Are collisions with electrons important for modeling the polarization of the lines of the C\textsubscript{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\textsubscript{2} molecule. Interpretation of the SSS is the only tool to obtain 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\textsubscript{2} states with electrons. The obtained formulae are applied to determine, for the first time, the polarization transfer rates between the C\textsubscript{2} states of the Swan band electronic system (a \textsuperscript{3}\Pi\textsubscript{u} – d \textsuperscript{3}\Pi\textsubscript{g}) and electrons for temperatures going up from 1000 to 10000 K. However, due to the closeness of the electronic states of the C\textsubscript{2} molecule, the two electronic d \textsuperscript{3}\Pi\textsubscript{g} and a \textsuperscript{3}\Pi\textsubscript{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 of the Swan band. Consequently, we also calculated the collisional polarization transfer rates in the case where the first eight electronic states of C\textsubscript{2} 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 us as second solar spectrum (SSS). Once the polarization is created, it can be modified by the Hanle effect of 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 to 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 second solar spectrum (SSS). These lines are almost absent in the ordinary intensity spectrum. The polarization is generated by anisotropic radiative scattering. Due to the richness of the 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 pratically in the same photospheric region. Thus, one can interpret the polarization of selected molecular lines by using the differenti al Hanle effect which leads to determination of solar magnetic field (e.g. Asensio Ramos & Trujillo Bueno 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 the analysis of the polarization of the molecular lines faced the clear lack of collisional data (eg Mohan Rao et al. 1999; Faurobert & Arnaud 2003; Trujillo Bueno et al. 2004). This long-time problem was strongly emphasized by the solar community (e.g. Trujillo Bueno et al. 2006). Since the beginnings of the 2000’s, the urgent need to collisional molecular data was highlighted, but from that time until now only very few works were dedicated to the understanding of this problem (see Derouich 2006, Qutub et al. 2019).

In the photosphere, there are two kinds of perturbers which are currently considered in the modeling of 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. 2019).

The effect of inelastic collisions with electrons on the polarization of solar molecules is unknown. From solar applications point of view, inelastic or elastic collisions are more known in the case of polarized atoms than polarized molecules. In fact, over more than 15 years we published tens of works concentrated on atomic collisions (e.g. Derouich et al. 2003; Derouich 2004; Derouich et al. 2004; Derouich & Barklem 2007; Sahal-Bréchet 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 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. there exist quantum coherences 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 $T^k_q$ (e.g. Sahal-Bréchet 1977, Trujillo Bueno 2001, Landi Degl’Innocenti & Landolfi 2004). Here $k$ is called the tensorial order and it is usually integer; $q$ quantifies the coherences between the zeeman-sublevels (e.g. Landi Degl’Innocenti & 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 criteria of validity is (e.g. Pack 1972):

$$E >> B N (N + 1)$$

(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 $T \sim 5800K$, the corresponding kinetic energy is $E \sim 4000 \text{cm}^{-1}$. The rotational constant $B$ is given, for many electronic states of the C$_2$ molecule, by Bornhauser et al. (2010, 2011) and in James et al. (2013). In fact, $B \sim 1.2 \text{cm}^{-1}$, thus for a typical value $N = 10$, $B N (N + 1) \sim 130 \text{cm}^{-1}$ 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 resonable computing time. In this sense, Derouich & Ben Abdallah (2009) compared polarization transfer cross-sections of the CH molecule obtained by full close-coupling method to those obtained by the IOS approximation and found that, for temperatures larger than 200K, the IOS is sufficient. The IOS approximation has been extensively tested and successfully used since it was proposed in the seventies.
By using the same coupling schemes presented in details, for example, by Harrison et al. (2013) (see also Corey & Smith 1985), we express the polarization transfer cross sections $\sigma^{k}_{\text{IOS}}(e_i, N_j \rightarrow e_f, N^\prime j^\prime, E)$ within the framework of the IOS approximation by:

$$\sigma^{k}_{\text{IOS}}(e_i, N_j \rightarrow e_f, N^\prime j^\prime, E) = \sum_{K} (-1)^{k+j^\prime+K+j+1}(2N+1)(2N^\prime+1)(2j^\prime+1)(2j+1) \left\{ \begin{array}{ccc} j & j^\prime & K \\ j & j & k \end{array} \right\} \times \left\{ \begin{array}{ccc} N & N^\prime & K \\ j & j & S_m \end{array} \right\} \left( \begin{array}{ccc} N^\prime & N & K \\ 0 & 0 & 0 \end{array} \right)^2 \sigma(e_i,0 \rightarrow e_f K, E),$$

where $E$ is the kinetic energy, and

- $N$ is the rotational angular momentum of the $C_2$;
- $S_m$ is the spin of the $C_2$ molecule;
- $j = N + S_m$;
- $l$ is the angular momentum of the electron relative to the $C_2$ molecule
- $L$ is the orbital momentum of the $C_2$ molecule
- $e_i$ and $e_f$ are the electronic lower and upper electronic $C_2$ states, respectively

The index $K$ can be identified as the amount of angular momentum transferred during the collision. The possible values of $K$ are given by the triangle inequalities contained in the 6 $j$-symbols of the Equation 2. We notice that due to the triangle conditions, the 3$j$-coefficients $\left( \begin{array}{ccc} N^\prime & N & K \\ 0 & 0 & 0 \end{array} \right)$ vanishes identically unless $N + N^\prime + K$ is of even parity. Note that the orbital momentums $l$ and $L$ do not appear explicitly in the expression of the IOS cross-section $\sigma^{k}_{\text{IOS}}(e_i, N_j \rightarrow e_f, N^\prime j^\prime)$; in fact they are included in the generalized cross-section $\sigma_{\text{IOS}}(e_i,0 \rightarrow e_f K)$. We assume that $\sigma_{\text{IOS}}(e_i,0 \rightarrow e_f K)$ is associated to the transition between two electronic levels with the same vibrational and rotational levels.

Calculations of $\sigma(e_i \rightarrow e_f)$ were performed by Halmová et al. (2006) and Halmová (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 $C_2$ molecules, we assume that $\sigma(e_i,0 \rightarrow e_f K) \simeq \sigma(e_i \rightarrow e_f)$ which can be considered as satisfactory assumption due to the closeness of the electronic states of the $C_2$ molecule.

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

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

$$C^{k}(e_i, N_j \rightarrow e_f, N^\prime j^\prime, T) = n_e \left( \frac{8}{\pi \mu k_B T^3} \right)^{1/2} \int_{0}^{\infty} \sigma^{k}_{\text{IOS}}(e_i, N_j \rightarrow e_f, N^\prime j^\prime, E) \exp \left( -\frac{E}{k_B T} \right) E dE,$$

where $\mu$ is the reduced mass of the system \{electron+C_2\} and $n_e$ is the density of the electrons.

Quantum description of the atomic and molecular states is suitably performed by using the density matrix elements $\rho^{k}_{ij}(e_i, N_j)$ expressed on the basis of irreducible tensorial operators (ITO) (e.g.
Sahal-Bréchot 1977; Landi Degl’Innocenti & 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):

\[
\frac{d \rho_{q}^{k}(e_{i}, Nj)}{dt} = -\rho_{q}^{k}(e_{i}, Nj) \sum_{e_{f} \neq e_{i}} \sum_{Nj'=1}^{2} \left( \frac{2j'+1}{2j+1} \right) C^{0}(e_{i}, Nj \rightarrow e_{f}, Nj') + \sum_{e_{f} \neq e_{i}} C^{k}(e_{f}, Nj' \rightarrow e_{i}, Nj) \rho_{q}^{k}(e_{f}, Nj')
\]

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 \( \text{C}_2 \) with neutral hydrogen atoms in order to obtain the complete contribution of collisions.

3 NUMERICAL CALCULATION

We are interested in the contribution of the \( \text{C}_2 \)-electron isotropic collisions in the formation of the polarization of the \((v=0, v=0)\) band of the Swan electronic system (\( d^{3}\Pi_u - a^{3}\Pi_g \)) of the \( \text{C}_2 \) 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 of the Swan band. As it can be seen in Table 1, the first eight electronic states \((X^{1}\Sigma_u^{-}, a^{3}\Pi_u, b^{3}\Sigma_g, A^{1}\Pi_u, c^{3}\Sigma_u, B^{1}\Delta_g, B'^{1}\Sigma_g, d^{3}\Pi_g)\) are remarkably close in the case of the \( \text{C}_2 \) solar molecule and they have to be taken into account in the modeling case. Note that this closeness of the electronic states is specific to the \( \text{C}_2 \) 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 \( a^{1}\Sigma_g \) state at the \( R_e = 2.548 \) a_0; \( R_e \) is the internuclear distance for equilibrium geometry. These physical realities make it important to not consider only 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 include in the SEE also the effect of other electronic states. In other words, reliable interpretation of the linear polarization degree that scattering processes produce in the Swan electronic system requires solving numerically the coupled set of the SEE of a multilevel system taking into account the eight electronic states given in Table 1. At the position of the equilibrium \( R_e = 2.548 \) a_0, the difference of energy between the ground state \( X^{1}\Sigma_u^{-} \) and the highest excited state \( d^{3}\Pi_u^{3} \) 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 \( X^{1}\Sigma_u^{-} \) and \( d^{3}\Pi_g \) is forbidden. As it can be seen in Halmová et al. (2006), collisional cross-sections corresponding to this transition is very weak if compared to the cross-sections associated to 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 are of 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 large number of electronic states in order to obtain the polarization transfer cross-sections. Results of Halmová et al. (2006) were obtained by using sophisticated quantum R-matrix method for a range of energy going from 0 to 10 eV which allow us to determine collision rates for temperatures up to 10000 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 the polarization transfer rates are reached for small values of \( \Delta j = |j' - j| \).

We provide in Figure 1 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 square fit of the polarization transfer rates presented in the Figure 1.
SSS formed in the photosphere of the Sun. Now on, one can consider that inelastic collisions with electrons can be safely neglected for lines of the solar molecules. From the C10 molecule, transfer rates can be obtained by using the following variation laws:

\[ \frac{dN}{dt} = k(a \rightarrow b)N_a - k(b \rightarrow a)N_b \]

where the values of \( k = 0 \) are comparable to the Einstein coefficient of the transition of the studied lines. Thus for typical photospheric electron densities \( N_e \approx 10^{12} \text{ cm}^{-3} \), the maximum value of \( k = 2 \) is obtained for \( T \) ranging from 1500K to 10000K. These coefficients allow the determination of the polarization transfer rates by collisions with electrons.

<table>
<thead>
<tr>
<th>level</th>
<th>energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^3\Pi_u )</td>
<td>-0.066</td>
</tr>
<tr>
<td>( X^1\Sigma_g^+ )</td>
<td>0.089</td>
</tr>
<tr>
<td>( A^1\Pi_u )</td>
<td>1.052</td>
</tr>
<tr>
<td>( c^3\Sigma_u^+ )</td>
<td>1.206</td>
</tr>
<tr>
<td>( B^1\Delta_g )</td>
<td>1.662</td>
</tr>
<tr>
<td>( B'^1\Sigma_u^+ )</td>
<td>1.879</td>
</tr>
<tr>
<td>( d^3\Pi_u )</td>
<td>2.507</td>
</tr>
</tbody>
</table>

As a result, transfer rates can be obtained by using the following variation laws:

\[ C^k(e_i \ N_j \rightarrow e_f \ N'j') = n_e \ [a_0 + a_1(\frac{T}{5000}) + a_2(\frac{T}{5000})^2] \]

where the values of \( a_0, a_1, \) and \( a_2 \) are provided in the 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 to the orientation terms with \( k = 1 \) and the linear polarization is associated to the alignment of the level \( (k = 2) \). The analytical relationships of the 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:

\[ C^k(e_f \ N'j' \rightarrow e_i \ Nj, T) = \left( \frac{2j + 1}{2j' + 1} \right) \exp \left( \frac{E_f - E_i}{k_B T} \right) \]

where \( E_f \) being the energy of the level \( (j) \) and \( k_B \) the Boltzmann constant.

### 4 ARE COLLISIONS WITH ELECTRONS IMPORTANT IN MODELING THE SSS OF C2?

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 Einstein \( A \) coefficient for the vibrational band (0-0) of the Swan band by using accurate quantum chemistry methods. They found that \( A = 7.626 \times 10^6 \text{ s}^{-1} \). For temperature \( T = 6000 \text{K} \), and for \( k = 0, 1 \) or 2, the largest value of \( C^k(e_f \ N'j' \rightarrow e_i \ Nj, T) \approx N_e \times 25.297 \times 10^{-10} \text{ s}^{-1} \). Thus for typical photospheric electron densities \( N_e = 10^{12} \text{ cm}^{-3} \), the maximum value of \( C^k(e_f \ N'j' \rightarrow e_i \ Nj, T) \approx 2.5 \times 10^3 \times 25.297 \times 10^{-10} \text{ s}^{-1} \). This quick comparison shows that the collisions with electrons cannot be important in the calculation of the scattering polarization of the 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.

### Table 1 Energy of the first electronic states of the C2 molecule (Halmová et al. 2006)

<table>
<thead>
<tr>
<th>level</th>
<th>energy (eV)</th>
</tr>
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<tbody>
<tr>
<td>( a^3\Pi_u )</td>
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</tr>
</tbody>
</table>

### Table 2 Coefficients \( a_0, a_1, \) and \( a_2 \) in \([\times 10^{-10} \text{ s}^{-1}]\) for temperatures ranging from 1500K to 10000K. These coefficients allow the determination of the polarization transfer rates by collisions with electrons.

<table>
<thead>
<tr>
<th>( X^1\Sigma_g^+ \rightarrow ) other states lower than ( d^3\Pi_u )</th>
<th>( a^3\Pi_u \rightarrow ) other states lower than ( d^3\Pi_u )</th>
<th>( a^3\Pi_u \rightarrow a^3\Pi_u )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>( a_0 )</td>
<td>( a_1 )</td>
</tr>
<tr>
<td>0</td>
<td>0.13565</td>
<td>12.2505</td>
</tr>
<tr>
<td>1</td>
<td>0.15025</td>
<td>9.4355</td>
</tr>
<tr>
<td>2</td>
<td>0.11385</td>
<td>7.152</td>
</tr>
</tbody>
</table>

As a result, transfer rates can be obtained by using the following variation laws:
other states of C2 lower than $d^3\Pi_g$

$C / n_e [10^{10} \text{cm}^{-3} \text{s}^{-1}]$

$T (K)$

$g_k = 0$

$g_k = 1$

$g_k = 2$

$a^3\Pi_u \rightarrow d^3\Pi_g$
5 CONCLUSION

Molecules have rich and complex spectra because their configurations are based on multiple electronic, vibrational and rotational states. This is reflected on 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. 2019). Collisions with electrons is another kind of collisions 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 C$_2$ 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$_2$ molecule. We conclude that for typical photospheric electron density, the polarization of the C$_2$ molecule is insensitive to collisions with electrons. Results of this work can be used as useful indication about cases of other solar molecules for which the polarization collisional rates are not known.

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