



Comprehensive Data for Depolarization of the Second Solar Spectrum by Isotropic Collisions with Neutral Hydrogen

M. Derouich

Astronomy and Space Science Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia; aldarwish@kau.edu.sa
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Abstract

Interpretation of the second solar spectrum (SSS) requires a complete determination of the depolarizing effect due to collisions with neutral hydrogen. In this paper, we provide comprehensive collision data for simple atoms, complex atoms, and atoms with hyperfine structure. Grids of interaction potentials were computed for a large range of effective quantum numbers n^* that characterize states of hypothetical simple atoms. After that, the Schrödinger equation is solved to calculate the collisional transition matrix for each value of n^* . Thus, we constructed a database of collisional polarization transfer and depolarization rates of all p -, d -, and f -states of simple atoms. The obtained results are fitted to deduce 48 variation laws, leading to the determination of all depolarization and polarization transfer rates of solar simple atoms. These laws are general and can be applied for any simple atom. We demonstrate how these laws can be used to efficiently obtain the collision rates associated with complex atoms, as well as with atoms with hyperfine structure. We show how the reader may use the variation laws to reproduce all new (de)polarization rates of this paper, as well as all rates of our previous papers published since 2003. Accuracy of our variation laws is discussed. Our analytical laws can be easily implemented in the numerical models developed to simulate the formation of the SSS.

Unified Astronomy Thesaurus concepts: [Solar physics \(1476\)](#)

1. Overview of the Collision Problem

To better explain some subtle aspects of (de)polarizing collisions that may not be trivial for nonspecialized readers, and in order to avoid ambiguities and confusion, we start by providing a brief overview of collisions and their effects on light polarization. We also explain how and why collisions must be included in the models of polarized line formation.

1.1. Basic Definitions and Framework

In the case where an atomic system (atom or molecule) is excited by isotropic radiation, all the Zeeman sublevels are equally populated, and as a result, the scattered radiation is unpolarized. Conversely, atomic systems excited by anisotropic radiation could emit polarized light. Such polarization is called scattering polarization (SP), and if it is observed close to the solar limb at the photospheric level, the SP is also called the second solar spectrum (SSS; e.g., Stenflo & Keller 1997; Gandorfer 2000; Stenflo et al. 2000). In fact, during spectral line formation, processes that break spherical symmetry could create polarization of the emitted light. However, several processes occurring in the medium where the line is formed can reduce this polarization. Isotropic processes intervening in the SP formation result in a partial or total polarization decrease (e.g., Sahal-Br  chot 1977; Trujillo Bueno 2001; Derouich et al. 2003b).

Isotropic collisions can have two effects on the observed radiation (e.g., Barklem & O'Mara 1997; Derouich et al. 2003b):

1. The observed line profile can be broadened.
2. The radiation polarization can be modified. If the variation corresponds to a decrease, it is called depolarization or relaxation. The depolarization corresponds to equalization of Zeeman sublevel populations and partial or total destruction of their coherences.

In this work, we focus our attention on the effect of collisions with hydrogen atoms. In photospheric conditions where the SSS is formed, the main collisional contribution comes from collisions with hydrogen, which is stronger than the contribution coming from collisions with electrons. Depolarization rates due to collisions with hydrogen atoms are often a fundamental ingredient in determining magnetic fields by interpreting their Hanle effect on the SP (e.g., Hanle 1924). The Hanle-based method is currently the only available approach to obtain weak and turbulent magnetic fields in the solar atmosphere (e.g., Landi Degl'Innocenti & Landolfi 2004).

Collisions with electrons are negligible in modeling the SSS. For example, at photospheric temperatures $T \sim 5000$ K, the de-excitation collision rate C for the Sr $\lambda 4607$ line is $\sim 2 \times 10^{-7} \times N_e$, where N_e is the electron density (Sahal-Br  chot 1969). Since $N_e \sim 10^{12} \text{ cm}^{-3}$ at the photosphere, $C \sim 2 \times 10^5 \text{ (s}^{-1}\text{)}$. The Einstein coefficient for spontaneous radiative de-excitation for the Sr $\lambda 4607$ line is $A = 2.01 \times 10^8 \text{ (s}^{-1}\text{)}$, and thus $C/A \sim 10^{-3} \ll 1$.

A quantum description of collisional depolarization is generally obtained by assuming that collisions are binary, complete, and well separated in time. This is an impact approximation where the collision duration is short as compared to the time interval between two collisions. The depolarization rates are computed by multiplying the hydrogen density and the collisional coefficients calculated for one binary collision.

1.2. Quantification of the Atomic Levels in the Solar Atmosphere

Consider an atomic state $|\alpha J M_J\rangle$ subject to the action of collisions where J is the total angular momentum, M_J is its projection along the quantization axis, and α represents a set of the other quantum numbers describing the electronic state.

Atomic linear polarization is nonzero only if the Zeeman sublevels having different absolute values $|M_J|$ are differently populated. On the other hand, the existence of circular polarization in the radiation is caused by differences of populations between Zeeman sublevels $|\alpha J + M_J\rangle$ and $|\alpha J - M_J\rangle$. In the case of the SSS, only the atomic linear polarization is of importance.

In order to describe the state of the emitting/absorbing atom (A), one resorts to the quantum mechanics, which tells us that at any instant t the atomic state is described by a wave function $|\psi_{(A)}(t)\rangle$. If $\{|\alpha JM_J\rangle\}$ is an orthonormal basis, $|\psi_{(A)}(t)\rangle$ can be written as a linear combination of vectors of this basis:

$$|\psi_{(A)}(t)\rangle = \sum_{\alpha JM_J} a_{\alpha JM_J}(t) |\alpha JM_J\rangle. \quad (1)$$

The probability of finding the atom in the state $|\alpha JM_J\rangle$ is given by

$$|\langle \alpha JM_J | \psi_{(A)}(t) \rangle|^2 = |a_{\alpha JM_J}(t)|^2. \quad (2)$$

The state of A can also be characterized by its density matrix $\rho^A(t)$, defined by

$$\rho^A(t) = |\psi_{(A)}(t)\rangle \langle \psi_{(A)}(t)|. \quad (3)$$

An important advantage of the density matrix $\rho^A(t)$ is that it allows a more general description than that given by a wave function $|\psi_{(A)}(t)\rangle$ (e.g., Trujillo Bueno 2001). If one considers a set of N systems that are identical and independent (in our case, N emitting solar atoms), one defines the total system density matrix as being the average of the density matrices of individual systems:

$$\bar{\rho}^A(t) = \frac{1}{N} \sum_{i=1}^N \rho^{A_i}(t). \quad (4)$$

The density matrix $\bar{\rho}^A$ then allows us to describe the “state of an average atom” or the “average state of an atom.” This is a useful and successful way to describe the overall system behavior, which is needed to model the SP formed in the Sun’s photosphere. Note that atomic states are described through the atomic density matrix ρ^A , but the emitted photons are described by another density matrix ρ^{photons} (see, e.g., Sahal-Brechot et al. 1998; Sahal-Brechot & Bommier 2014).

From now on, we will use the notation ρ instead of $\bar{\rho}^A(t)$ for short. The diagonal element $\langle \alpha JM_J | \rho | \alpha JM_J \rangle$ is the average population of the level $|\alpha JM_J\rangle$. The nondiagonal elements $\langle \alpha JM_J | \rho | \alpha J' M_J' \rangle$ are the average of the coherence (interference) between the states $|\alpha JM_J\rangle$ and $|\alpha J' M_J'\rangle$.

We note that in the standard basis $\{|\alpha JM_J\rangle\}$ there is no difference in physical meaning between diagonal elements (populations) and nondiagonal elements (coherences). The distinction between populations and coherences depends on the choice of the quantization axis along which the momentum J is projected (e.g., Landi Degl’Innocenti & Landolfi 2004). In fact, the irreducible tensor operators (ITO) basis has been shown to be the most suitable to model the formation of the SP.

In the case of collisions with neutral hydrogen treated in this work, transitions with $\alpha \neq \alpha'$ are not of interest since they do not have any effect on the SSS. Thus, from now on, we omit the label α for the sake of brevity, and we restrict our notations to involve only the J number and its projection M_J .

1.3. Irreducible Tensor Operators Basis and Statistical Equilibrium Equations (SEEs)

1.3.1. Irreducible Tensor Operators Basis

Development of the density matrix over the basis of the ITO is dictated by the symmetries of the studied problem (e.g., Landi Degl’Innocenti & Landolfi 2004). In fact, the ITO basis is particularly well adapted to the study of problems with spherical or axial symmetry and allows a noncomplicated formulation of the SEEs. In addition, quantities expressed in the ITO have a measurable physical meaning. The passage relation from the standard basis to the ITO basis is (e.g., Sahal-Brechot 1977; Landi Degl’Innocenti & Landolfi 2004)

$${}^{J,J'} T_q^{k_J} = \sum_{M_J, M_J'} (-1)^{J-M_J} \sqrt{2k_J + 1} \begin{pmatrix} J & k_J & J' \\ -M_J & q & M_J' \end{pmatrix} \times |JM_J\rangle \langle J'M_J'|, \quad (5)$$

where the entity between parentheses is a $3j$ -coefficient. According to the selection rules, one has $|J - J'| \leq k_J \leq J + J'$, $-k_J \leq q \leq k_J$, and $q = M_J - M_J'$. Let us mention that k_J is the tensorial order and q quantifies the coherence rate between the Zeeman sublevels.

The density matrix of an “average atom” is ρ . The density matrix elements in the ITO basis ${}^J \rho_q^{k_J}$ are commonly referred to as multipolar terms or elements. The importance of the ITO basis is apparent from the fact that certain multipolar terms are directly proportional to the J -level population and, therefore, we do not need to know the population of each Zeeman sublevel. We also note that the limiting case, where the light polarization is neglected, is retrieved by simple restriction of the equations to the order $k_J = 0$. Under the impact approximation, the effect of collisions on the atomic density matrix ρ is proportional to the depolarization (relaxation) matrix.

1.3.2. Statistical Equilibrium Equations

We consider the SEEs for atomic levels that undergo effects of several physical processes. Let us denote the density matrix variation rate under the effect of the process i as $\left(\frac{d^J \rho_q^{k_J}}{dt} \right)_i$. In the photosphere where the SSS is formed, the label i is used to refer to collisions with hydrogen atoms, radiative processes, and the Hanle effect of a magnetic field. If natural widths of fine-structure levels are smaller than separations between different fine levels, one has to solve the SEEs for J -levels. Therefore, the SEEs, describing the effect of these different processes on atomic states, can be written as

$$\sum_i \left(\frac{d^J \rho_q^{k_J}}{dt} \right)_i = 0. \quad (6)$$

The incident unpolarized but anisotropic radiation that illuminates the emitting atom at the solar atmosphere does not create multipolar elements ${}^J \rho_q^{k_J}$ with odd k_J (e.g., Trujillo Bueno 2001; Landi Degl’Innocenti & Landolfi 2004). Thus, the subsystem solution that corresponds to the values of odd k_J is

$${}^J \rho_0^{k_J} = 0, \quad k_J \text{ odd integer}, \quad (7)$$

which also means that $N_{JM_J} = N_{J-M_J}$. As a result, none of the atomic levels are circularly polarized, i.e., the SP is linear.

To interpret the SP, one needs only even values of k_J . Although the radiation does not contain tensorial orders larger than 2, orders higher than 2 (if they exist) should be taken into account in the SEEs. In other words, even if one observes only the linear polarization associated with $k_J = 2$, density matrix elements $^J\rho_q^{k_J}$ with $k_J > 2$ are coupled to the orders $k_J = 0, 2$ via the SEEs and therefore cannot be ignored. One needs, for theoretical calculation of linear polarization, all the multipolar terms of the atomic density matrix of orders $k_J = 0, 2, 4, \dots$

2. Different Types of (De)Polarizing Collisions

Collisions can be divided into three types:

1. Purely elastic collisions, where the atomic angular momentum J does not change during the collision. These collisions mix Zeeman substates (JM_J) inside a given J -level.
2. Quasi-elastic collisions, which change the value of J but *without* changing the electronic state. These collisions mix Zeeman substates (JM_J) and ($J'M_J'$) with $J \neq J'$.
3. Inelastic collisions, which correspond to cases where initial and final electronic states are different.

Let us mention that, during a given binary collision between a hydrogen atom and the emitting atom, only off-diagonal elements of the interaction potential matrix are able to vary the polarization (see, e.g., Derouich et al. 2005a). This is because off-diagonal elements contain the anisotropic part of the interaction potential since it depends on the projection M_J of J . This property is general, i.e., regardless of whether the emitting atom is in the s -, p -, d -, or f -state, only the anisotropic part of the interaction potential affects the atomic polarization. A detailed explanation of this property for an atom in an s -state interacting with the hydrogen atom in its ground s -state is given in Section 2 of Derouich et al. (2005a) (see also Derouich & Barklem 2007). However, the anisotropy of the interaction potential should not be confused with the fact that the collisions are isotropic, i.e., the relative velocity distribution during the collisions is isotropic (and, more precisely, chosen to be Maxwellian in our depolarization rate calculations).

3. Depolarization and Polarization Transfer Rate

In the impact approximation one assumes that the collisions are binary and uncorrelated. Hence, the collisional depolarization is proportional to the hydrogen atom density. Evolution of the perturbed atom states is governed by the SEEs, which give the variation of the density matrix elements $^J\rho_0^{k_J}$ due to isotropic collisions with hydrogen atoms (see, e.g., Sahal-Br  chot 1977; Derouich et al. 2003a):

$$\left(\frac{d^J \rho_q^{k_J}}{dt} \right)_{\text{coll}} = -^J\rho_q^{k_J} \times [D^{k_J}(J, T) + \sum_{J' \neq J} \sqrt{\frac{2J'+1}{2J+1}} D^0(J \rightarrow J', T)] + \sum_{J' \neq J} D^{k_J}(J \rightarrow J', T) ^{J'}\rho_q^{k_J}. \quad (8)$$

Collisions with neutral hydrogen atoms are elastic or quasi-elastic, i.e., occur inside the same electronic state.

Atomic state orientation is quantified by the density matrix elements with odd tensorial orders k_J ($k_J = 1, k_J = 3$, etc.),

while the alignment is given by the even orders ($k_J = 2, k_J = 4$, etc.) (e.g., Landi Degl'Innocenti & Landolfi 2004). The population of the J -level is given by density matrix elements with $k_J = 0$. Isotropic collisions affect multipolar elements $^J\rho_q^{k_J}$ ($q \neq 0$) in the same way that they affect $^J\rho_0^{k_J}$. $D^{k_J}(J, T)$ is the collisional depolarization rate of the order k_J of the level J . In particular,

1. $D^0(J, T)$ is the population destruction rate. We can verify that it is identically zero. This means that purely elastic collisions do not change the population of the level J .
2. $D^1(J, T)$ is the destruction rate of the orientation, which is directly related to the circular polarization.
3. $D^2(J, T)$ is the destruction rate of alignment, which is of interest, particularly in the interpretation of the SSS, since it is associated with the linear polarization.

For a complete study of the effect of isotropic collisions with neutral hydrogen atoms, we must also consider the polarization transfer rates between J and J' atomic levels $D^{k_J}(J \rightarrow J', T)$. The tensorial order k_J is between zero and $2J$ if $J < J'$, and if $J > J'$, $0 \leq k_J \leq 2J'$. The rates $D^{k_J}(J \rightarrow J', T)$ result from an integration over the Maxwellian velocity distribution of $[n_H \times v \times \sigma^{k_J}(J \rightarrow J', v)]$, where $\sigma^{k_J}(J \rightarrow J', v)$ is the polarization transfer cross section, v is the relative velocity, and n_H is the hydrogen density. $D^{k_J}(J \rightarrow J', T)$ is a linear combination of the usual rates of collisional transitions between the Zeeman sublevels $C(JM_J \rightarrow J'M_J', T)$ (e.g., Sahal-Br  chot 1977; Derouich et al. 2003a).

By using the general equation giving $D^{k_J}(J \rightarrow J', T)$ (see Derouich et al. 2003a), one can deduce, for the particular case where $k_J = 0$, that

$$D^0(J \rightarrow J', T) = \frac{1}{\sqrt{(2J+1)(2J'+1)}} \times \sum_{M_J, M_J'} C(JM_J \rightarrow J'M_J', T) = \sqrt{\frac{2J+1}{2J'+1}} C(J \rightarrow J', T). \quad (9)$$

For $J = J'$ one finds that

$$D^0(J \rightarrow J, T) = C(J \rightarrow J, T). \quad (10)$$

In addition,

$$D^{k_J}(J, T) = D^0(J \rightarrow J, T) - D^{k_J}(J \rightarrow J, T). \quad (11)$$

4. Collisions of Simple Atoms with Neutral Hydrogen

4.1. General Considerations and Variation Laws

We denote as ‘‘a simple atom’’ an atom having only one valence electron in a p -, d -, or f -state above a filled subshell (e.g., Na I or K I) or above an electron in an s -state (Sr I or Ca I). Derouich–Sahal-Br  chot–Barklem (DSB) developed a general semiclassical theory of calculation of depolarization rates of lines of simple atoms by isotropic collisions with neutral atoms of hydrogen (see, e.g., Derouich et al. 2003a, 2003b, 2015, 2017; Derouich 2004, 2017, 2019; Sahal-Br  chot et al. 2007).

The energy of the valence electron in an excited level is denoted as E_{level} , and the ionization energy of the perturbed atom in its fundamental state is E_∞ . Thus, the ionization energy

of the atom in its excited level is $(E_\infty - E_{\text{level}})$. The effective quantum number associated with the excited level is defined by (see, e.g., Derouich et al. 2003b)

$$n^* = [2(E_\infty - E_{\text{level}})]^{-1/2}, \quad (12)$$

where E_∞ and E_{level} are in a.u. and are tabulated in atomic databases. Following the DSB method, n^* characterizes the atomic state. As an example, by using Equation (12), one finds $n^* = 2.030$ for the Mg $3p$ level, $n^* = 2.077$ for Ca $4p$, and $n^* = 2.117$ for Na $3p$.

The DSB semiclassical theory of collisions is justified by the fact that, in the solar temperatures, the process of depolarization depends essentially on intermediate interatomic distances. This theory is general, i.e., it is not specific to a given atom and, thus, allows depolarization rate determination for all neutral simple atoms. Comparisons to some specific calculations of quantum chemistry validate DSB general theory (see, e.g., Derouich et al. 2003b). In fact, at $T = 5000$ K, for p - and d -states, the difference between our results and those of quantum chemistry obtained by Kerkeni (2002) is 11% for Mg I, 8% for Ca I, 13% for Na I, and 3%–5% for Ca II.

Let us mention that in the ITO basis, each atomic level is characterized by the total angular momentum J , the tensorial order k , the orbital momentum l , and the effective principal quantum number n^* . Our numerical code allows us to calculate all rates of depolarization of levels of simple atoms for a large range of n^* values.

Calculation of $D^{kj}(J, T)$ and $D^{kj}(J \rightarrow J', T)$ advances through the following steps:

1. Calculation of the Coulomb wave functions of the perturbed atom and the interaction potentials between the perturbed atom and hydrogen.
2. Resolution of the Schrödinger equation, which leads to the calculation of the transition matrix between the Zeeman sublevels.
3. Calculation of the transition probabilities in the ITO basis.
4. Integration on impact parameters and relative velocities to finally obtain the depolarization and polarization transfer rates.

These steps are grouped in an interactive code.

We determined a set of data that includes thousands of (de) polarization cross sections. Then, after averaging over velocities, we obtained 2400 rates $D^{kj}(J, T)$ and $D^{kj}(J \rightarrow J', T)$ in the case of states p ($l = 1$), d ($l = 2$), and f ($l = 3$).

We show that these rates generally follow power-law behaviors with n^* that fit by

$$D^{kj}(J \rightarrow J', T = 5000 \text{ K}) = n_{\text{H}} \times 10^{-10} a^{kj}(J \rightarrow J') \times n^{*b^{kj}(J \rightarrow J')}$$

$$D^{kj}(J, T = 5000 \text{ K}) = n_{\text{H}} \times 10^{-10} a^{kj}(J) \times n^{*b^{kj}(J)}, \quad (13)$$

where the hydrogen density n_{H} is in cm^{-3} and D^{kj} rates are in s^{-1} . We notice that laws of Equation (13) are based on a least-squares method. These laws, characterized by tabulated values of a_j^k (in $\text{cm}^3 \text{s}^{-1}$) and b_j^k , are based on 50 hypothetical values of n^* since $1.5 \leq n^* \leq 3$ for $l = 1$, $2.5 \leq n^* \leq 4$ for $l = 2$, and $3.3 \leq n^* \leq 5$ for $l = 3$. We adopt a step size of 0.1 in the variation of n^* . The n^* chosen values cover the majority of the

Table 1
Values of $a^{kj}(J \rightarrow J')$ and $b^{kj}(J \rightarrow J')$ Coefficients for the p -states

p -states: P_1	J	J'	k	$a^{kj}(J \rightarrow J')$	$b^{kj}(J \rightarrow J')$
$P_{1/2}$ and $P_{3/2}$	1/2	1/2	1	5.1	2.3241
	1	1	1	18.00	2.8711
	1	1	2	16.32	2.8100
	3/2	3/2	1	6.21	2.5101
	3/2	3/2	2	12.229	2.7517
	3/2	3/2	3	8.44	2.667
	1/2	3/2	0	9.75	2.7054
	1/2	3/2	1	1.485	2.7211

Note. The a^{kj} coefficients are given in $\text{cm}^3 \text{s}^{-1}$.

SSS lines. All 48 possible values of (a_j^k, b_j^k) are tabulated in the next subsections.

To infer the rates (at $T = 5000$ K) corresponding to a real simple atom, one has to determine the value of n^* and, then, can apply the laws of Equation (13). As we discussed in our previous papers (e.g., Derouich et al. 2015), the depolarization and polarization transfer rates have temperature dependence of $T^{0.38}$. Thus, one can assume that

$$D^{kj}(J \rightarrow J', T) = D^{kj}(J \rightarrow J', T = 5000 \text{ K}) \times \left[\frac{T}{5000} \right]^{0.38}$$

$$D^{kj}(J, T) = D^{kj}(J, T = 5000 \text{ K}) \times \left[\frac{T}{5000} \right]^{0.38}. \quad (14)$$

4.2. p -states

Grids of collisional rates are computed for 16 values of n^* in the interval $[1.5, 3]$ with a step size of 0.1. Each value of n^* corresponds to a hypothetical simple atom. For simple atoms in the p -states, one needs to consider the states $^2P_{1/2}$, 1P_1 , and $^2P_{3/2}$. All nonzero rates associated with simple atoms in the p -states are as follows:

1. $D^1(\frac{1}{2})$: orientation destruction rate of the state $^2P_{1/2}$.
2. $D^1(1)$ and $D^2(1)$: orientation and alignment destruction rate of the state 1P_1 , respectively.
3. $D^1(\frac{3}{2})$ and $D^2(\frac{3}{2})$: orientation and alignment destruction rate of the state $^2P_{3/2}$, respectively; and $D^3(\frac{3}{2})$: linked indirectly to circular polarization via the SEEs.
4. $D^0(\frac{1}{2} \rightarrow \frac{3}{2})$ and $D^1(\frac{1}{2} \rightarrow \frac{3}{2})$: population transfer and orientation transfer from the level $^2P_{1/2}$ to the level $^2P_{3/2}$, respectively.

After establishing the variation laws of Equation (13), we obtain the a^{kj} and b^{kj} values corresponding to the p -states. These values are given in Table 1.

4.3. d -states

We consider a collision problem between an atom in its d -state and neutral hydrogen, which, during the entire collision, remains in its fundamental state $1s$. By using our numerical code, we obtain general results of any depolarization and polarization transfer rates for values of n^* ranging from 2.5 to 4. All nonzero a^{kj} and b^{kj} values associated with the d -states of simple atoms are provided in Table 2.

Table 2Values of $a^{kj}(J \rightarrow J')$ and $b^{kj}(J \rightarrow J')$ Coefficients for the d -states

d -states: D_2 $D_{3/2}$ and $D_{5/2}$	J	J'	k	$a^{kj}(J \rightarrow J')$	$b^{kj}(J \rightarrow J')$
	3/2	3/2	1	1.5878	2.3375
	3/2	3/2	2	3.0478	3.5063
	3/2	3/2	3	2.143	3.0124
	2	2	1	4.3625	2.7534
	2	2	2	7.6841	3.1696
	2	2	3	5.88876	3.0531
	2	2	4	5.37	2.8001
	5/2	5/2	1	3.280	2.6001
	5/2	5/2	2	6.2336	2.9796
	5/2	5/2	3	4.77716	2.7831
	5/2	5/2	4	4.653	2.8018
	5/2	5/2	5	5.044	2.7934
	3/2	5/2	0	3.8599	3.2736
	3/2	5/2	1	-0.257	3.3078
	3/2	5/2	2	6.6651	3.4573
	3/2	5/2	3	-0.126	3.3111

Note. The a^{kj} coefficients are given in $\text{cm}^3 \text{s}^{-1}$.

4.4. f -states

As in the case of states p ($l=1$) and d ($l=2$), the rates calculated for f -states ($l=3$) generally follow the laws of Equation (13). The values of n^* range from 3.3 to 5. It is obvious that the values of n^* , which are of interest for f -states, are larger than those for p - and d -states. Values of a^{kj} and b^{kj} are shown in Table 3.

5. Depolarization Rates for Atoms with Hyperfine Structure

If an atom possesses a nuclear spin I , the hyperfine components of a fine J -level can show interesting, and sometimes unexpected, profiles in the SSS. For example, Na I has a spin nuclear $I = 3/2$, and therefore two hyperfine levels are possible in the case of level $^2P_{1/2}$: $F = 1$ and 2. Although the level $^2P_{1/2}$ is not linearly polarizable since $J = 1/2$ does not allow the creation of a tensorial order $k_J = 2$ inside the fine level, hyperfine levels $F = 1$ and 2 are linearly polarizable by scattering of anisotropic radiation and thus can be observed in the SSS.

Intricate and complex structures of SSS profiles, such as Na $\lambda 5896$, K $\lambda 7699$, Li $\lambda 6707$, Ba $\lambda 4554$, etc., should be elucidated in terms of hyperfine-structure effects. Theoretical works and observations (e.g., Stenflo & Keller 1997; Stenflo et al. 2000; Smitha et al. 2014; Belluzzi et al. 2015; Sampoorana et al. 2019) show the importance of hyperfine structures in the SSS. In this context, it is important to include collisional (de) polarization rates of a large number of hyperfine levels in the SSS modeling to infer interesting information about the solar photosphere.

In previous works (see Derouich et al. 2017), we elaborated the main steps of two methods, direct and indirect calculation of (de)polarization rates for atoms with hyperfine structure. We explained why it is convenient to adopt the indirect method. According to the indirect method, one assumes that during the collision the emitting atom nuclear spin is conserved (e.g., Derouich et al. 2017). This is the frozen nuclear spin approximation, where depolarization and polarization transfer rates of hyperfine levels can be expressed as a linear combination of rates associated with the fine levels. In fact,

Table 3Values of $a^{kj}(J \rightarrow J')$ and $b^{kj}(J \rightarrow J')$ Coefficients for the f -states

f -states: F_3 $F_{5/2}$ and $F_{7/2}$	J	J'	k	$a^{kj}(J \rightarrow J')$	$b^{kj}(J \rightarrow J')$
	5/2	5/2	1	1.29859	3.35014
	5/2	5/2	2	1.5521	3.5642
	5/2	5/2	3	1.3590	3.5667
	5/2	5/2	4	1.4630	3.5330
	5/2	5/2	5	1.01188	3.4677
	3	3	1	2.97391	3.1598
	3	3	2	3.4327	3.4048
	3	3	3	3.12132	3.1780
	3	3	4	3.17449	3.0056
	3	3	5	2.87098	2.9978
	3	3	6	2.99018	2.7797
	7/2	7/2	1	2.42326	3.1009
	7/2	7/2	2	2.6984	3.2119
	7/2	7/2	3	2.51373	2.9235
	7/2	7/2	4	2.59771	2.8799
	7/2	7/2	5	1.87740	3.1354
	7/2	7/2	6	2.01073	2.9980
	7/2	7/2	7	1.73455	2.7087
	5/2	7/2	0	2.6867	3.2718
	5/2	7/2	1	-0.602019	3.4501
	5/2	7/2	2	2.0001	3.5076 ^a
	5/2	7/2	3	-0.408094	3.0087
	5/2	7/2	4	1.20930	2.8709
	5/2	7/2	5	-0.367204	3.6086

Notes. The a^{kj} coefficients are given in $\text{cm}^3 \text{s}^{-1}$.^a This law is valid for $3.3 \leq n^* \leq 4.3$.

the polarization transfer rates can be written as (e.g., Nienhuis 1976; Omont 1977)

$$\begin{aligned}
& \mathcal{D}^{k_F}((JI)FF' \rightarrow (J'I)F''F''', T) \\
&= \sqrt{(2F+1)(2F'+1)(2F''+1)(2F''' + 1)} \\
& \quad \times \sum_{k_J} (2k_J + 1) D^{k_J}(J \rightarrow J', T) \\
& \quad \times \sum_{k_I} (2k_I + 1) \left\{ \begin{matrix} J & I & F \\ J & I & F' \\ k_J & k_I & k_F \end{matrix} \right\} \left\{ \begin{matrix} J' & I & F'' \\ J' & I & F''' \\ k_J & k_I & k_{F'} \end{matrix} \right\}. \quad (15)
\end{aligned}$$

Equation (15) is valid for cases where initial level $|(JI)FF'$ and final level $|(J'I)F''F'''$ are different. In addition, Equation (15) takes into account the possibility of coherences between hyperfine levels F and F' inside the same fine level J .

In the cases of purely elastic collisions, where initial and final hyperfine levels are the same, the depolarization of the hyperfine level $|(JI)FF$ is given by

$$\begin{aligned}
\mathcal{D}^{k_F}((JI)F, T) &= \mathcal{D}^0((JI)FF \rightarrow (JI)FF, T) \\
& \quad - \mathcal{D}^{k_F}((JI)FF \rightarrow (JI)FF, T). \quad (16)
\end{aligned}$$

Depolarization and polarization transfer rates can be obtained by using Tables 1–3 together with Equation (15).

If the coherence between the hyperfine levels F and F' inside the same fine J -level is neglected, we denote $\mathcal{D}^{k_F}((JI)F, T)$ by $\mathcal{D}^{k_F}(JF)$ and $\mathcal{D}^{k_F}((JI)FF' \rightarrow (J'I)F''F''', T)$ by $\mathcal{D}^{k_F}(JF \rightarrow J'F')$. Variation of the density matrix elements

due to the isotropic collisions with neutral hydrogen becomes

$$\left[\frac{d\rho_q^{k_F}(JF)}{dt} \right]_{\text{coll}} = \sum_{J'F' \neq JF} \mathcal{D}^{k_F}(JF \leftarrow J'F') \times \rho_q^{k_F}(J'F') - \left[\sum_{J'F' \neq JF} \sqrt{\frac{2F+1}{2F'+1}} \mathcal{D}^{(0)}(JF \rightarrow J'F') + \mathcal{D}^{k_F}(JF) \right] \times \rho_q^{k_F}(JF). \quad (17)$$

6. Complex Atoms

Extension of our results from simple to complex atoms is motivated by the fact that a complete study of the SSS necessarily requires the interpretation of spectra of complex atoms (Manso Sainz & Landi Degl'Innocenti 2002; Derouich et al. 2005b; Sahal-Br  chot et al. 2007). In fact, more than 85% of the polarized lines presented in Gandorfer (2000) are associated with complex atoms.

Calculation of the depolarization and transfer polarization rates for levels of complex atoms requires determination of the collision matrix. Such a calculation corresponds to the resolution of the Schr  dinger equation, which implies that the interaction potential elements must be determined. This is the so-called direct method, which is very complicated. This method might be even impossible in most of the cases. In fact, it is very complicated to undertake the problem of collisions between a complex atom like Ti I or Fe I and hydrogen in solar temperature conditions.

To solve this problem, Derouich et al. (2005b) proposed an indirect method based on the frozen core approximation. In the framework of this indirect method, the complex atom is assumed to be composed of the following:

1. Electrons in an internal subshell where their total orbital momentum is zero.
2. Outer incomplete (open) shell containing electrons with nonzero total orbital momentum denoted as L_c and a total spin S_c . This shell is called the core of the complex atom.
3. An optical electron with orbital angular momentum l and spin s ($s = 1/2$).

We adopt the frozen core approximation, that is, the core angular momentum is conserved during the collision. Therefore, the collisional transition matrix elements between levels of complex atoms are linear combinations of transition matrix elements between levels of simple atoms. We have established the equation giving the coefficients of this linear combination (Equation (8) of Derouich et al. 2005b). Similarly, by applying the frozen core approximation in the ITO basis, one can also find that the depolarization and polarization transfer rates for complex atoms are given by linear combination of those associated with simple atoms given by Tables 1–3. Coefficients of the linear combination are similar to those given by Derouich et al. (2005a) and by Sahal-Br  chot et al. (2007).

Note that the total orbital moment is given by $\mathbf{L} = \mathbf{L}_c + \mathbf{l}$ and the total spin $\mathbf{S} = \mathbf{S}_c + \mathbf{s}$. Atoms or ions are considered to be simple if $L_c = 0$. Simple atoms have an electronic configuration with only one valence electron above a completely filled subshell or above a subshell having an electron in an s -state.

We suppose that only the valence electrons undergo the effect of the interaction with neutral hydrogen. The internal electrons are not affected by the collisions in the sense that L_c , S_c , and $\mathbf{J}_c = \mathbf{L}_c + \mathbf{S}_c$ are conserved in the framework of the frozen core approximation.

We consider that $\mathcal{J} = \mathbf{J} + \mathbf{J}_c$ is the total level angular momentum of the complex atom. The polarization transfer rates $\mathcal{D}^{k_J}(\mathcal{J} \rightarrow \mathcal{J}')$ are readily obtained by carrying out the formal substitutions $F \rightarrow \mathcal{J}$ and $I \rightarrow J_c$ on Equation (15). Thus, rates of complex atoms $\mathcal{D}^{k_J}(\mathcal{J} \rightarrow \mathcal{J}')$ are given by the following linear combination of the rates of simple atoms $D^{k_J}(J \rightarrow J', T)$:

$$\begin{aligned} \mathcal{D}^{k_J}(\mathcal{J} \rightarrow \mathcal{J}') &= (2\mathcal{J} + 1)(2\mathcal{J}' + 1) \\ &\times \sum_{k_J} (2k_J + 1) D^{k_J}(J \rightarrow J', T) \\ &\times \sum_{k_{J_c}} (2k_{J_c} + 1) \left\{ \begin{matrix} J & J_c & \mathcal{J} \\ J & J_c & \mathcal{J} \\ k_J & k_{J_c} & k_{\mathcal{J}} \end{matrix} \right\} \left\{ \begin{matrix} J' & J_c & \mathcal{J}' \\ J' & J_c & \mathcal{J}' \\ k_J & k_{J_c} & k_{\mathcal{J}} \end{matrix} \right\}. \end{aligned} \quad (18)$$

We particularly note that rates of levels of complex atoms $\mathcal{D}^{k_J}(\mathcal{J} \rightarrow \mathcal{J}')$ with even tensorial order k_J , which affect the linear polarization of complex atoms, can be expressed as a function of rates $D^{k_J}(J \rightarrow J', T)$ that affect circular polarization of simple atoms. For example, for $\mathcal{J} = 1$ and $k_J = 2$, if one has $J = 3/2$, odd values $k_J = 1$ and 3 are involved in the summation of Equation (18).

For depolarization rates of complex atoms we apply

$$D^{k_J}(\mathcal{J}, T) = \mathcal{D}^0(\mathcal{J} \rightarrow \mathcal{J}) - \mathcal{D}^{k_J}(\mathcal{J} \rightarrow \mathcal{J}). \quad (19)$$

7. Recovering Previous Results

We determined a set of data that includes thousands of (de) polarization cross-section values.¹ Instead of publishing collisional data as they are, we make the choice to collect them in a more compact form as 48 variation laws characterized by the tabulated a_J^k and b_J^k values.

Readers should be able to derive all data presented in our previous papers from the comprehensive data provided in this manuscript in the form of variations laws. In addition to the data that have been published previously, one can find additional new data that are published in the present manuscript for the first time. The data of this work are applicable for any simple atom, any complex atom, and any atom with hyperfine structure provided that $l = 1, 2$, or 3. Hence, these data cover the majority of polarized lines associated with neutral atoms in the SSS.

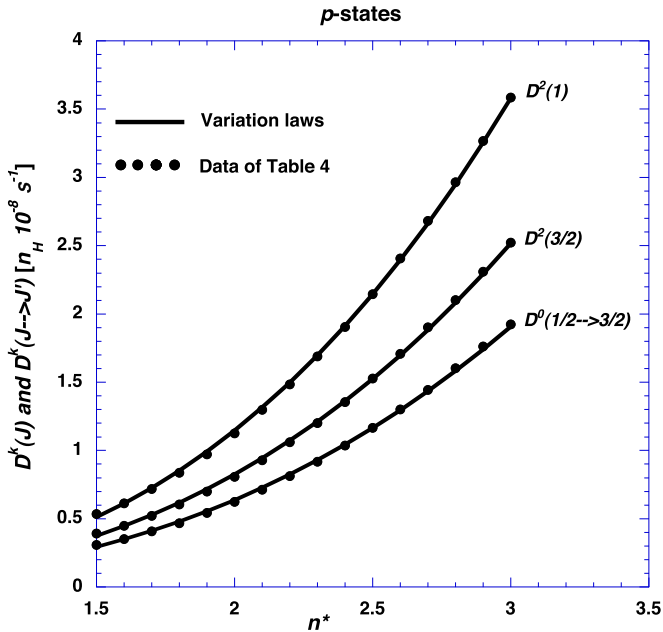
Using our variation laws, all data of our previous papers published since 2003 can be recovered. For example, previous results concerned with p -states of Derouich et al. (2003b) and Derouich (2004) are recalled in Table 4. Figure 1 presents a confrontation between results of Table 4 and results obtained by applying our variation laws determined in this work. It is straightforward to see that both curves are very similar, which means that results of Derouich et al. (2003b) and Derouich (2004) are nothing but particular cases of our variation laws.

In fact, our intention in this work is to produce for the reader, in a single document and in a compact way, practically all the

¹ Every (de)polarization cross-section calculation requires a determination of the interaction potential and a Schr  dinger equation resolution by using our numerical code of collisions.

Table 4(De)polarization Rates for Even k per Unit Hydrogen Density as a Function of n^* and for the Local Temperature $T = 5000$ K

n^*	$D^2(1)/n_H$	$D^2(\frac{3}{2})/n_H$	$D^0(\frac{1}{2} \rightarrow \frac{3}{2})/n_H$
1.5	0.5338	0.3931	0.3087
1.6	0.6135	0.4477	0.3508
1.7	0.7188	0.5220	0.4068
1.8	0.8363	0.6047	0.4686
1.9	0.9716	0.7000	0.5415
2.0	1.1260	0.8084	0.6230
2.1	1.2971	0.9289	0.7129
2.2	1.4844	1.0599	0.8113
2.3	1.6875	1.2021	0.9181
2.4	1.9043	1.3563	1.0360
2.5	2.1452	1.5270	1.1648
2.6	2.4065	1.7086	1.2999
2.7	2.6814	1.9010	1.4427
2.8	2.9634	2.1015	1.6026
2.9	3.2665	2.3097	1.7622
3.0	3.5842	2.5237	1.9251

Note. Rates are given in 10^{-8} s^{-1} and hydrogen density n_H in cm^{-3} (Derouich 2004).**Figure 1.** Examples of variation laws vs. original data for the case of p -states.

depolarization and polarization transfer rates of interest within the framework of neutral atom SSS study.

Let us now take some important particular cases in the SSS. We apply our method to the depolarization calculation for the levels Mg I $3p^1P_1$, Ca I $4p^1P_1$, and Na I $3p^2P_{3/2}$. We compare depolarization rates D^2 of these levels, previously calculated in Derouich et al. (2003b), to the rates calculated by applying our

Table 5 D^2/n_H for the Mg, Ca, and Na due to Collisions with Hydrogen Atoms at $T = 5000$ K

Atomic State	Mg $3p^1P_1$	Ca $4p^1P_1$	Na $3p^2P_{3/2}$
n^*	2.030	2.077	2.117
D^2/n_H (Derouich et al. 2003b)	1.2009	1.2818	0.9702
D^2/n_H (current work)	1.2153	1.2727	0.9631

Note. Rates D^2 are given in 10^{-8} s^{-1} and hydrogen density n_H in cm^{-3} .

variation laws in cases of values of n^* for Mg I $3s\ 3p$, Ca I $4s\ 4p$, and Na I $3p$. Results are provided in Table 5. It can be easily concluded that our variation laws permit us to retrieve, with good precision, depolarization rates D^2 previously published.

8. Concluding Remarks

In this work, new data were obtained with our numerical code of collisions. Then, by using a least-squares fit of all numerical data (i.e., new data and data published since 2003), we obtained 48 new variation laws that allow us to obtain depolarization and polarization transfer rates for all simple atoms in their p -, d -, and f -states. The quality of the fit may be evaluated in the example of Figure 1.

Using our variation laws, polarization transfer and depolarization rates of hyperfine levels can be easily obtained through linear combinations on the basis of algebraic coefficients and quantum numbers. The same line of reasoning allows indirect determination of rates associated with J -levels of complex atoms. This work is thus a comprehensive collection of depolarizing collisional data that can be implemented in modeling the SSS for solar spectropolarimetric applications.

Readers should be able to derive all data presented in our previous DSB papers from the comprehensive data provided in this manuscript in the form of variation laws. In addition to the data published earlier, one can find additional new data that are published in the present manuscript for the first time. The data set presented in this work covers the majority of polarized lines associated with neutral atoms in the SSS.

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ORCID iDs

M. Derouich <https://orcid.org/0000-0003-3549-885X>

References

- Barklem, P. S., & O'Mara, B. J. 1997, *MNRAS*, **290**, 102
- Belluzzi, L., Landi Degl'Innocenti, E., & Trujillo Bueno, J. 2015, *ApJ*, **812**, 73
- Derouich, M. 2004, PhD thesis, Paris VII-Denis Diderot Univ. <https://tel.archives-ouvertes.fr/tel-00331859>
- Derouich, M. 2017, *NewA*, **51**, 32
- Derouich, M. 2019, *MNRAS*, **481**, 2444
- Derouich, M., & Barklem, P. S. 2007, *A&A*, **462**, 1171
- Derouich, M., Barklem, P. S., & Sahal-Br  chot, S. 2005a, *A&A*, **441**, 395
- Derouich, M., Basurah, H., & Badruddin, B. 2017, *PASA*, **34**, 8
- Derouich, M., Radi, A., & Barklem, P. S. 2015, *A&A*, **584**, 8
- Derouich, M., Sahal-Br  chot, S., & Barklem, P. S. 2003a, *A&A*, **409**, 369
- Derouich, M., Sahal-Br  chot, S., & Barklem, P. S. 2005b, *A&A*, **434**, 779

- Derouich, M., Sahal-Br  chot, S., Barklem, P. S., & O'Mara, B. J. 2003b, [A&A](#), **404**, 763
- Gandorfer, A. 2000, The Second Solar Spectrum: A High Spectral Resolution Polarimetric Survey of Scattering Polarization at the Solar Limb in Graphical Representation, Vol. 1: 4625    to 6995    (Zurich: vdf Hochschulverlag)
- Hanle, W. 1924, [ZPhy](#), **30**, 93
- Kerkeni, B. 2002, [A&A](#), **390**, 783
- Landi Degl'Innocenti, E., & Landolfi, M. 2004, [ASSL](#), **307**
- Manso Sainz, R., & Landi Degl'Innocenti, E. 2002, [A&A](#), **394**, 1093
- Nienhuis, G. 1976, [JPhB](#), **9**, 167
- Omont, A. 1977, [PQE](#), **5**, 69
- Sahal-Br  chot, S. 1969, [A&A](#), **1**, 91
- Sahal-Br  chot, S. 1977, [ApJ](#), **213**, 887
- Sahal-Brechot, S., & Bommier, V. 2014, [AdSpR](#), **54**, 1164
- Sahal-Brechot, S., Bommier, V., & Feautrier, N. 1998, [A&A](#), **340**, 579
- Sahal-Br  chot, S., Derouich, M., Bommier, V., & Barklem, P. S. 2007, [A&A](#), **465**, 667
- Sampoorna, M., Nagendra, K. N., Sowmya, K., Stenflo, J. O., & Anusha, L. S. 2019, [ApJ](#), **883**, 188
- Smitha, H. N., Nagendra, K. N., Stenflo, J. O., Bianda, M., & Ramelli, R. 2014, [ApJ](#), **794**, 30
- Stenflo, J. O., & Keller, C. U. 1997, [A&A](#), **321**, 927
- Stenflo, J. O., Keller, C. U., & Gandorfer, A. 2000, [A&A](#), **355**, 789
- Trujillo Bueno, J. 2001, in ASP Conf. Ser. 236, Advanced Solar Polarimetry: Theory, Observations, and Instrumentation, ed. M. Sigwarth (San Francisco, CA: ASP), 161