Ortho-para transition in molecular hydrogen

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The radiative ortho-para transition in the molecular hydrogen is studied. This highly forbidden transition is very sensitive to relativistic and subtle nonadiabatic effects. Our result for the transition rate in the ground vibrational level $\Gamma(J=1\rightarrow J=0) = 6.20(62)\cdot 10^{-14}$ year^{-1} is significantly lower in comparison to all the previous approximate calculations. Experimental detection of such a weak line by observation of, for example, the cold interstellar molecular hydrogen is at present unlikely.

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The hydrogen molecule in the ground electronic state can exist in a nuclear triplet state ($S=1$, *ortho*-H_2) with the odd angular momentum L, or in a singlet state ($S=0$, *para*-H_2) with the even L. The question we rise is, what are the physical mechanisms for possible transitions between these two classes of states. The nonradiative transition, for example, in the interstellar molecular hydrogen is mostly induced by collisions with atomic H. The corresponding rates were obtained by Sun and Dalgarno in [1]. The radiative transition which is much weaker can in principle take place at sufficiently low densities and temperatures. The relativistic spin-orbit interaction (nuclear spin and the electron momenta) is the most obvious source of this transition as it mixes slightly the o-H_2 and p-H_2 states, see Eq. (1). This effect has been considered in the original work of Raich and Good in [2], although not in a complete and systematic way. It has happened that a tiny nonadiabatic correction to the total H_2 wave function significantly changes the theoretical predictions for this rate. Moreover, the spin-orbit mixing is not the only one effect, which makes this transition possible. There are also relativistic corrections to the $E1$ coupling to the electromagnetic field which is barely known in literature. These corrections in the context of H_2 molecule have been derived for the first time by Dodelson in [3] using the Feinberg-Sucher formalism. Here we rederive this result in a much simpler way. Because of the summation over the infinite H_2 spectrum, the calculations of ortho-para transition amplitude are not completely trivial. The most elaborate so far calculations by Raich and Good [2] including Dodelson corrections [3] gave the rate of $1.85(46)\cdot 10^{-13}$ year^{-1}, which did not include all important contributions. The purpose of this work is to present a complete theoretical description of the radiative ortho-para conversion of H_2 molecule, including the results of direct numerical calculations of the transition probability for the lowest rotational levels.

The interaction of an arbitrary molecule with the electromagnetic field, whose characteristic wavelength is much larger than the size of this molecule, including the relevant spin-orbit interaction is [4]

$$\begin{aligned}\delta H &= -\sum_A e_A\,\vec{x}_A\cdot\vec{E} - \sum_b e_b\,\vec{x}_b\cdot\vec{E} - \sum_A \frac{e_A}{2\,m_A}\\ &\quad\times\Big[g_A\,x_A^i\,s_A^j\,B^j_{,i} + (g_A-1)\,\vec{s}_A\times\vec{x}_A\cdot\partial_t\vec{E}\Big]\\ &\quad+\sum_{A,b}\frac{e_A\,e_b}{4\,\pi}\,\frac{1}{2\,x_{Ab}^3}\left[\frac{g_A}{m_A\,m_b}\,\vec{s}_A\cdot\vec{x}_{Ab}\times\vec{p}_b\right.\\ &\quad\left.-\frac{(g_A-1)}{m_A^2}\,\vec{s}_A\cdot\vec{x}_{Ab}\times\vec{p}_A\right]. \end{aligned}\tag{1}$$

In the above, A,b are the indices of the nuclei and electrons respectively, x_A, x_b are the coordinates of the nuclei and electrons with respect to the mass center, $\vec{x}_{Ab}=\vec{x}_A-\vec{x}_b$, and g_A is the nuclear g-factor. Moreover, the electromagnetic fields $\vec{E},\vec{B}$ and their derivatives are assumed in Eq. (1) to be at the mass center.

For o-H_2 (the first excited rotational state) the nuclear spin $S=1$ couples to the orbital angular momentum $J=1$ of the nuclei, giving the total angular momentum characterized by quantum numbers $F=0,1,2$. In the p-H_2 (the ground rotational state) the total angular momentum is $F=0$, therefore the one photon ortho-para transition from any other $F=0$ level is strictly forbidden, while $F=1$ level decays by $E1$ transition and $F=2$ level decays by the $M2$ transition.

Let us first consider the $M2$ transition from $F=2$ level of o-H_2, to $F=0$ level of p-H_2. This transition comes from the following interaction with the electromagnetic field, which is obtained from Eq. (1)

$$\delta H = -\frac{e\,g_p}{4\,m_p}\,(s_A^j - s_B^j)\,\mathcal{R}^i\,B^j_{,i}\,, \tag{2}$$

with $\mathcal{R} = x_A - x_B$ and the proton g-factor $g_p = 5.585\,694\,713(46)$ [5]. From this Hamiltonian one obtains

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the transition rate $\Gamma(M2) \equiv \Gamma_2$

$$\begin{aligned}\Gamma_2 &= 2\,\alpha\,\omega\,\frac{1}{5}\sum_{m_F}\bigg|\bigg\langle{}^1\Sigma_0\bigg|\frac{g_p}{4\,m_p}\,(\vec{k}\cdot\vec{\mathcal{R}})\,(\vec{s}_A-\vec{s}_B)\times\vec{k}\\ &\quad\bigg|{}^3\Pi_2, m_F\bigg\rangle\bigg|^2\\ &\approx \frac{1}{120}\,\alpha\,\omega^5\left(\frac{g_p\,\mathcal{R}_0}{m_p}\right)^2. \end{aligned} \tag{3}$$

where $\mathcal{R}_0$ is the average distance between protons, and the last equation holds for the nuclear H_2 wave function which is strongly peaked around $\mathcal{R}_0$, as it is the case for the lowest rovibrational levels.

The calculation of the rate for $E1$ transition from $F = 1$ level of o-H_2 to $F = 0$ level of p-H_2 is more complicated as it includes corrections to the wave function coming from the spin-orbit interaction. Since it is $\Delta F = 1$ transition, the operators in the interaction Hamiltonian in Eq. (1) can be simplified, namely $x^i_A\, s^j_A \to \epsilon^{ijk}\,(\vec{x}_A\times\vec{s}_A)^k/2$ and this Hamiltonian becomes

$$\begin{aligned}\delta H &= H_{LS} + e\,(\vec{x}_{1C}+\vec{x}_{2C})\cdot\vec{E}\\ &\quad+\frac{e}{4\,m_p}\left(\frac{g_p}{2}-1\right)\vec{\mathcal{R}}\times(\vec{s}_A-\vec{s}_B)\cdot\partial_t\vec{E}\,, \end{aligned}\tag{4}$$

$$H_{LS} = -\frac{i}{2}\,\vec{H}_{LS}\cdot(\vec{s}_A-\vec{s}_B), \tag{5}$$

$$\vec{H}_{LS} = \frac{g_p\,\alpha}{2\,m_p\,m}\,\vec{h}_1 - \frac{(g_p-1)\,\alpha}{2\,m_p^2}\,\vec{h}_2\times\vec{\nabla}_{\mathcal{R}} \tag{6}$$

$$\vec{h}_1 = \left(\frac{\vec{x}_{1A}}{x^3_{1A}}-\frac{\vec{x}_{1B}}{x^3_{1B}}\right)\times\vec{\nabla}_1 + \left(\frac{\vec{x}_{2A}}{x^3_{2A}}-\frac{\vec{x}_{2B}}{x^3_{2B}}\right)\times\vec{\nabla}_2, \tag{7}$$

$$\vec{h}_2 = \frac{\vec{x}_{1A}}{x^3_{1A}}+\frac{\vec{x}_{1B}}{x^3_{1B}}+\frac{\vec{x}_{2A}}{x^3_{2A}}+\frac{\vec{x}_{2B}}{x^3_{2B}}\,. \tag{8}$$

The resulting transition rate $\Gamma(E1) \equiv \Gamma_1$ is

$$\begin{aligned}\Gamma_1 &= \frac{4}{3}\,\alpha\,\omega\,\frac{1}{3}\sum_{m_F}|\langle{}^1\Sigma_0|\vec{Q}\times\frac{(\vec{s}_A-\vec{s}_B)}{2}|{}^3\Pi_1, m_F\rangle|^2\\ &= \frac{2}{9}\,\alpha\,\omega|\langle\Sigma|Q^k|\Pi^k\rangle|^2\,, \end{aligned}\tag{9}$$

where

$$\begin{aligned}Q^k &= \frac{1}{2\,m_p}\left(\frac{g_p}{2}-1\right)\omega^2\,\mathcal{R}^k\\ &\quad-\frac{\omega}{2}\,\epsilon^{ikj}\,(x^i_{1C}+x^i_{2C})\,\frac{1}{E_\Pi-H}\,H^j_{LS}\\ &\quad-\frac{\omega}{2}\,\epsilon^{ikj}\,H^j_{LS}\,\frac{1}{E_\Sigma-H}\,(x^i_{1C}+x^i_{2C}), \end{aligned}\tag{10}$$

and H is the 4-body nonrelativistic Hamiltonian. In order to simplify the evaluation of Q^k we perform the adiabatic expansion, namely the expansion of the resolvent in the kinetic energy of the nuclei

$$\begin{aligned}\frac{1}{E_\Pi-H} &= \frac{1}{E_{\rm BO}-H_{\rm BO}} - \frac{1}{E_{\rm BO}-H_{\rm BO}}\,(\delta E_\Pi-\delta H_M)\\ &\quad\times\frac{1}{E_{\rm BO}-H_{\rm BO}}+\ldots \end{aligned}\tag{11}$$

similarly for $\frac{1}{E_\Sigma-H}$, and the expansion of the wave function

$$\phi_\Sigma = \psi(\vec{x}_{1C},\vec{x}_{2C};\mathcal{R})\,\lambda_0(\mathcal{R})/\sqrt{4\,\pi}+\delta\phi_\Sigma, \tag{12}$$

$$\phi^k_\Pi = \psi(\vec{x}_{1C},\vec{x}_{2C};\mathcal{R})\,\lambda^k_1(\vec{\mathcal{R}})/\sqrt{4\,\pi}+\delta\phi_\Pi, \tag{13}$$

with $\lambda^k_1 = \lambda_1\,\mathcal{R}^k/\mathcal{R}$ and with normalization

$$\int d\mathcal{R}\,\mathcal{R}^2\,\lambda_0^2(\mathcal{R}) = \int d\mathcal{R}\,\mathcal{R}^2\,\lambda_1^2(\mathcal{R}) = 1\,. \tag{14}$$

While the exact nonadiabatic correction to the wave function is unknown, we need only the first order m/m_p part of the correction, which explicitly depends on the nuclear state [6]

$$\delta\phi_\Sigma = -\frac{2}{m_p}\,\frac{1}{E_{BO}-H_{BO}}\,\nabla^l_{\mathcal{R}}\psi\,\nabla^l\lambda_0/\sqrt{4\,\pi}, \tag{15}$$

$$\delta\phi^k_\Pi = -\frac{2}{m_p}\,\frac{1}{E_{BO}-H_{BO}}\,\nabla^l_{\mathcal{R}}\psi\,\nabla^l\lambda^k_1/\sqrt{4\,\pi}. \tag{16}$$

We introduce now the perturbed electronic wave functions

$$\psi^i_1 = \frac{1}{E_{\rm BO}-H_{\rm BO}}\,(x^i_{1C}+x^i_{2C})\,\psi, \tag{17a}$$

$$\psi^j_2 = \frac{1}{E_{\rm BO}-H_{\rm BO}}\,h^j_1\,\psi, \tag{17b}$$

$$\psi^l_3 = \frac{1}{E_{\rm BO}-H_{\rm BO}}\,\nabla^l_{\mathcal{R}}\,\psi, \tag{17c}$$

to simplify the matrix elements of Q^k in Eq. (10)

$$\begin{aligned}\langle\Sigma|Q^k|\Pi^k\rangle &= \frac{1}{2\,m_p}\left(\frac{g_p}{2}-1\right)\omega^2\,\mathcal{R}_0 - \frac{\omega\,(g_p-1)}{m_p^2\,\mathcal{R}_0}\\ &\quad+\ \omega^2\,\frac{g_p\,\alpha}{4\,m_p\,m}\,X_1 - \omega\,\frac{g_p\,\alpha}{4\,m_p^2\,m\,\mathcal{R}_0}\,(X_2+2\,X_3) \end{aligned}\tag{18}$$

where we used the commutator

$$i\,\big[p^k_1+p^k_2, H_{BO}-E_{BO}\big] = \alpha\,h^k_2, \tag{19}$$

and

$$X_1 = \epsilon^{ikj}\,n^k\,\langle\psi^i_1\,|\,\psi^j_2\rangle_{\mathcal{R}_0}, \tag{20a}$$

$$\begin{aligned}X_2 &= (\delta^{kl}-n^k\,n^l)\,\epsilon^{ikj}\\ &\quad\times\Big[\langle\partial^l_{\mathcal{R}}\psi^i_1\,|\,\psi^j_2\rangle - \langle\psi^i_1\,|\,\partial^l_{\mathcal{R}}\psi^j_2\rangle\Big]_{\mathcal{R}_0}, \end{aligned}\tag{20b}$$

$$\begin{aligned}X_3 &= (\delta^{kl}-n^k\,n^l)\,\epsilon^{ikj}\,\Big[\langle\psi^l_3|(x^i_{1C}+x^i_{2C})|\psi^j_2\rangle\\ &\quad+\langle\psi^l_3|h^j_1|\psi^i_1\rangle\Big]_{\mathcal{R}_0}, \end{aligned}\tag{20c}$$

with $\vec{n} \equiv \vec{\mathcal{R}}_0/\mathcal{R}_0$. One notes that derivatives of nonlinear and linear parameters in ψ, see Eq. (24), with respect to $\mathcal{R}$ do not contribute to the above matrix elements, which significantly simplifies the numerical computations.

Results for X_i can be expressed in terms of dimensionless factors F_i

$$X_1 = -\frac{9}{m^2\,\alpha^4\,\mathcal{R}^2}\,F_1(m\,\alpha\,\mathcal{R}), \tag{21a}$$

$$X_2 = \frac{9}{m^2\,\alpha^4\,\mathcal{R}^3}\,F_2(m\,\alpha\,\mathcal{R}), \tag{21b}$$

$$X_3 = -\frac{2\,m}{\alpha}\,F_3(m\,\alpha\,\mathcal{R}), \tag{21c}$$

which are chosen in such a way, that $F_i(m\,\alpha\,\mathcal{R})$ vanish at $\mathcal{R}=0$ and approach 1 for $\mathcal{R}\to\infty$. However, in the case of F_2 this large $\mathcal{R}$ limit is only a rough approximation, since we have not been able to perform this limit analytically. We can now return to Eq. (18) and obtain a compact formula for the matrix element in the transition rate Γ_1 of Eq. (9)

$$\begin{aligned}\langle\Sigma|Q^k|\Pi^k\rangle &= \frac{\omega^2\,\mathcal{R}_0}{2\,m_p}\left[\left(\frac{g_p}{2}-1\right)-\frac{9}{2}\,\frac{g_p\,F_1}{(m\,\alpha\,\mathcal{R}_0)^3}\right] \\ &- \frac{\omega}{m_p^2\,\mathcal{R}_0}\left[(g_p-1)-g_p\,F_3+\frac{9}{4}\,\frac{g_p\,F_2}{(m\,\alpha\,\mathcal{R}_0)^3}\right].\end{aligned} \tag{22}$$

Numerical evaluation of the Γ_2 rate according to formula (3) is straightforward. To obtain the ortho-para energy spacing ω and the average internuclear distance $\mathcal{R}_0$, we employed the accurate Kołos-LeRoy-Schwartz interaction potential [7] which includes the adiabatic and relativistic energy corrections. With this potential we solved numerically the radial Schrödinger equation to obtain the energies and wave functions corresponding to the lowest ortho and para levels. The numerical values used here are $\omega = 2\pi\cdot 118.49$ cm^{-1} and $\mathcal{R}_0 = 1.449$ au, and the resulting $M2$ transition rate with physical constants from Ref. [5] is

$$\Gamma_2 = 1.07(1)\cdot 10^{-14}\,\mathrm{year}^{-1}\,. \tag{23}$$

The accurate evaluation of Γ_1 and the corresponding electronic matrix elements F_i in Eqs. (21) is a challenging task. We have represented the electronic ground state wave function as well as the first order perturbed functions defined by Eqs. (17), in the form of properly symmetrized linear combinations $\psi = \sum_k c_k \hat{P}_{\mathrm{g,u}}\phi_k$ of Gaussian geminals

$$\begin{aligned}\phi_k &= \Xi_k \\ &\times \exp\left(-\alpha_k\,x_{1A}^2-\beta_k\,x_{1B}^2-\zeta_k\,x_{2A}^2-\eta_k\,x_{2B}^2-\gamma_k\,x_{12}^2\right).\end{aligned} \tag{24}$$

The projection operators

$$\hat{P}_{\mathrm{g,u}} = \frac{1}{4}\,(1+\hat{P}_{12})\,(1\pm\hat{\imath}) \tag{25}$$

ensure the proper symmetry with respect to the exchange of the electrons and with respect to the inversion operation, yielding singlet *gerade* or *ungerade* functions. Required Σ^+, Σ^-, or Π symmetry of the electronic wave function was imposed by the Cartesian prefactor Ξ_k. The linear and the nonlinear parameters were optimized variationally with the goal function being the ground state energy in the case of the unperturbed wave function ψ or pertinent Hylleraas functional

$$\mathcal{J}[\psi_k^i] = \langle\psi_k^i|E_{\mathrm{BO}}-H_{\mathrm{BO}}|\psi_k^i\rangle + 2\langle\psi|\hat{\mathcal{O}}|\psi_k^i\rangle \tag{26}$$

in the case of the perturbed functions ψ_k^i. Table I shows explicitly the elements defining particular functions with the assumption that the molecule is placed along the Cartesian X axis. The unperturbed wave function has been expanded in 600-term basis set which enables the electronic ground state energy to be obtained with an error of only $3\cdot10^{-9}$ a.u. A 1200-term expansions have been employed to represent the perturbed functions. Values of the $\mathcal{J}$ functionals corresponding to the optimum parameters are displayed in Table II.

TABLE I: The definitions of the functions used in the computations.

	Ξ_k	$\hat{P}$, Eq. (25)	$\hat{\mathcal{O}}$, Eq. (26)
ψ	1	gerade	–
ψ_1^x	$x_1,\,x_2$	ungerade	x_1+x_2
ψ_1^y	$y_1,\,y_2$	ungerade	y_1+y_2
ψ_1^z	$z_1,\,z_2$	ungerade	z_1+z_2
ψ_2^x	$y_1z_2-y_2z_1$	ungerade	h_1^x
ψ_2^z	$y_1,\,y_2$	ungerade	h_1^z
ψ_3^y	$y_1,\,y_2$	gerade	$\partial_{\mathcal{R}}^y$

The general formulas (20), in the particular case of the molecule oriented along the X axis, can be explicitly written as follows

$$X_1 = -2\big\langle\psi_1^y\,|\,\psi_2^z\big\rangle_{\mathcal{R}_0}, \tag{27a}$$

$$X_2 = 4\Big[\big\langle\partial_{\mathcal{R}}^y\psi_1^x\,|\,\psi_2^z\big\rangle-\big\langle\partial_{\mathcal{R}}^y\psi_1^z\,|\,\psi_2^x\big\rangle\Big]_{\mathcal{R}_0}, \tag{27b}$$

$$\begin{aligned}X_3 &= 2\Big[\langle\psi_3^y|(x_{1C}^x+x_{2C}^x)|\psi_2^z\rangle-\langle\psi_3^y|(x_{1C}^z+x_{2C}^z)|\psi_2^x\rangle \\ &\quad+\langle\psi_3^y|h_1^z|\psi_1^x\rangle-\langle\psi_3^y|h_1^x|\psi_1^z\rangle\Big]_{\mathcal{R}_0}.\end{aligned} \tag{27c}$$

Table II contains all the expectation values appearing in Eqs. (27) as well as the final X_i and F_i values computed at $\mathcal{R}_0 = 1.449$ bohr. To check the correctness of our codes we performed additional calculations at large internuclear distance ($\mathcal{R} = 12.0$ bohr) and compared the resulting goal functions and the expectation values with analytically derived asymptotic values. This comparison is presented in Table II.

Using Eqs. (9), (22), and the Table II one obtains the numerical value for the $E1$ transition rate

$$\Gamma_1 = 1.68(17)\cdot10^{-13}\ \mathrm{year}^{-1}\,, \tag{28}$$

and finally the rate averaged over the total angular momentum F

$$\Gamma = (5\,\Gamma_2+3\,\Gamma_1)/9 = 6.20(62)\cdot10^{-14}\ \mathrm{year}^{-1}\,. \tag{29}$$

TABLE II: Numerical values of the optimum goal functions Eq. (26) and the expectation values comprising the X_i factors Eqs. (27) in atomic units.

	$\mathcal{R}_0 = 1.449$	$\mathcal{R} = 12.0$	Asymp.
$E_{\rm BO}$	$-1.174\,073\,569$	$-1.000\,002\,546$	-1.0
$\mathcal{J}[\psi_1^x]$	-3.3582	-4.5241	-4.5
$\mathcal{J}[\psi_1^y]$	-2.3684	-4.4885	-4.5
$\mathcal{J}[\psi_2^x]$	-7.87×10^{-3}	-2.22×10^{-7}	0.0
$\mathcal{J}[\psi_2^z]$	-0.4925	-5.06×10^{-5}	0.0
$\mathcal{J}[\psi_3^y]$	-2.90×10^{-2}	-0.2500	-0.25
$\langle \psi_1^y \mid \psi_2^z \rangle$	0.7824	0.0312	
X_1	-1.5649	-0.0623	
F_1	0.3651	0.9975	1.0
$\langle \partial_{\mathcal{R}}^y \psi_1^x \mid \psi_2^z \rangle$	0.7467	0.0014	
$\langle \psi_1^z \mid \partial_{\mathcal{R}}^y \psi_2^x \rangle$	0.0034	0.0002	
X_2	3.0003	0.0062	
F_2	1.0142	1.1989	
$\langle\psi_3^y\vert(x_{1C}^x+x_{2C}^x)\vert\psi_2^z\rangle$	0.0707	-0.0029	
$\langle\psi_3^y\vert(x_{1C}^z+x_{2C}^z)\vert\psi_2^x\rangle$	-0.0010	-0.0001	
$\langle\psi_3^y\vert h_1^z\vert\psi_1^x\rangle$	-0.2579	-0.5026	
$\langle\psi_3^y\vert h_1^x\vert\psi_1^z\rangle$	0.1066	0.4980	
X_3	-0.3984	-2.0037	
F_3	0.1992	1.0019	1.0

Our result for the averaged transition rate is in disagreement with the result of Dodelson [3], $\Gamma = 1.85(46)\cdot 10^{-13}\,\text{year}^{-1}$, which is in turn based on the former work of Raich and Good [2] and included direct coupling of nuclear spin to the radiation field. We confirm in this work the existence of these additional couplings, which here are expressed by the 3rd term in Eq. (1). In our opinion, the difference from our result is due to the omission of the $M2$ transition, the omission of the nonadiabatic contributions corresponding to X_2 and X_3 in Eq. (20), less accurate ω, and due to a lower accuracy of the numerical calculation of the matrix elements in Ref. [2]. In particular, without X_3 the overall rate Γ would be about 24% larger.

The possibility of the experimental detection of the *o*-*p* H_2 line is questionable. Much stronger $E2$ lines have already been observed at the *Infrared Space Observatory* ISO and served for estimation of the temperature of interstellar hydrogen clouds and of the ratio of abundance *o*-H_2 to *p*-H_2, which sometimes differs significantly from the equilibrium one [8]. The much weaker $E1$ line has not been observed yet. In fact there is a potential opportunity related with the Herschel Space Observatory to be launched in 2008 [9]. Its spectral range covers the *o*-*p* line at 84.4 μm, but its resolution is, probably, not high enough at this wavelength.

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