6269	-0.6287	[28]
$GK^1\Sigma_g^+$	-0.6250	-0.6265	[28]
$D^1\Pi_u$	-0.6220	-0.6236	[29]
$B''^1\Sigma_u^+$	-0.5965	-0.6025	[28]
$D'^1\Pi_u$	-0.5927	-0.6002	[30]

The 694-, 884- and 1013-state grand total cross section (GTCS) and total ionisation cross section (TICS) are presented in Figs. 1 and 2 respectively. These results are practically the same and hence the 1013-state calculations are converged in the target state expansion for both the number of Laguerre basis functions N_l and maximum orbital angular momentum $l_{\max}$. The convergence of the 694- and 1013-state calculations indicate that the $l_{\max} = 6$ pseudostates model is sufficiently accurate enough to describe the long-range correlations and (virtual) Ps-formation (in the low-energy region and) above the ionisation threshold. Note that the sharp rise in the TICS just above the ionisation threshold is from the Ps-formation and direct ionisation flux captured by the open positive-energy pseudostates. Hence a larger CCC calculation is expected to have sharper TICS rise just above the ionisation threshold. CCC results presented from here onwards are calculated with the 1013-state model.

3.2. Convergence of the partial-wave expansion

Convergence of the GTCS and TICS is investigated in Figs. 3 and 4 with respect to the size of the projectile partial-wave expansion. The 1013-state CCC calculations at the fixed-nuclear distance of $R_m = 1.448$ a_0 were performed for partial-wave expansions with $L_{\max} = M_{\max} = 7$, $L_{\max} = M_{\max} = 8$ and $L_{\max} = M_{\max} = 9$, which were then topped-up using the analytic Born subtraction method. A noticeable difference is seen at the TICS peak, where the $L_{\max} = M_{\max} = 7$ cross section is approximately 2.5% and 3.8% lower than the $L_{\max} = M_{\max} = 8$ and $L_{\max} = M_{\max} = 9$ results respectively. Further investigation indicates that the incomplete coupling of the $L_{\max} = M_{\max} = 7$ partial-wave expansion to the $|m| = 8$ states is not the major contributor to this difference. The $L_{\max} = M_{\max} = 8$ and $L_{\max} = M_{\max} = 9$ GTCS maximum is within 1% of each other and the $L_{\max} = M_{\max} = 8$ and $L_{\max} = M_{\max} = 9$ TICS maximum is within 1.3% of each other. The $L_{\max} = M_{\max} = 8$ and $L_{\max} = M_{\max} = 9$ TICS and GTCS are practically the same across the entire energy-range and are therefore converged.

4. Conclusion

The 1013-state CCC results presented here for positron-H_2 scattering are converged in both the projectile partial-wave and close-coupling (target state) expansions. Convergence studies suggest that the present fixed-nuclei $R_m = 1.448$ a_0 1013-state CCC results are accurate to within 5% for the GTCS and TICS. This accuracy estimate does not include uncertainty associated with the fixed-nuclei approximation. However adiabatic-nuclei results show a very minor difference.

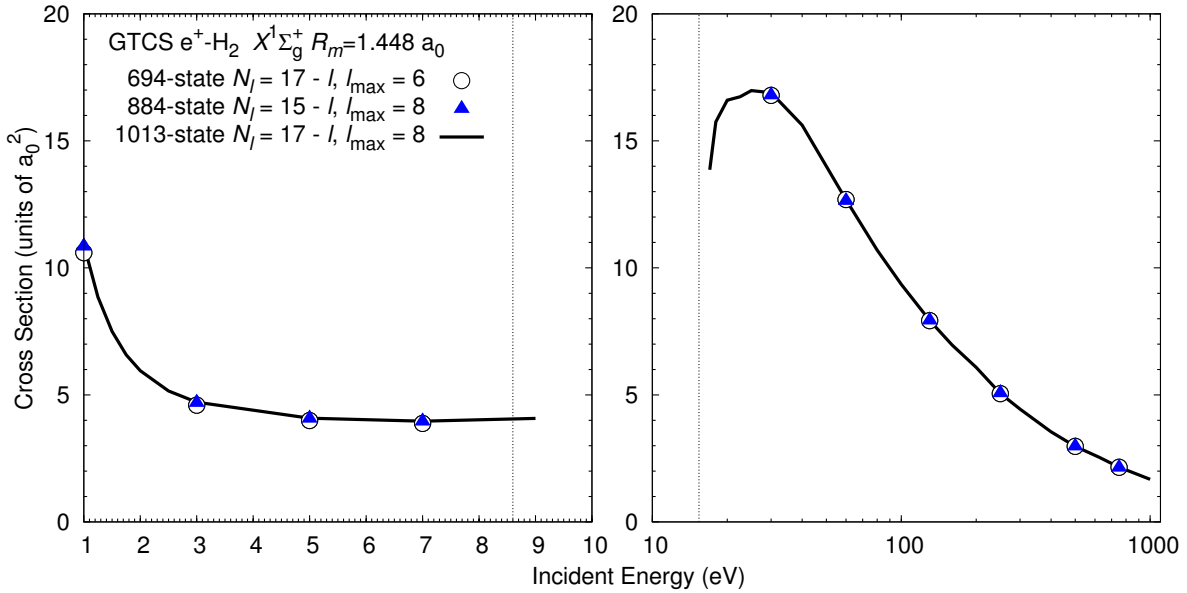

Figure 1. Convergence studies of positron scattering from H_2 at the mean vibrational ground state fixed-nuclear distance of $R_m = 1.448\ a_0$. 694-, 884- and 1013-state convergent close-coupling (CCC) calculations are presented for the grand total cross section (GTCS). A Laguerre basis with N_l functions for each orbital angular momentum l up to $l_{\max}$ is used to construct the one-electron orbitals. The dotted vertical lines at 8.6 and 15.4 eV indicate the positronium-formation and ionisation thresholds of H_2 in the ground state.

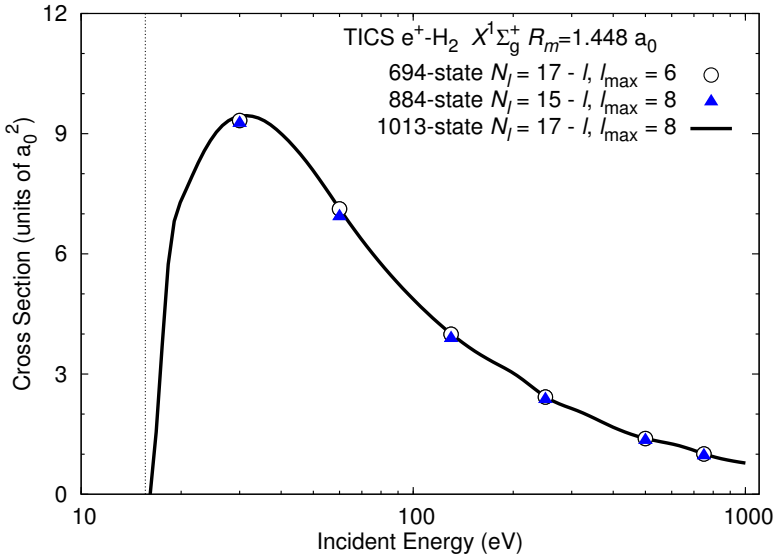

Figure 2. Convergence studies of positron scattering from H_2 at the mean vibrational ground state fixed-nuclear distance of $R_m = 1.448\ a_0$. 694-, 884- and 1013-state convergent close-coupling (CCC) calculations are presented for the total ionisation cross section (TICS). A Laguerre basis with N_l functions for each orbital angular momentum l up to $l_{\max}$ is used to construct the one-electron orbitals. The dotted vertical line at 15.4 eV indicates the ionisation threshold of H_2 in the ground state.

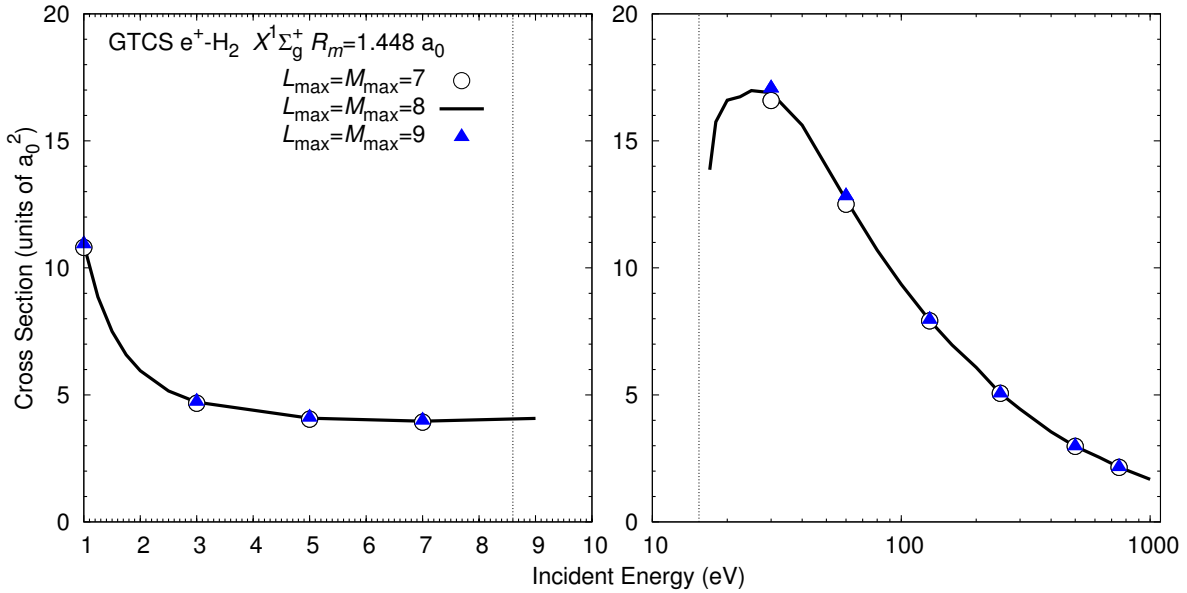

Figure 3. Convergence studies of the grand total cross section (GTCS) for positron scattering from H_2 at the mean vibrational ground state fixed-nuclear distance of $R_m = 1.448\ a_0$. 1013-state convergent close-coupling (CCC) results are calculated using a partial-wave expansion with maximum orbital angular momentum $L_{\max}$ and maximum orbital angular projection $M_{\max}$. An orientationally averaged analytic Born subtraction method is used to top-up results. The dotted vertical lines at 8.6 and 15.4 eV indicate the positronium-formation and ionisation thresholds of H_2 in the ground state.

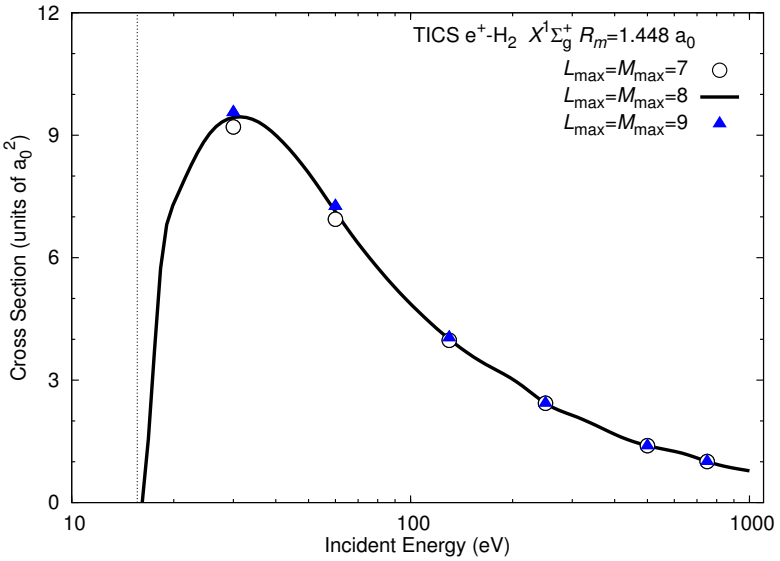

Figure 4. Convergence studies of the total ionisation cross section (TICS) for positron scattering from H_2 at the mean vibrational ground state fixed-nuclear distance of $R_m = 1.448\ a_0$. 1013-state convergent close-coupling (CCC) results are calculated using a partial-wave expansion with maximum orbital angular momentum $L_{\max}$ and maximum orbital angular projection $M_{\max}$. An orientationally averaged analytic Born subtraction method is used to top-up results. The dotted vertical line at 15.4 eV indicates the ionisation threshold of H_2 in the ground state.

Although not presented, similar convergence studies have been performed for CCC calculations of electron scattering from H_2^+ [12]. The equilibrium distance fixed-nuclei $R_0 = 2.0$ a_0 results in Ref. [12] demonstrated the same level of convergence and are estimated to be accurate to within 5% for the dissociative excitation cross section.

As a first attempt at electron- and positron-molecule CCC calculations, the method has shown great promise. Integrated cross sections for the major scattering processes are in good agreement with experiment over a broad energy-range [12, 13]. The accurate structure models used in these calculations are calculated from a complete Laguerre basis. Achieving convergent results with respect to the size of the projectile partial-wave and target state (Laguerre basis) expansions indicate that scattering cross sections are accurate. With this solid foundation the CCC method is expected to be successful in describing more complicated molecular collision systems.

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