

Electron-Impact Double Ionization of the H_2 Molecule

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ABSTRACT: A time-dependent close-coupling method in spherical polar coordinates is developed to calculate the electron-impact double ionization of the H_2 molecule. The full wavefunction is represented by an expansion in products of six-dimensional radial-angular numerical functions and analytic rotational functions. A test calculation finds good agreement between the new method and a previous frozen core method for the single ionization of H_2 for the $M = l_0 = 0$ partial wave and an impact energy of 100.0 eV. A test calculation is also made for the double ionization of H_2 for the same partial wave and impact energy.

I. INTRODUCTION

A time-dependent close-coupling (TDCC) method was originally developed to calculate the electron-impact single ionization of H_2^+ [1]. The full wavefunction was represented by an expansion in products of four-dimensional radial-angular numerical functions and analytic rotational functions. When the close-coupling results for low angular momentum are combined with distorted-wave results for high angular momentum, the total cross section was found to be in excellent agreement with experiment [2]. A frozen-core TDCC method was then used to calculate the electron-impact single ionization of H_2 [3]. The total cross section was again found to be in excellent agreement with experiment [4]. The frozen core TDCC method has also been used to calculate the electron-impact single ionization of Li_2 [5].

In this article we develop a time-dependent close-coupling method to calculate the electron-impact double ionization of H_2 . We note that a TDCC method for atoms has been previously applied to calculate the electron-impact double ionization of He [6], [7], Mg [8], Be [9], and [10]. For H_2 the full wavefunction is represented by an expansion in products of six-dimensional radial-angular numerical functions and analytic rotational functions. Test calculations are made on a relatively small numerical lattice for one partial wave and one incident energy. Details of the TDCC method of H_2 are presented in Section II, test calculations are presented in Section III, and a brief summary of future plans is given in Section IV. Unless otherwise stated, all quantities are given in atomic units.

II. THEORY

A. Relaxation to the Ground State

The Six-dimensional wavefunction $\bar{\Psi}^0$ for the ground state of H_2 is obtained by relaxation of the time-dependent Schrodinger equation in imaginary time (τ):

$$-\frac{\partial \bar{\Psi}^0(\vec{r}_1, \vec{r}_2, \tau)}{\partial \tau} = \sum_i \left(-\frac{1}{2} \nabla_i^2 + V(\vec{r}_i) \right) \bar{\Psi}^0(\vec{r}_1, \vec{r}_2, \tau) + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \bar{\Psi}^0(\vec{r}_1, \vec{r}_2, \tau), \quad (1)$$

where $V(\vec{r})$ is a single particle interaction with the target nuclei. The wavefunction $\bar{\Psi}^0$ is represented by an expansion in simple products of four-dimensional radial-angular functions $\bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau)$ and rotational functions:

$$\bar{\Psi}^0(\vec{r}_1, \vec{r}_2, \tau) = \sum_{m_1} \sum_{m_2} \frac{\bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau)}{r_1 r_2 \sqrt{\sin \theta_1} \sqrt{\sin \theta_2}} \times \Phi_{m_1}(\phi_1) \Phi_{m_2}(\phi_2), \quad (2)$$

where $\Phi_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}$ and $m_1 + m_2 = 0$. The angular reduction of the time-dependent Schrodinger equation in imaginary time yields a set of close-coupling equations given by:

$$\begin{aligned} & \frac{\partial \bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau)}{\partial \tau} \\ & = \sum_i T_{m_i}(r_i, \theta_i) \bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau) \\ & + \sum_{m_1} \sum_{m_2} V_{m_1 m_2, m'_1 m'_2}^{M=0}(r_1, \theta_1, r_2, \theta_2) \bar{P}_{m'_1 m'_2}(r_1, \theta_1, r_2, \theta_2, \tau). \end{aligned} \quad (3)$$

The single particle operator in the close-coupling equations is given by:

$$T_{m_i}(r_i, \theta_i) = K(r_i) + \bar{K}(r_i, \theta_i) + A_{m_i}(r_i, \theta_i) + N(r_i, \theta_i), \quad (4)$$

where $K(r)$ and $K(r, \theta)$ are kinetic energy operators [1]. The axial angular momentum operator is given by:

$$A_m(r, \theta) = \frac{m^2}{2r^2 \sin^2 \theta}. \quad (5)$$

The nuclear interaction operator for is given by:

$$N(r, \theta) = -\frac{1}{\sqrt{r^2 + \frac{1}{4}R^2 - rR \cos \theta}} - \frac{1}{\sqrt{r^2 + \frac{1}{4}R^2 + rR \cos \theta}}, \quad (6)$$

where R is the internuclear separation, which is aligned along the z axis. The two particle operator in the close-coupling equations is given by:

$$\begin{aligned} V_{m_i m_j, m'_i m'_j}^M & = \sum_{\lambda} \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} \sum_q \frac{(\lambda - |q|)}{(\lambda + |q|)} P_{\lambda}^{|q|}(\cos \theta_i) P_{\lambda}^{|q|}(\cos \theta_j) \times \\ & \langle (m_i, m_j) M | e^{iq(\phi_j - \phi_i)} | (m'_i, m'_j) M \rangle, \end{aligned} \quad (7)$$

where $P_{\lambda}^{|q|}(\cos \theta)$ is an associated Legendre function.

At time $\tau = 0$ the radial-angular functions are given by:

$$\bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau) = P_{1s0}(r_1, \theta_1) P_{1s0}(r_2, \theta_2) \delta_{m_1, 0} \delta_{m_2, 0}, \quad (8)$$

where the radial-angular orbital, $P_{1s0}(r, \theta)$, is obtained by matrix diagonalization of the Hamiltonian, $T_m = 0(r, \theta)$. Upon relaxation in imaginary time of Eq.(3), an accurate wavefunction for the ground state of H_2 is obtained.

B. Propagation of the Scattering State

The nine-dimensional wavefunction Ψ^M for electron ionization of the ground state of H₂ is obtained by solving the time-dependent Schrodinger equation:

$$i \frac{\partial \Psi^M(\vec{r}_1, \vec{r}_2, \vec{r}_3, t)}{\partial t} = \sum_i \left(-\frac{1}{2} \nabla_i^2 + V(\vec{r}_i) \right) \Psi^M(\vec{r}_1, \vec{r}_2, \vec{r}_3, t) + \sum_{i < j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \Psi^M(\vec{r}_1, \vec{r}_2, \vec{r}_3, t). \quad (9)$$

The wavefunction Ψ^M for a given M symmetry is represented by an expansion in simple products of six-dimensional radial-angular functions $P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t)$ and rotational functions:

$$\begin{aligned} \Psi^M(\vec{r}_1, \vec{r}_2, \vec{r}_3, t) &= \sum_{m_1} \sum_{m_2} \sum_{m_3} \frac{P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t)}{r_1 r_2 r_3 \sqrt{\sin \theta_1} \sqrt{\sin \theta_2} \sqrt{\sin \theta_3}} \\ &\times \Phi_{m_1}(\phi_1) \Phi_{m_2}(\phi_2) \Phi_{m_3}(\phi_3), \end{aligned} \quad (10)$$

where $M = m_1 + m_2 + m_3$. The angular reduction of the time-dependent Schrodinger equation yields a set of time-dependent close-coupling equations given by:

$$\begin{aligned} i \frac{\partial P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t)}{\partial t} &= \sum_i T_{m_i}(r_i, \theta_i) P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t) \\ &+ \sum_{m'_1} \sum_{m'_2} V_{m_1 m_2, m'_1 m'_2}^M(r_1, \theta_1, r_2, \theta_2) P_{m'_1 m'_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t) \\ &+ \sum_{m'_1} \sum_{m'_2} V_{m_1 m_3, m'_1 m'_2}^M(r_1, \theta_1, r_3, \theta_3) P_{m_1 m_2 m'_2}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t) \\ &+ \sum_{m'_2} \sum_{m'_3} V_{m_2 m_3, m'_2 m'_3}^M(r_2, \theta_2, r_3, \theta_3) P_{m_1 m_2 m'_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t). \end{aligned} \quad (11)$$

At time $t = 0$ the radial-angular functions are given by:

$$\begin{aligned} P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t = 0) &= \sum_{m_1} \sum_{m_2} \bar{P}_{m_1 m_2}(r_1, \theta_1, r_2, \theta_2, \tau \rightarrow \infty) \times G_{k_0 l_0 m_3}(r_3, \theta_3) \delta_{m_3, M}. \end{aligned} \quad (12)$$

The Gaussian wavepacket is given by:

$$G_{k_0 l_0 m_3}(r, \theta) = \frac{e^{-\frac{(r-a)^2}{2\omega^2}}}{(\omega^2 \pi)^{\frac{1}{4}}} e^{i(k_0 r - l_0 \pi/2)} \sqrt{2\pi \sin \theta} Y_{l_0 m_3}(\theta, \phi = 0), \quad (13)$$

where a is the localization radius, ω is the packet width, l_0 is the incident angular momentum, and the incident energy equals $k_0^2/2$.

Following propagation in real time of Eq. (11), momentum space amplitudes are calculated using:

$$\begin{aligned}
& A_{l_2 m_2 l_3 m_3}^M(k_2, k_3) \\
&= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\pi dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3 \\
&\times P_{1s0}^*(r_1, \theta_1) \tilde{P}_{k_2 l_2 m_2}^*(r_2, \theta_2) \tilde{P}_{k_3 l_3 m_3}^*(r_3, \theta_3) \\
&\times P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \rightarrow \infty),
\end{aligned} \tag{14}$$

$$\begin{aligned}
& A_{l_1 m_1 l_3 m_3}^M(k_1, k_3) \\
&= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3 \\
&\times \tilde{P}_{k_1 l_1 m_1}^*(r_1, \theta_1) P_{1s0}^*(r_2, \theta_2) \tilde{P}_{k_3 l_3 m_3}^*(r_3, \theta_3) \\
&\times P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \rightarrow \infty),
\end{aligned} \tag{15}$$

$$\begin{aligned}
& A_{l_1 m_1 l_2 m_2}^M(k_1, k_1) \\
&= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3 \\
&\times \tilde{P}_{k_1 l_1 m_1}^*(r_1, \theta_1) \tilde{P}_{k_2 l_2 m_2}^*(r_2, \theta_2) P_{1s0}^*(r_3, \theta_3) \\
&\times P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \rightarrow \infty),
\end{aligned} \tag{16}$$

$$\begin{aligned}
& B_{l_1 m_1 l_2 m_2 l_3 m_3}^M(k_1, k_2, k_3) \\
&= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3 \\
&\times P_{k_1 l_1 m_1}^*(r_1, \theta_1) P_{k_2 l_2 m_2}^*(r_2, \theta_2) P_{k_3 l_3 m_3}^*(r_3, \theta_3) \\
&\times P_{m_1 m_2 m_3}^M(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \rightarrow \infty),
\end{aligned} \tag{17}$$

where the radial-angular orbitals, $P_{klm}(r, \theta)$, are obtained by matrix diagonalization of the Hamiltonian, $T_m(r, \theta)$. In addition, the radial-angular orbitals, $\tilde{P}_{klm}(r, \theta)$, are obtained by matrix diagonalization of the Hamiltonian, $T_m(r, \theta) + V_{HS}(r, \theta)$, where $V_{HS}(r, \theta)$ is the Hartree-Slater potential [3].

C. Cross Sections

The total single ionization cross section leaving in the ground state is given by:

$$\sigma_1 = \frac{\pi}{2k_0^2} \sum_M \sum_{l_0} 2 \sum_{i < j} \sum_{l_i m_i} \sum_{l_j m_j} \int_0^\infty dk_i \int_0^\infty dk_j \left| A_{l_i m_i l_j m_j}^M(k_i, k_j) \right|^2. \tag{18}$$

The total double ionization cross section is given by:

$$\sigma_2 = \frac{\pi}{2k_0^2} \sum_M \sum_{l_0} 2 \sum_{l_1 m_1} \sum_{l_2 m_2} \sum_{l_3 m_3} \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3 \left| B_{l_1 m_1 m_2 l_3 m_3}^M(k_1, k_2, k_3) \right|^2. \tag{19}$$

The energy differential double ionization cross section is given by:

$$\begin{aligned} \frac{d\sigma_2}{d\alpha d\beta} &= \frac{\pi}{2k_0^2} \sum_M \sum_{l_0} 2 \sum_{l_1 m_1} \sum_{l_2 m_2} \sum_{l_3 m_3} \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3 \\ &\times \delta\left(\alpha - \arctan \frac{k_2}{k_1}\right) \delta\left(\beta - \arctan \frac{k_3}{\sqrt{k_1^2 + k_2^2}}\right) \\ &\times \left| B_{l_1 m_1 l_2 m_2 l_3 m_3}^M(k_1, k_2, k_3) \right|^2, \end{aligned} \quad (20)$$

where α is an angle in the (k_1, k_2) hyperspherical plane and β is an angle in the plane perpendicular to the (k_1, k_2) hyperspherical plane, both defined from 0 to $\pi/2$. The energy and angle differential double ionization cross section is given by:

$$\begin{aligned} \frac{d\sigma_2}{d\alpha d\beta d\Omega_1 d\Omega_2 d\Omega_3} &= \frac{\pi}{2k_0^2} 2 \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3 \\ &\times \delta\left(\alpha - \arctan \frac{k_2}{k_1}\right) \delta\left(\beta - \arctan \frac{k_3}{\sqrt{k_1^2 + k_2^2}}\right) \times \left| \sum_M \sum_{l_0} i^{l_0} Y_{l_0 M}^*(\theta_e, \phi_e) \right. \\ &\times \sum_{l_1 m_1} \sum_{l_2 m_2} \sum_{l_3 m_3} (-i)^{l_1+l_2+l_3} e^{i(\sigma_{l_1}+\sigma_{l_2}+\sigma_{l_3})} B_{l_1 m_1 l_2 m_2 l_3 m_3}^M(k_1, k_2, k_3) \\ &\left. \times Y_{l_1 m_1}(\hat{k}_1) Y_{l_2 m_2}(\hat{k}_2) Y_{l_3 m_3}(\hat{k}_3) \delta_{m_1+m_2+m_3, M} \right|^2, \end{aligned} \quad (21)$$

where the incoming electron beam is oriented at angles (θ_e, ϕ_e) with respect to the z axis, $Y_{lm}(\theta, \phi)$ is a spherical harmonic, and σ_l is the Coulomb phase shift.

III. RESULTS

As a simple numerical test of the theory, we use a radial-angular grid of $\Delta r_i = 0.40$ with and with $N_r = 72$ and $\Delta\theta_i = 0.125\pi$ with $N_\theta = 8$. The internuclear separation is $R = 1.4$.

Bound and continuum radial-angular orbitals for H_2^+ are found upon matrix diagonalization of $T_m(r, \theta)$. For $m = 0$ we obtained 29 bound states, beginning with $P_{1s0}(r, \theta)$ at -35.8 eV, and 230 continuum states ranging from 0.06 eV to 148.9 eV. For $m = 1$ we obtained 23 bound states, beginning with $P_{2p1}(r, \theta)$ at -12.5 eV, and 229 continuum states ranging from 0.09 eV to 147.3 eV.

Bound and continuum radial-angular orbitals for H_2 are found upon matrix diagonalization of $T_m(r, \theta) + V_{HS}(r, \theta)$. For $m = 0$ we obtained 16 bound states, beginning with $\tilde{P}_{1s0}(r, \theta)$ at -15.4 eV, and 241 continuum states ranging from 0.03 eV to 149.9 eV. For $m = 1$ we obtained 10 bound states, beginning with $\tilde{P}_{2p1}(r, \theta)$ at -3.8 eV, and 240 continuum states ranging from 0.05 eV to 147.5 eV. The choice of the parameter α in the local exchange potential allows adjustment of the $1s0$ binding energy to be near the experimental value.

For relaxation to the ground state, we use a numerical lattice of $(72 \times 8)^2$ points partitioned over 324 parallel computer cores and the 3 coupled channels found in Table I. At time $\tau = 0$ the radial-angular functions of Eq.(8)

yield an energy of -49.3 eV. Following 1000 time steps at $\Delta\tau = 0.01$ the radial-angular functions of Eq.(3) yield an energy of -52.5 eV.

For propagation of the scattering state, we use a numerical lattice of $(72 \times 8)^3$ points partitioned over 5832 parallel computer cores and the 7 coupled channels found in Table II. At time $t = 0$ we choose a Gaussian wavepacket of Eq. (13) with a localization radius $\alpha = 14.4$, a packet width $\omega = 3.6$, an incident angular momentum $l_0 = 0$, and an incident energy of $E_0 = 100.0$ eV. Following 1500 time steps at $\Delta t = 0.01$ the radial angular functions of Eq. (11) are used to calculate the $3 \times (481)^2$ momentum space amplitudes of Eqs.(14)-(16) and the $(459)^3$ momentum space amplitudes of Eq. (17).

The total single ionization cross section leaving H_2^+ in the ground state from Eq. (18) is found to be 2.25 Mbarns for $M = l_0 = 0$ at 100.0 eV incident energy. The total double ionization cross section from Eq.(19) is found to be 29.5 Kbarns for $M = l_0 = 0$ at 100.0 eV incident energy.

To check our total single ionization cross section, we carried out frozen-core TDCC calculations [3], as outlined in the Appendix. The initial state is the bound radial-angular orbital $\tilde{P}_{1s0}(r, \theta)$ at -15.4 eV. For propagation of the scattering state, we use a numerical lattice of $(72 \times 8)^2$ points partitioned over 324 parallel computer cores and the 3 coupled channels found in Table I. Following 1500 time steps at $\Delta t = 0.01$ the radial-angular functions of Eq. (24) are used to calculate the $(481)^2$ momentum space amplitudes of Eq.(26). The total single ionization cross section from Eq. (27) is found to be 2.01 Mbarns for $M = l_0 = 0$ at 100.0 eV incident energy, including both the $S = 0$ singlet and $S = 1$ triplet contributions.

IV. SUMMARY

In the future we plan to apply the TDCC method to a full calculation of the electron-impact double ionization of H_2 . We will choose an impact energy above the full breakup energy of 52.5 eV and the number of Ml_0 partial waves will include $M \leq 3$ and $l_0 \leq 4$. We plan on using a radial-angular grid of $\Delta r_i = 0.20$ with $N_r = 144$ and $\Delta\theta_i = 0.0833\pi$ with $N_\theta = 12$. The numerical lattice of $(144 \times 12)^3$ points will be partitioned over 46,656 parallel computer cores. The number of coupled channels for relaxation and propagation will also be increased to at least include $m_i = \pm 2$.

Acknowledgments

This work was supported in part by grants from the US Department of Energy and the US National Aeronautics and Space Administration. Computational work was carried out at the National Energy Research Scientific Computing Center (NERSC) in Berkeley, California and the High Performance Computing Center (HLRS) in Stuttgart, Germany.

APPENDIX

The six-dimensional wavefunction Ψ^M for electron ionization of one active electron in the ground state of H_2 is obtained by solving the time-dependent Schrodinger equation:

$$i \frac{\partial \Psi^M(\vec{r}_1, \vec{r}_2, t)}{\partial t} = \sum_i \left(-\frac{1}{2} \nabla_i^2 + V(\vec{r}_i) \right) \Psi^M(\vec{r}_1, \vec{r}_2, t) + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \Psi^M(\vec{r}_1, \vec{r}_2, t). \quad (22)$$

The wavefunction Ψ^M for a given M symmetry is represented by an expansion in simple products of four-dimensional radial-angular functions $P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t)$ and rotational functions:

$$\Psi^M(\vec{r}_1, \vec{r}_2, t) = \sum_{m_1} \sum_{m_2} \frac{P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t)}{r_1 r_2 \sqrt{\sin \theta_1} \sqrt{\sin \theta_2}} \times \Phi_{m_1}(\phi_1) \Phi_{m_2}(\phi_2), \quad (23)$$

where $M = m_1 + m_2$. The angular reduction of the time-dependent Schrodinger equation yields a set of time-dependent close-coupling equations given by:

$$\begin{aligned}
 & i \frac{\partial P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t)}{\partial t} \\
 &= \sum_i \left(T_{m_i}(r_i, \theta_i) + V_{HS}(r_i, \theta_i) \right) P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t) \\
 &+ \sum_{m'_1} \sum_{m'_2} V_{m_1 m_2, m'_1 m'_2}^M(r_1, \theta_1, r_2, \theta_2) P_{m'_1 m'_2}^M(r_1, \theta_1, r_2, \theta_2, t).
 \end{aligned}$$

At time $t = 0$ the radial-angular functions are given by:

$$\begin{aligned}
 & P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t = 0) \\
 &= \sqrt{1/2} [\tilde{P}_{1s0}(r_1, \theta_1) G_{k_0 l_0 m_2}(r_2, \theta_2) \delta_{m_1, 0} \delta_{m_2, M} \\
 &+ (-1)^S G_{k_0 l_0 m_1}(r_1, \theta_1) \tilde{P}_{1s0}(r_2, \theta_2) \delta_{m_1, M} \delta_{m_2, 0}]
 \end{aligned} \tag{25}$$

Momentum space amplitudes are calculated using:

$$\begin{aligned}
 & B_{l_1 m_1 l_2 m_2}^M(k_1, k_2) \\
 &= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \times \tilde{P}_{k_1 l_1 m_1}^*(r_1, \theta_1) \tilde{P}_{k_2 l_2 m_2}^*(r_2, \theta_2) \\
 &\times P_{m_1 m_2}^M(r_1, \theta_1, r_2, \theta_2, t \rightarrow \infty).
 \end{aligned} \tag{26}$$

The total single ionization cross section is given by:

$$\sigma_1 = \frac{\pi \omega_t}{k_0^2} \sum_M \sum_{l_0} \sum_S \frac{(2S+1)}{4} \sum_{l_1 m_1} \sum_{l_2 m_2} \int_0^\infty dk_1 \int_0^\infty dk_2 |B_{l_1 m_1 l_2 m_2}^M(k_1, k_2)|^2, \tag{27}$$

where the subshell occupation number $\omega_t = 2$ for the ground state of H₂.

Table I
4D Coupled Channels

	m_1	m_2
1	0	0
2	1	-1
3	-1	1

Table II
6D Coupled Channels

	m_1	m_2	m_3
1	0	0	0
2	1	-1	0
3	-1	1	0
4	1	0	-1
5	-1	0	1
6	0	1	-1
7	0	-1	1

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