Complete Solution of Electronic Excitation and Ionization in Electron-Hydrogen Molecule Scattering

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A complete solution of electronic excitation and ionization in electron-hydrogen molecule scattering

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The convergent close-coupling method has been used to solve the electron-hydrogen molecule scattering problem in the fixed-nuclei approximation. Excellent agreement with experiment is found for the grand total, elastic, electronic-excitation, and total ionization cross sections from the very low to the very high energies. This shows that for the electronic degrees of freedom the method provides a complete treatment of electron scattering on molecules as it does for atoms.

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Molecular hydrogen H_2 is the simplest two-electron molecule. It is the most abundant molecule in the universe; particularly in interstellar space and in the atmospheres of gas giants and the outermost planets in our solar system. It is present at the edge region of fusion devices and widely used in plasma processing. A range of applications require accurate and comprehensive electron-collision data of molecular hydrogen in order to interpret spectroscopic data and model astrophysical and technological plasmas. Yet, this most fundamental few-body problem (e-H_2 scattering) has remained unsolved by theoretical methods, and a reliable dataset of collision cross sections is significantly lacking in accuracy and range of scattering processes.

Experimentally cross sections have been measured for elastic scattering, vibrational and electronic excitations, ionization and dissociative processes of the ground state. A number of articles have given an extensive overview of the available experimental data and provided a recommended set of cross sections [1–4]. The most recent recommended data set [1] comes predominantly from experimental measurements, which is problematic as theoretical and experimental results vary significantly for electronic excitation cross sections. In addition experimental uncertainties in the measurement of electronic excitation cross sections are relatively large, generally 20-25%.

For theorists the H_2 molecule offers a unique testing ground for the development of computational techniques. With wavefunctions known to high accuracy for this simple molecule the challenge is to treat the collision dynamics accurately. A large number of theoretical methods have been applied to calculate electron collisions with the H_2 molecule. Among the most advanced and general are calculations based on the Schwinger variational principle [5], Kohn variational method [6], R-matrix method [7–11], and time-dependent close-couplig method (TDCC) [12]. Agreement between theory and experiment for this most fundamental of all molecules is mixed at best. To date, no theoretical method has been able to describe the e-H_2 collision processes consistently across all transitions and incident electron energies.

There is of course a good reason for this; experience gained over the last few decades in electron-atom scattering suggests the importance of inter-channel coupling between all reaction channels including ionization. Another important point is the complete account of polarization effects in the scattering calculations. Within the close-coupling approach these can be achieved by using a near-complete expansion of both the discrete and continuum spectrum of the target. This is the approach adopted in the *ab initio* convergent close-coupling (CCC) method [13] and R-matrix with pseudo-states method (RMPS) [14]. A sufficiently large expansion has to be used to accurately model the coupling between all reaction channels and avoid the pseudo-resonance problem.

This strategy is difficult to implement for molecules due to the lack of spherical symmetry and reaction channels related to molecular vibrations and rotations. Even within the Born-Oppenheimer approximation and performing fixed-nuclei calculations the close-coupling expansion for the electronic part of the total wavefunction was often limited to just a few low-lying states of the H_2 molecule. For example, R-matrix calculations [7, 8] had seven states, the Kohn variational method [6] had four states and the Schwinger multichannel (SMC) calculations [5] had nine states. Such calculations are limited to low energies and their accuracy (convergence) is difficult to estimate. The notable exception is the molecular formulation of the RMPS method [11] that used a set of pseudostates to model the coupling to the ionization channels. The total number of states was 41 in the biggest calculation, however, only two states, the ground and first excited states, were represented accurately. For other molecules the situation is similar to H_2. Typically, electron-molecule calculations include just a few states in the close-coupling expansion and convergence studies are not performed.

This is very different to the electron-atom scattering field, which has undergone considerable progress over the last two decades. Large-scale close-coupling calcula-

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tions are common, convergence studies are routinely conducted and results of calculations are increasingly being presented with uncertainty estimates.

To enable large close-coupling calculations for molecular targets the computational implementation is important. The RMPS method as well as other techniques (Kohn and Schwinger methods) use Slater and Gaussian orbitals. This is helpful in dealing with the multicentre nature of the molecular wavefunctions but at the same time they are notorious for linear dependence problems for large expansions. This limits the size of the calculations and the range of its applicability. The CCC method makes use of the Sturmian (Laguerre) basis that has no linear dependence problems and allows us to conduct large-scale calculations. Another important difference is the adoption of a single-centre description of the target molecule in the CCC calculations. The advantage of the single-centre approach is the ability to evaluate all matrix elements in a straightforward manner. This works particularly well for the H_2 molecule with the accuracy of the wavefunctions better or comparable than in previous calculations [5, 7, 11].

The present approach has already been applied to positron scattering from the H_2 molecule [15–17] and electron scattering from H_2^+ and its isotopologues [18, 19]. In the latter case we conducted adiabatic-nuclei calculations, which allowed us to obtain collision data for scattering from the hot (vibrationally excited) target. In both cases we have explicitly demonstrated the convergence of the calculations with respect to the number of the target states in the close-coupling expansion and the size of the projectile partial wave expansion.

Here we apply the CCC method to the e-H_2 scattering problem. To demonstrate the accuracy of the method we present the grand total, ionization, and elastic scattering integrated cross sections. We also present differential cross sections (DCS) for elastic scattering and excitations of a number of low lying states at 17.5 eV. This energy is just above the H_2 ionization threshold, where the electronic excitations and ionization processes are dominant and their correct account is crucial.

The CCC method is formulated in a spherical coordinate system where the origin is set at the midpoint between the two nuclei and the z axis is chosen to align along the internuclei axis $\boldsymbol{R}$ (body-frame). The body-frame total scattering wavefunction is expanded in a set of target states. This leads to coupled Lippmann-Schwinger equations for the body-frame T-matrix. These equations are solved in momentum space via a K-matrix formulation, which enforces unitarity. In the case of homonuclear diatomic molecules like H_2 the partial wave expansion of the projectile wavefunctions allows one to solve the Lippmann-Schwinger equations per partial wave of total orbital angular momentum projection M, spin S and parity Π. Body-frame T-matrix elements are then transformed into the lab-frame using standard techniques and cross sections are calculated [20]. For details of the molecular CCC method see Ref. [18].

The CCC method requires a set of target (pseudo)states that should form a near-complete basis. The H_2 target electronic Hamiltonian $H_{\mathrm{T}}^{\mathrm{Elec}}$ in the Born-Oppenheimer approximation describes two electrons in the Coulomb potential of two protons that are fixed at a distance R and is defined as (atomic units are used throughout the paper)

$$H_{\mathrm{T}}^{\mathrm{Elec}} = H_1^{\mathrm{Elec}} + H_2^{\mathrm{Elec}} + V_{12} + 1/R, \tag{1}$$

where H_i^{Elec} is the one-electron electronic Hamiltonian of H_2^+

$$H_i^{\mathrm{Elec}} = -\frac{1}{2}\nabla_i^2 - \frac{1}{\left|\boldsymbol{r}_i + \frac{\boldsymbol{R}}{2}\right|} - \frac{1}{\left|\boldsymbol{r}_i - \frac{\boldsymbol{R}}{2}\right|}, \tag{2}$$

V_{12} is the electron-electron potential and $1/R$ is the internuclear Coulomb repulsion term. The H_2 electronic target states are characterised by their orbital angular momentum projection m, parity π and spin s. The target Hamiltonian (1) is diagonalised for each (m,π,s) term in a set of antisymmetrised two-electron configurations, where one-electron orbitals are represented by Laguerre basis functions. We designate N_l as the number of Laguerre basis functions per orbital angular momentum l up to $l_{\max}$.

The H_2 structure model needs to allow for an expansion over the two electrons $(nlm, n'l'm')$. The structure model chosen here represents the "outer" electron $(n'l'm')$ by one-electron orbitals. These one-electron orbitals were constructed from a Laguerre basis that had $N_l = 17 - l$ functions up to $l_{\max} = 3$. Exponential fall-offs were chosen such that positive-energy pseudostates were open just above ionization threshold and were $\alpha_{l=0} = 0.76$; $\alpha_{l=1} = 0.765$; $\alpha_{l=2} = 0.79$ and $\alpha_{l=3} = 0.85$. The "inner" electron is expanded by all $n \leq 2$ one-electron orbitals. These orbitals $(n \leq 2)$ are constructed from short-ranged Laguerre functions that have exponential fall-offs of $\alpha_l = 1.85$. However, the $1s\sigma_g$ orbital $(n = 1)$ is represented by a converged molecular-orbital of H_2^+ that was constructed from a Laguerre basis that had $N_l = 60 - l$, $\alpha_l = 0.9$ functions up to $l_{\max} = 8$. This molecular-orbital allows us to obtain an accurate ionization threshold within a single-centre expansion.

Diagonalising the target Hamiltonian with the model described above, $N = 491$ target states were constructed and used in the scattering calculations. Of these 491 states, 92 states were in the discrete spectrum and 399 states were in the continuum. In Table I the two-electron energies and vertical excitation energies at the equilibrium distance of $R_0 = 1.4\ a_0$ are presented for a number of low-lying states and compared with highly accurate structure calculations [21–26]. The length gauge oscillator strengths for the $X^1\Sigma_g^+ \to B^1\Sigma_u^+$ and $X^1\Sigma_g^+ \to C^1\Pi_u$ transitions are 0.277 and 0.337, which compares well with the accurate theoretical values 0.301 [25] and 0.351 [27], respectively. The static dipole polarisability is $\alpha_{\parallel} = 6.427\ a_0^3$ and $\alpha_{\perp} = 4.637\ a_0^3$ for the ground state, which are both in good agreement with the accurate calculations of Kolos and Wolniewicz [28] ($\alpha_{\parallel} = 6.380\ a_0^3$ and $\alpha_{\perp} = 4.578\ a_0^3$).

TABLE I: Two-electron energy E of electronic target states of H_2 and the vertical electronic excitation energy from the ground state ΔE at the internuclear distance of $R_0 = 1.4\ a_0$. Comparisons are made with accurate structure calculations [21–26].

	E (a.u.)		ΔE (eV)	
State	Present	Ref.	Present	Ref.
$X^1\Sigma_g^+$	-1.162	-1.174 [21]		
$b^3\Sigma_u^+$	-0.770	-0.784 [22]	10.67	10.62 [22]
$a^3\Sigma_g^+$	-0.710	-0.714 [23]	12.32	12.54 [23]
$c^3\Pi_u$	-0.701	-0.707 [24]	12.56	12.73 [24]
$B^1\Sigma_u^+$	-0.697	-0.706 [25]	12.66	12.75 [25]
$EF^1\Sigma_g^+$	-0.687	-0.692 [25]	12.92	13.13 [25]
$C^1\Pi_u$	-0.683	-0.689 [26]	13.03	13.22 [26]

To model scattering from the ground vibrational state in the fixed-nuclei approximation more accurately, the equilibrium distance is replaced by the mean internuclear distance of the vibrational ground state [29]. For scattering calculations we use the mean internuclear distance of H_2 $R_m = 1.448\ a_0$. It is also important to note that in the fixed-nuclei approximation the closure-method is effectively used to analytically sum over all vibrational and rotational excitations.

Scattering calculations were performed from 0.1 to 300 eV. With the $R_m = 1.448\ a_0$ fixed-nuclei structure model the ionization threshold is at 15.97 eV. For energies above the ionization threshold the 491-state model was used. This is the intermediate energy region where *ab initio* calculations are most difficult to perform. Below the ionization threshold a smaller model is sufficient. In this energy region we use the same model described above except the "outer" electron $(n'l'm')$ orbitals were constructed from a Laguerre basis that had $N_l = 10 - l$ functions up to $l_{\max} = 2$. We have conducted convergence studies at selected energies to verify the accuracy of the results as a function of the size of the Laguerre basis and projectile partial wave expansions. Detailed convergence studies will be presented elsewhere.

The present results have been calculated using a projectile partial-wave expansion with maximum orbital angular momentum $L_{\max} = 8$. The total spin $S = 1/2$, odd and even parity Π and total orbital angular projection $|M| \leq 8$ channels were included. Below the ionization threshold fewer projectile partial-waves are required. For inelastic scattering, the orientationally averaged analytic Born subtraction method was used to top-up the projectile partial-wave expansion for integrated cross sections [18].

The grand total cross section (GTCS) for electron scattering from the ground state of the H_2 molecule is presented in Fig. 1. The CCC results are compared with the measurements of Ferch *et al.* [30], van Wingerden *et al.* [31], Hoffman *et al.* [32], Deuring *et al.* [33], Jones [34], Subramanian and Kumar [35], Nickel *et al.* [36] and Zhou *et al.* [37]. As far as we are aware these are the only *ab initio* results of the GTCS across the intermediate-energy region that are in excellent agreement with all experiments. The small experimental uncertainties suggest that the CCC formalism is correct across the entire energy range, with elastic, excitation and ionization cross sections being taken into account accurately.

Our best estimate for the scattering length is 1.30 a_0 with uncertainty of about 10%. These values are in agreement with other calculations (1.24 a_0[38], 1.27 a_0 [39], 1.29 a_0 [40], 1.30 a_0 [41]). Detailed analysis of low-energy e-H_2 collisions will be conducted elsewhere.

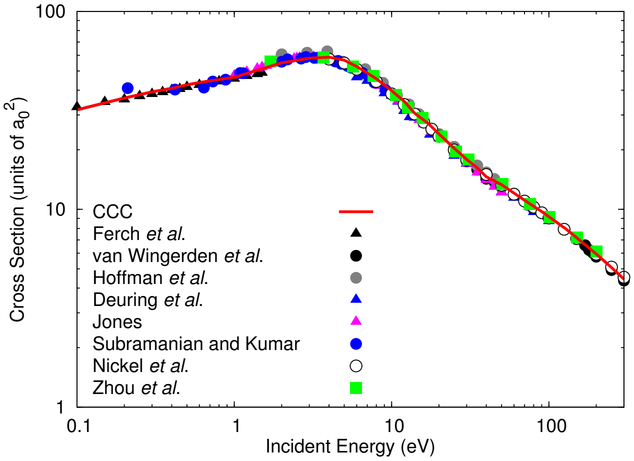

FIG. 1: Grand total cross section of electron scattering from H_2. CCC results are compared with the measurements of Ferch *et al.* [30], van Wingerden *et al.* [31], Hoffman *et al.* [32], Deuring *et al.* [33], Jones [34], Subramanian and Kumar [35], Nickel *et al.* [36] and Zhou *et al.* [37].

In Fig. 2 total single ionization cross sections of H_2 are presented. CCC H_2^+ production results are compared with the H_2^+ production measurements of Krishnakumar and Srivastava [42] and Straub *et al.* [43] and the total ionization cross section (TICS) measurements of Rapp and Englander-Golden [44], Lindsay and Mangan [2] and calculations using the RMPS [11] and TDCC [12] methods. CCC results have been multiplied by the appropriate Franck-Condon [45] factor to calculate the production of H_2^+ (≈98.5% of the fixed-nuclei cross section) and not dissociative ionization. Comparing with experiment, the CCC results are in excellent agreement with all experiments from the ionization threshold to the cross section maximum. For high energies CCC results favour the measurements of Krishnakumar and Srivastava [42]. The excellent agreement between the CCC results and measurements of the GTCS and TICS indicates that the electron flux has been correctly distributed to the continuum and discrete spectrum. Hence elastic and electronic excitation cross sections should be accurate if the scattering calculation uses accurate target states, as is the case with the present model.

Comparing with other calculations, CCC results are in excellent agreement with the *ab initio* RMPS [11] and TDCC [12] results. The RMPS results are available from the ionization threshold to 30 eV and TDCC results are only available at 25, 50 and 75 eV. In the RMPS calculations there was a problem with pseudo-resonances and an averaging procedure was used to smooth over the results. The one-electron TDCC method utilises the local-exchange approximation and uses smaller partial wave expansion together with a polinomial extrapolation technique. Despite these differences the agreement with CCC is remarkable.

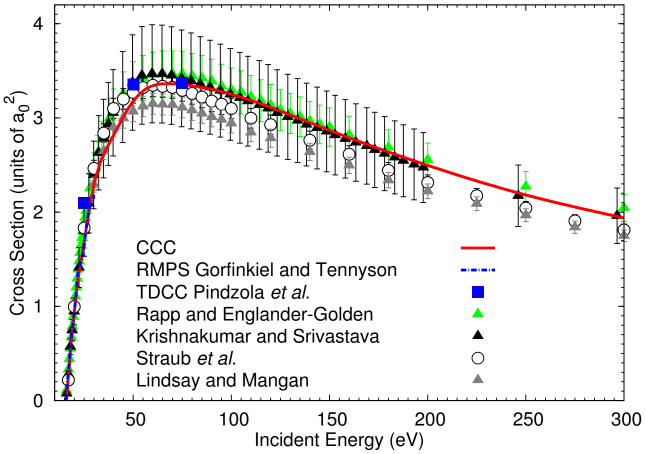

FIG. 2: Ionization cross sections of electron scattering from H_2. Convergent close-coupling (CCC) results are compared with the H_2^+ production measurements of Krishnakumar and Srivastava [42], Straub *et al.* [43] and the total ionization cross section measurements of Rapp and Englander-Golden [44] and Lindsay and Mangan [2]. RMPS [11] results end at 30 eV and are indistinguishable from CCC results. TDCC [12] results are available only at 25, 50 and 75 eV.

The elastic integrated cross section is presented in Fig. 3 from 10 to 100 eV (for lower energies see Fig. 1). The fixed-nuclei CCC results are in excellent agreement with the measurements of Shyn and Sharp [46], Nishimura *et al.* [47], Khakoo and Trajmar [48] across the entire energy range considered. The measurements of Srivastava *et al.* [49] are consistently lower than the CCC results and the other measurements.

To complete our presentation we consider an example of DCS. In Fig. 4 the 17.5 eV incident electron energy DCS are presented for elastic scattering and low-lying electronic excitations. Starting with the top-left panel the CCC elastic DCS are compared with the measurements of Khakoo and Trajmar [48] and the 7-state R-matrix calculations of Branchett *et al.* [8]. The CCC results are in good agreement with experiment and the R-matrix results, with some variation between the two theories at the forward angles. Measurements of the electronic excitations of H_2 are exceptionally difficult due to the overlapping electronic-vibrational manifolds in the energy loss spectrum. Considering this difficulty the CCC results are in excellent agreement with experiment [50] for all transitions considered. CCC results are also compared with the SMC calculations of da Costa *et al.* [5] for excitation to the $B^1\Sigma_u^+$; $c^3\Pi_u$ and $C^1\Sigma_u$ states.

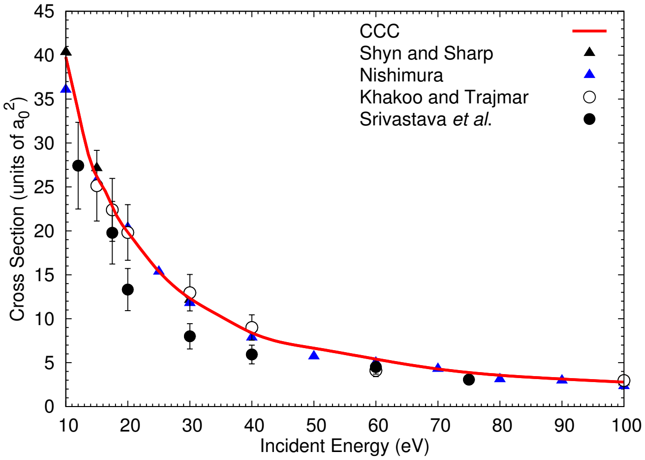

FIG. 3: Elastic cross section of electron scattering from H_2. CCC results are compared with the measurements of Shyn and Sharp [46], Nishimura *et al.* [47], Khakoo and Trajmar [48] and Srivastava *et al.* [49].

In conclusion we have performed CCC calculations of electron-H_2 scattering over a very broad energy range yielding excellent agreement with experiment. The CCC formalism provides a complete solution of the electron-molecular hydrogen scattering problem in the fixed-nuclei approximation, irrespective of the projectile energy or the electronic transition of interest. The fixed-nuclei approximation is the foundation on which techniques are built to describe vibrational and rotational excitations, resonance and dissociative processes in molecules [9, 10, 20, 51] . This will allow us to model such processes and address some long standing problems, such as the controversy over the vibrational excitation cross sections for molecular hydrogen [3]. While we appreciate that molecular hydrogen is the simplest molecule of practical interest, the CCC formalism is general and can readily be extended to other molecules where the interaction is dominated by one- or two-electron excitations. We are now in a position for molecular targets where we were for atomic targets two decades ago.

In addition to extending the CCC method to more complicated molecules we are also extending the method to make use of the spheroidal coordinate system. This will allow us to study diffuse molecules like Li_2 and scattering from hot (vibrationally excited) molecules. All this extensive data will be made available via the LXCat database and should be useful in astrophysical, plasma and transport modelling.

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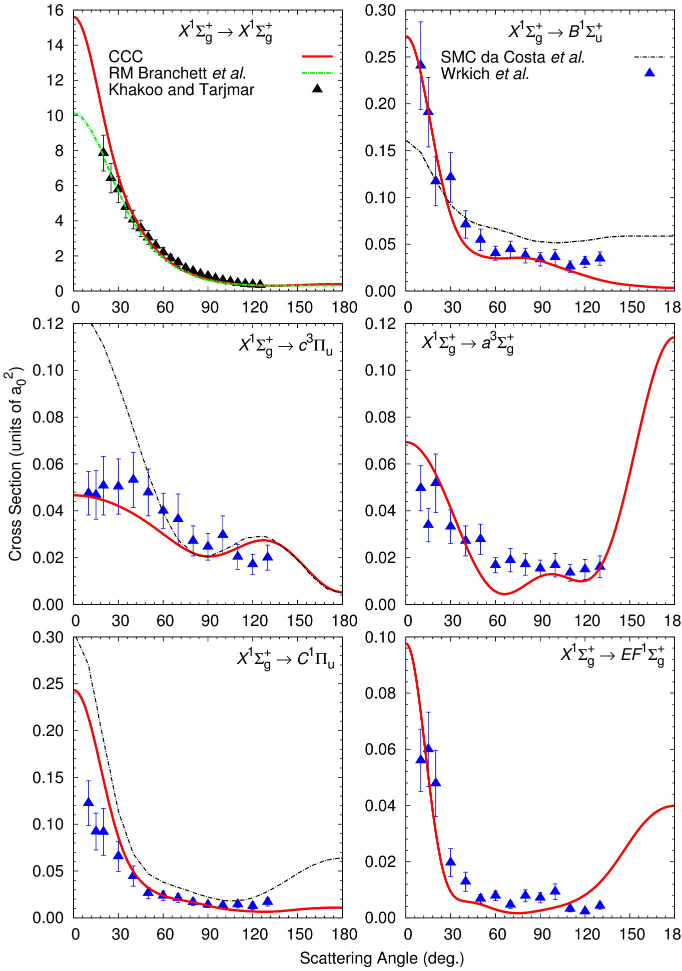

FIG. 4: Elastic and electronic excitation e-H_2 differential cross sections (DCS) at 17.5 eV. CCC results are compared with the elastic DCS measurements of Khakoo and Trajmar [48], with the measurements of Wrkich *et al.* [50] for electronic excitations of the $B^1\Sigma_u^+$; $c^3\Pi_u$; $a^3\Sigma_g^+$; $C^1\Sigma_u$ and $EF^1\Sigma_g^+$ states. CCC results are also compared with the R-matrix (RM) calculations of Branchett *et al.* [8] and SMC calculations of da Costa *et al.* [5].

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