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 B$^+$ [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 $\overline{\Psi}^0$ for the ground state of H_2 is obtained by relaxation of the time-dependent Schrodinger equation in imaginary time (τ):

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

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:

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

where $\Phi_m(\phi) = \dfrac{e^{im\phi}}{\sqrt{2\pi}}$ 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:

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

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

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

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

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

The nuclear interaction operator for H_2 is given by:

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

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:

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

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

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

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

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 wave function Ψ^M for electron ionization of the ground state of H_2 is obtained by solving the time-dependent Schrodinger equation:

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

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:

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

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:

$$i\frac{\partial P_{m_1 m_2 m_3}^M(r_1,\theta_1,r_2,\theta_2,r_3,\theta_3,t)}{\partial t}$$

$$= \sum_i T_{m_i}(r_i,\theta_i)P_{m_1 m_2 m_3}^M(r_1,\theta_1,r_2,\theta_2,r_3,\theta_3,t)$$

$$+ \sum_{m_1'}\sum_{m_2'} V_{m_1 m_2,m_1' m_2'}^M(r_1,\theta_1,r_2,\theta_2)P_{m_1' m_2' m_3}^M(r_1,\theta_1,r_2,\theta_2,r_3,\theta_3,t)$$

$$+ \sum_{m_1'}\sum_{m_2'} V_{m_1 m_3,m_1' m_3'}^M(r_1,\theta_1,r_3,\theta_3)P_{m_1' m_2 m_3'}^M(r_1,\theta_1,r_2,\theta_2,r_3,\theta_3,t)$$

$$+ \sum_{m_2'}\sum_{m_3'} V_{m_2 m_3,m_2' m_3'}^M(r_2,\theta_2,r_3,\theta_3)P_{m_1 m_2' m_3'}^M(r_1,\theta_1,r_2,\theta_2,r_3,\theta_3,t). \tag{11}$$

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

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

The Gaussian wavepacket is given by:

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

where a is the localization radius, w 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:

$$A^M_{l_2 m_2 l_3 m_3}(k_2, k_3)$$

$$= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3$$

$$\times P^*_{1s0}(r_1, \theta_1) \tilde{P}^*_{k_2 l_2 m_2}(r_2, \theta_2) \tilde{P}^*_{k_3 l_3 m_3}(r_3, \theta_3)$$

$$\times P^M_{m_1 m_2 m_3}(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \to \infty), \tag{14}$$

$$A^M_{l_1 m_1 l_3 m_3}(k_1, k_3)$$

$$= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3$$

$$\times \tilde{P}^*_{k_1 l_1 m_1}(r_1, \theta_1) P^*_{1s0}(r_2, \theta_2) \tilde{P}^*_{k_3 l_3 m_3}(r_3, \theta_3)$$

$$\times P^M_{m_1 m_2 m_3}(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \to \infty), \tag{15}$$

$$A^M_{l_1 m_1 l_2 m_2}(k_1, k_1)$$

$$= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3$$

$$\times \tilde{P}^*_{k_1 l_1 m_1}(r_1, \theta_1) \tilde{P}^*_{k_2 l_2 m_2}(r_2, \theta_2) P^*_{1s0}(r_3, \theta_3)$$

$$\times P^M_{m_1 m_2 m_3}(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \to \infty), \tag{16}$$

$$B^M_{l_1 m_1 l_2 m_2 l_3 m_3}(k_1, k_2, k_3)$$

$$= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \int_0^\infty dr_3 \int_0^\pi d\theta_3$$

$$\times P^*_{k_1 l_1 m_1}(r_1, \theta_1) P^*_{k_2 l_2 m_2}(r_2, \theta_2) P^*_{k_3 l_3 m_3}(r_3, \theta_3)$$

$$\times P^M_{m_1 m_2 m_3}(r_1, \theta_1, r_2, \theta_2, r_3, \theta_3, t \to \infty), \tag{17}$$

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 H_2^+ in the ground state is given by:

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

The total double ionization cross section is given by:

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

The energy differential double ionization cross section is given by:

$$\frac{d\sigma_2}{d\alpha d\beta} = \frac{\pi}{2k_0^2} \sum_M \sum_{l_0} 2 \sum_{l_1 m_1} \sum_{l_2 m_2} \sum_{l_3 m_3} \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3$$

$$\times \delta\left(\alpha - \arctan\frac{k_2}{k_1}\right)\delta\left(\beta - \arctan\frac{k_3}{\sqrt{k_1^2 + k_2^2}}\right)$$

$$\times \left| B^M_{l_1 m_1 l_2 m_2 l_3 m_3}(k_1, k_2, k_3) \right|^2, \tag{20}$$

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:

$$\frac{d\sigma_2}{d\alpha d\beta d\Omega_1 d\Omega_2 d\Omega_3}$$

$$= \frac{\pi}{2k_0^2} 2 \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3$$

$$\times \delta\left(\alpha - \arctan\frac{k_2}{k_1}\right)\delta\left(\beta - \arctan\frac{k_3}{\sqrt{k_1^2 + k_2^2}}\right) \times |\sum_M \sum_{l_0} i^{l_0} Y^*_{l_0 M}(\theta_e, \phi_e)$$

$$\times \sum_{l_1 m_1} \sum_{l_2 m_2} \sum_{l_3 m_3} (-i)^{l_1+l_2+l_3} e^{i\left(\sigma_{l_1} + \sigma_{l_2} + \sigma_{l_3}\right)} B^M_{l_1 m_1 l_2 m_2 l_3 m_3}(k_1, k_2, k_3)$$

$$\times Y_{l_1 m_1}(\hat{k}_1) Y_{l_2 m_2}(\hat{k}_2) Y_{l_3 m_3}(\hat{k}_3)\delta_{m_1+m_2+m_3,M}|^2, \tag{21}$$

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 $N_r = 72$ 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 $(72\times8)^2$ 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 $(72\times8)^3$ 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 $a = 14.4$, 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 $(72\times8)^2$ 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 $M \leq 2$ and $l_0 \leq 6$. 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 $(144 \times 8)^3$ 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 $m_i = \pm 2$.

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:

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

The wavefunction Ψ^M for a given M symmetry is represented by an expansion in simple products of four-dimensional radial-angular functions $P_{m_1m_2}^M(r_1,\theta_1,r_2,\theta_2,t)$ and rotational functions:

$$\Psi^M(\vec{r}_1,\vec{r}_2,t) = \sum_{m_1}\sum_{m_2}\frac{P_{m_1m_2}^M(r_1,\theta_1,r_2,\theta_2,t)}{r_1\,r_2\,\sqrt{\sin\theta_1}\,\sqrt{\sin\theta_2}}\times\Phi_{m_1}(\phi_1)\Phi_{m_2}(\phi_2), \tag{23}$$

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:

$$i \frac{\partial P^M_{m_1 m_2} (r_1, \theta_1, r_2, \theta_2, t)}{\partial t}$$

$$= \sum_i \left(T_{m_i} (r_i, \theta_i) + V_{HS} (r_i, \theta_i) \right) P^M_{m_1 m_2} (r_1, \theta_1, r_2, \theta_2, t)$$

$$+ \sum_{m_1'} \sum_{m_2'} V^M_{m_1 m_2, m_1' m_2'} (r_1, \theta_1, r_2, \theta_2) P^M_{m_1' m_2'} (r_1, \theta_1, r_2, \theta_2, t).$$

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

$$P^M_{m_1 m_2} (r_1, \theta_1, r_2, \theta_2, t = 0)$$

$$= \sqrt{1/2} [\tilde{P}_{1s0}(r_1, \theta_1) G_{k_0 l_0 m_2} (r_2, \theta_2) \delta_{m_1, 0} \delta_{m_2, M}$$

$$+ (-1)^S G_{k_0 l_0 m_1} (r_1, \theta_1) \tilde{P}_{1s0}(r_2, \theta_2) \delta_{m_1, M} \delta_{m_2, 0}] \tag{25}$$

Momentum space amplitudes are calculated using:

$$B^M_{l_1 m_1 l_2 m_2} (k_1, k_2)$$

$$= \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \times \tilde{P}^*_{k_1 l_1 m_1} (r_1, \theta_1) \tilde{P}^*_{k_2 l_2 m_2} (r_2, \theta_2)$$

$$\times P^M_{m_1 m_2} (r_1, \theta_1, r_2, \theta_2, t \to \infty). \tag{26}$$

The total single ionization cross section is given by:

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

where the subshell occupation number $w_t = 2$ for the ground state of H_2.

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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