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# Are collisions with electrons important for modeling the polarization of the lines of the $C_2$ solar molecule?

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Abstract Observations of the second solar spectrum (SSS) revealed the existence of prominent linear polarization signals due to lines of the C<sub>2</sub> molecule. Interpretation of the SSS is the only tool to obtain the weak and turbulent magnetic field which is widespread in the Quiet Sun. However, this interpretation is conditioned by the determination of accurate collisional data. In this context, we present a formulation of the problem of the calculation of the polarization transfer rates by collisions of polarized C<sub>2</sub> states with electrons. The obtained formulae are applied to determine, for the first time, the polarization transfer rates between the C<sub>2</sub> states of the Swan band electronic system ( $a^{3}\Pi_{u} - d^{3}\Pi_{g}$ ) and electrons for temperatures going up from 1000 to 10 000 K. However, due to the closeness of the electronic states of the C<sub>2</sub> molecule, the two electronic  $d^{3}\Pi_{g}$  and  $a^{3}\Pi_{u}$  cannot be disconnected from the other electronic levels and, thus, a model based on only two states is not sufficient to describe the formation of the lines in the Swan band. Consequently, we also calculated the collisional polarization transfer rates in the case where the first eight electronic states of C<sub>2</sub> are taken into account. All rates are given as functions of the temperature by power laws. Our results should be useful for future solar applications.

Key words: Collisions — Sun: photosphere — atomic processes — line: formation — polarization

## **1 INTRODUCTION**

Close to the solar limb, scattering processes of incident anisotropic radiation can create linear polarization in spectral lines without the need for magnetic fields. This linear polarization is usually referred to as a second solar spectrum (SSS). Once the polarization is created, it can be modified by the Hanle effect of a weak and turbulent magnetic field. Interpretation of the SSS, in terms of magnetic fields, means that theoretical polarization should be fitted to the observed one. The best fit is obtained through an iterative method by first adjusting the polarization profile with a magnetic field value B, and then repeating the procedure by varying the B-value until the difference between theoretical and observed profiles reaches its minimum. This yields a value of the magnetic field B, which is thus uniquely determined. This technique is known nowadays to be the only tool for obtaining the turbulent and weak magnetic field.

Molecular lines observed in the solar photosphere have, in general, peaks of polarization in the SSS. These lines are almost absent in the ordinary intensity spectrum. The polarization is generated by anisotropic radiative scattering. Due to the richness of internal structure of the molecules, in a single band of an electronic transition, one can find many molecular polarized lines of the SSS which are formed practically in the same photospheric region. Thus, one can interpret the polarization of selected molecular lines by using the differential Hanle effect, which leads to determination of the solar magnetic field (e.g., Asensio & Trujillo 2005; Berdyugina & Fluri 2004).

To model the formation of the SSS, one should take into account all the relevant physical processes present during its formation. However, all works dedicated to analysis of the polarization of the molecular lines faced a clear lack of collisional data (e.g., Mohan Rao & Rangarajan 1999; Faurobert & Arnaud 2003; Trujillo Bueno et al. 2004). This long-term problem was strongly emphasized by the solar community (e.g., Trujillo Bueno et al. 2006). Since the beginning of the 2000s, the urgent need for collisional molecular data was highlighted, but from that time until now, only very few works focused on investigating this problem (see Derouich 2006; Derouich et al. 2019; Qutub et al. 2020).

In the photosphere, there are two kinds of perturbers which are currently considered in modeling the solar molecular polarization, (a) hydrogen atoms which induce elastic collisions (i.e., collisions within an electronic state) and (b) electrons inducing inelastic collisions (i.e., collisions involving two electronic states). Recently, we presented the first calculations of the (de)polarization rates by elastic collisions with hydrogen atoms for a solar molecule, namely the CN molecule (Qutub et al. 2020).

The effect of inelastic collisions with electrons on the polarization of solar molecules is unknown. From a solar

applications point of view, inelastic or elastic collisions have been more thoroughly researched in the case of polarized atoms than polarized molecules. In fact, over more than 15 years we published tens of works concentrating on atomic collisions (e.g., Derouich et al. 2003; Derouich 2004; Derouich et al. 2004; Derouich & Barklem 2007; Sahal-Bréchot et al. 2007, Derouich et al. 2015; Derouich 2018; Derouich 2019). Our aim in this work is to provide, for the first time, collisional polarization rates due to collisions between electrons and the  $C_2$  solar molecule in its ground and excited states.

# 2 DEFINITION OF THE POLARIZATION TRANSFER CROSS-SECTIONS

We consider a  $C_2$  molecular level subjected to the action of collisions with electrons. This level is assumed to be polarized, i.e., quantum coherences exist among its Zeeman sub-levels which are also unevenly populated. The signature of such a polarization is observed in the SSS. In the photosphere where the SSS forms, collisions with electrons are mainly isotropic. In order to define the collisional polarization transfer cross-sections and rates, one should consider suitable coupling schemes and adopt the tensorial basis  $T_q^k$  (e.g., Sahal-Bréchot 1977; Trujillo Bueno 2001; Landi & Landolfi 2004). Here k is called the tensorial order and it is usually an integer; q quantifies the coherences between the Zeeman sublevels (e.g., Landi & Landolfi 2004). Due to the isotropy of the collisions, all polarization transfer cross-sections and rates are q-independent.

In the framework of the infinite order sudden (IOS) approach, the rotation of the  $C_2$  molecule during the collision is neglected. Its criterion of validity is (e.g., Pack 1974)

$$E >> B N (N+1), \tag{1}$$

where E is the kinetic energy, B is the rotational constant of the molecule and N is the rotational number. For solar temperatures where  $T \sim 5800$  K, the corresponding kinetic energy is  $E \sim 4000 \text{ cm}^{-1}$ . The rotational constant B is given, for many electronic states of the C<sub>2</sub> molecule, in Bornhauser et al. (2010, 2011) and in Brooke et al. (2013). In fact,  $B \sim 1.2 \text{ cm}^{-1}$ , thus for a typical value N = 10,  $BN(N+1) \sim 130 \text{ cm}^{-1}$  which is effectively much smaller than  $E \sim 4000 \text{ cm}^{-1}$ , implying that the IOS is well validated.

Furthermore, as we are interested in the solar temperatures, where the kinetic energies of collisions are high, one can expect that some simplifications regarding the coupling effects, like the IOS approximation invoked in this work, can be adopted in order to obtain results with acceptable accuracy in reasonable computing time. In this sense, Derouich & Ben Abdallah (2009) compared polarization transfer cross-sections of the CH molecule obtained by the full close-coupling method to those obtained by the IOS approximation and found that, for temperatures larger than 200 K, the IOS is sufficient. The IOS approximation has been extensively tested and successfully applied since it was proposed in the seventies (e.g., Goldflam et al. 1977; Corey & Alexander 1985; Corey et al. 1986; Derouich 2006; Lique et al. 2006).

By implementing the same coupling schemes presented in detail, for example, by Harrison et al. (2013) (see also Corey & Smith 1985), we express the polarization transfer cross sections  $\sigma_{IOS}^k(e_i \ Nj \rightarrow e_f \ N'j', E)$  within the framework of the IOS approximation by

$$\sigma_{IOS}^{k}(e_{i} \ Nj \to e_{f} \ N'j', E) = \sum_{K} (-1)^{k+j'+K+j+1} (2N+1)(2N'+1)(2j'+1)(2j+1) \left\{ \begin{array}{c} j \ j' \ K \\ j' \ j \ k \end{array} \right\} \times \left\{ \begin{array}{c} N \ N' \ K \\ j' \ j \ S_{m} \end{array} \right\}^{2} \left( \begin{array}{c} N' \ N \ K \\ 0 \ 0 \ 0 \end{array} \right)^{2} \sigma(e_{i}0 \to e_{f}K, E),$$

$$(2)$$

where E is the kinetic energy, and

- N is the rotational angular momentum of  $C_2$ ;

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- $S_m$  is the spin of the C<sub>2</sub> molecule;
- $-j = N + S_m;$
- -l is the angular momentum of the electron relative to the C<sub>2</sub> molecule
- L is the orbital momentum of the C<sub>2</sub> molecule
- $-e_i$  and  $e_f$  are the electronic lower and upper electronic C<sub>2</sub> states, respectively

The index K can be identified as the amount of angular momentum transferred during the collision. The possible values of K are provided by the triangle inequalities contained in the six *j*-symbols of Equation (2). We notice that due to the triangle conditions, the three *j*-coefficients  $\binom{N' \ N \ K}{0 \ 0 \ 0}$  vanish identically unless N + N' + K is of even parity. Note that the orbital momentums *l* and *L* do not appear explicitly in the expression for the IOS cross-section  $\sigma_{IOS}^k(e_i \ Nj \rightarrow e_f \ N'j')$ ; in fact they are included in the generalized cross-section  $\sigma_{IOS}(e_i 0 \rightarrow e_f K)$ . We assume that  $\sigma_{IOS}(e_i 0 \rightarrow e_f K)$  is associated with the transition between two electronic levels with the same vibrational and rotational levels.

Calculations of the  $\sigma(e_i \to e_f)$  were performed by Halmová et al. (2006) and Halmova (2008) in the context of a sophisticated quantum chemistry R-matrix formalism based on a 26-state close-coupling expansion. In order to exploit their results and to estimate, for the first time, polarization transfer rates by collisions between electrons and C<sub>2</sub> molecules, we assume that  $\sigma(e_i 0 \to e_f K) \simeq \sigma(e_i \to e_f)$  which can be considered as a satisfactory assumption due to the closeness of the electronic states of the C<sub>2</sub> molecule.

As has been explained, for example, in Harrison & Tennyson (2012) and Harrison et al. (2012), who treated collisions between electrons and diatomic molecules, the IOS approximation is useful since it greatly reduces computation time while keeping an acceptable precision when the collision energy is large. In addition, it is advantageous for our purpose in this work because only in the framework of the IOS approximation is it possible to express the polarization transfer cross-sections  $\sigma_{IOS}^k(e_i \ Nj \to e_f \ N'j', E)$  as a linear combination of the standard collisional cross-sections  $\sigma(e_i \to e_f)$ (Eq. (2)).

By averaging  $\sigma_{IOS}^k(e_i N j \rightarrow e_f N' j', E)$  over a Maxwellian distribution of relative kinetic energies E, one obtains the polarization transfer rates

$$C^{k}(e_{i} Nj \to e_{f} N'j', T) = n_{e} \left(\frac{8}{\pi\mu k_{B}^{3}T^{3}}\right)^{1/2} \int_{0}^{\infty} \sigma_{IOS}^{k}(e_{i} Nj \to e_{f} N'j', E) \exp\left(-\frac{E}{k_{B}T}\right) EdE,$$
(3)

where  $\mu$  is the reduced mass of the system {electron+C<sub>2</sub>} and  $n_e$  is the density of the electrons.

Quantum description of the atomic and molecular states is suitably performed by utilizing the density matrix elements  $\rho_q^k(e_i \ Nj)$  expressed in the basis of irreducible tensorial operators (ITOs) (e.g., Sahal-Bréchot 1977; Landi & Landolfi 2004). In the ITO basis, the rate of variation of  $\rho_q^k(e_i \ Nj)$  due to isotropic collisions with electrons can be written as (e.g., Derouich 2006)

$$\frac{d \ \rho_q^k(e_i \ Nj)}{dt} = -\rho_q^k(e_i \ Nj) \sum_{e_f \neq e_i} \sum_{N'j'} \sqrt{\frac{2j'+1}{2j+1}} C^0(e_i \ Nj \to e_f \ N'j') + \sum_{e_f \neq e_i} \sum_{N'j'} C^k(e_f \ N'j' \to e_i \ Nj) \ \rho_q^k(e_f \ N'j').$$
(4)

Equation (4) is a part of the contribution of the collisions in the statistical equilibrium equations (SEE). It is necessary to add the contribution of collisions of  $C_2$  with neutral hydrogen atoms in order to obtain the complete contribution of collisions.

#### **3 NUMERICAL CALCULATION**

We are interested in the contribution of the C<sub>2</sub>-electron isotropic collisions to the formation of the polarization of the (v = 0, v = 0) band for the Swan electronic system  $(d \ ^3\Pi_g - a \ ^3\Pi_u)$  of the C<sub>2</sub> solar molecule; v denotes the vibrational level. However, the two electronic states  $a \ ^3\Pi_u$  and  $d \ ^3\Pi_g$  cannot be disconnected from the other close electronic states. A model based only on two states is not sufficient to describe the formation of the lines in the Swan band. As can be seen in Table 1, the first eight electronic states  $(X \ ^1\Sigma_g, a \ ^3\Pi_u, b \ ^3\Sigma_g, A \ ^1\Pi_u, c \ ^3\Sigma_u, B \ ^1\Delta_g, B' \ ^1\Sigma_g, d \ ^3\Pi_g)$  are remarkably close in the case of the C<sub>2</sub> solar molecule and they have to be taken into account in the modeling process. Note that this

closeness of the electronic states is specific to the  $C_2$  molecule and is not necessarily present in the cases of other solar molecules.

According to Halmová et al. (2006), the first excited state  $a {}^{3}\Pi_{u}$  lies 0.066 eV lower than the ground state  $a {}^{1}\Sigma_{g}$  at  $R_{e} = 2.548 a_{0}$ ;  $R_{e}$  is the internuclear distance for equilibrium geometry. These physical realities make it important to not only consider the effect of the collisional rate between the two states  $(d {}^{3}\Pi_{g} - a {}^{3}\Pi_{u})$  of the Swan electronic system, but one has to also include the effect of other electronic states in the SEE. In other words, reliable interpretation of the linear polarization degree that scattering processes produce in the Swan electronic states given in Table 1. At the position of the equilibrium  $R_{e} = 2.54 a_{0}$ , the difference in energy between the ground state  $X^{1}\Sigma_{g}^{+}$  and the highest excited state  $d^{1}\Pi_{q}^{-}$  is 2.507 eV.

We notice that some electronic transitions between the eight electronic states are forbidden due to the dipolar selection rules. For instance, the transition between two first levels  $X^{-1}\Sigma_g$  and  $d^{-3}\Pi_g$  is forbidden. As can be seen in Halmová et al. (2006), collisional cross-sections corresponding to this transition are very weak if compared to the cross-sections associated with the permitted transition  $a^{-3}\Pi_u - d^{-3}\Pi_g$ . Although the collisional processes do not obey strong selection rules like electric dipole radiative transitions, it is usually found that collisions with electron rates produce weak values for the forbidden lines.

We used the excitation cross-sections  $\sigma(e_i \rightarrow e_f)$  calculated by Halmová et al. (2006) for a large number of electronic states in order to obtain the polarization transfer cross-sections. Results of Halmová et al. (2006) were obtained by following the sophisticated quantum R-matrix method for a range of energy going from 0 to 10 eV which allows us to determine collision rates for temperatures up to 10 000 K.

In this work, for illustrative purposes, we choose to show only the polarization transfer rates between the levels j' = 6 (upper electronic state) and j = 6 (lower electronic state). We verified that our conclusions in this work will not be affected by this choice of the values j and j'. Let us mention also that the maximum values of polarization transfer rates are reached for small values of  $\Delta j = |j' - j|$ .

In Figure 1, we provide polarization transfer rates from the state  $a {}^{3}\Pi_{u}$  to  $d {}^{3}\Pi_{g}$ , and from  $a {}^{3}\Pi_{u}$  or  $a {}^{3}\Sigma_{g}$  to other electronic states lower than  $d {}^{3}\Pi_{g}$ . All rates are given for k = 0, k = 1 and k = 2. It is possible to provide a good least squares fit for the polarization transfer rates presented in Figure 1. As a result, transfer rates can be obtained by employing the following variation laws

$$C^{k}(e_{i} N j \to e_{f} N' j') = n_{e} \left[a_{0} + a_{1}\left(\frac{T}{5000}\right) + a_{2}\left(\frac{T}{5000}\right)^{2}\right],$$
 (5)

where the values of  $a_0$ ,  $a_1$  and  $a_2$  are provided in Table 2. The rates are given for tensorial orders k = 0, k = 1 and k = 2. Let us recall that the population of the *j*-level is related to the order k = 0, the circular polarization is associated with the orientation terms with k = 1 and the linear polarization is associated with the alignment of the level (k = 2). The analytical relationships expressed in Equation (5), giving the rates as functions of the temperatures, are obtained with a correlation coefficient R > 0.99. These relationships are useful for solar applications and can be easily included in the radiative transfer numerical codes.

Deexcitation collisional rates  $C^k(e_f N'j' \rightarrow e_i Nj)$  can be retrieved by applying the detailed balance relation

$$C^{k}(e_{f} \ N'j' \to e_{i} \ Nj, T) = \frac{2j+1}{2j'+1} \exp\left(\frac{E_{j} - E_{j'}}{k_{B}T}\right) \ C^{k}(e_{i} \ Nj \to e_{f} \ N'j', T),$$
(6)

where  $E_j$  is the energy of level (j) and  $k_B$  the Boltzmann constant.

# 4 ARE COLLISIONS WITH ELECTRONS IMPORTANT IN MODELING THE SSS OF C<sub>2</sub>?

In order to model the formation of molecular lines, theoretically, collisions with electrons have to be taken into account. But, the effect of these collisions is important only if the values of their rates are comparable to the Einstein coefficient of the transition of the studied lines. Brooke et al. (2013) calculated the Einstein A coefficient for the vibrational band (0-0) of the Swan band by utilizing accurate quantum chemistry methods. They found that  $A = 7.626 \times 10^6 \text{ s}^{-1}$ . For temperature T = 6000 Kand for k = 0, 1 or 2, the largest value of  $C^k(e_f N'j' \rightarrow e_i Nj, T) = N_e 25.297 \times 10^{-10} \text{ s}^{-1}$ . Thus for typical photospheric electron densities  $N_e = 10^{12} \text{ cm}^{-3}$ , the maximum value of  $C^k(e_f N'j' \rightarrow e_i Nj, T) \simeq 2.5 \times 10^3$ << A. This quick comparison demonstrates that the colli-



Fig. 1 Polarization transfer rates by collisions with electrons as a function of temperatures going from 1000 K to 10 000 K for different electronic states of  $C_2$  and for k = 0, k = 1 and k = 2.

Table 1 Energy of the First Electronic States of the C2 Molecule (Halmová et al. 2006)

Energy (eV)
-0.066
0.
0.089
1.052
1.206
1.662
1.879
2.507

**Table 2** Coefficients  $a_0$ ,  $a_1$  and  $a_2$  in [×10<sup>-10</sup> s<sup>-1</sup>] for temperatures ranging from 1500 K to 10 000 K. These coefficients allow the determination of the polarization transfer rates by collisions with electrons.

$X \ ^1\Sigma_g \rightarrow$ other states lower than $d \ ^3\Pi_g$				$a {}^{3}\Pi_{u} \rightarrow$ other states lower than $d {}^{3}\Pi_{g}$			$a \ ^3\Pi_u \rightarrow a \ ^3\Pi_u$		
k	$a_0$	$a_1$	$a_2$	$a_0$ .	$a_1$	$a_2$	$a_0$ .	$a_1$	$a_2$
0	0.1956	12.2505	9.80275	-0.46216	-1.61935	7.079	0.79943	-3.36875	2.958
1	0.15025	9.4355	7.54875	-0.35588	-1.24715	5.45175	0.61567	-2.59435	2.27793
2	0.11385	7.152	5.72175	-0.26984	-0.9451	4.13225	0.46665	-1.9664	1.7266

sions with electrons cannot be important in the calculation of scattering polarization for solar molecules. From now on, one can consider that inelastic collisions with electrons can be safely neglected for lines of the SSS formed in the photosphere of the Sun.

## **5** CONCLUSIONS

Molecules have rich and complex spectra because their configurations are based on multiple electronic, vibrational and rotational states. This is reflected in the fact that, within a narrow spectral window, many lines are contained in one band of an electronic transition and can be covered by simultaneous observations. Thus, for example, one can efficiently apply the differential Hanle effect to extract the magnetic field of the Sun. However, to correctly interpret the observed polarization, depolarizing and polarizing collisions of the molecular states should be known without ambiguity.

Unfortunately, especially for solar molecules, many collisional problems are still open. Only recently, a first paper was concerned with collisions of the solar CN molecule with neutral hydrogen (Qutub et al. 2020). Collisions with electrons is another kind of collision for which the effect on the solar molecular polarization is still unknown. In this work, we proposed a quantum determination of the collisional polarization transfer rates by collisions of the C2 solar molecule with electrons. Our main concern in this work is to answer the question about the efficiency of the electron collisions on the polarization of the C<sub>2</sub> molecule. We conclude that for typical photospheric electron density, the polarization of the C2 molecule is insensitive to collisions with electrons. Results of this work can be regarded as a useful indication about cases of other solar molecules for which the polarization collisional rates are not known.

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