



General model of depolarization and transfer of polarization of singly ionized atoms by collisions with hydrogen atoms



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HIGHLIGHTS

- We computed the depolarization rates for large number of n^* and E_p .
- Genetic programming has been utilized to obtain strongly non-linear relationships
- These relationships reproduce the original data with accuracy better than 10%.
- General model is obtained to allow calculations of the depolarization rates
- Complex ions and the hyperfine levels can be easily derived from our results.

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ABSTRACT

Simulations of the generation of the atomic polarization is necessary for interpreting the second solar spectrum. For this purpose, it is important to rigorously determine the effects of the isotropic collisions with neutral hydrogen on the atomic polarization of the neutral atoms, ionized atoms and molecules. Our aim is to treat in generality the problem of depolarizing isotropic collisions between singly ionized atoms and neutral hydrogen in its ground state. Using our numerical code, we computed the collisional depolarization rates of the p -levels of ions for large number of values of the effective principal quantum number n^* and the Unsöld energy E_p . Then, genetic programming has been utilized to fit the available depolarization rates. As a result, strongly non-linear relationships between the collisional depolarization rates, n^* and E_p are obtained, and are shown to reproduce the original data with accuracy clearly better than 10%. These relationships allow quick calculations of the depolarizing collisional rates of any simple ion which is very useful for the solar physics community. In addition, the depolarization rates associated to the complex ions and to the hyperfine levels can be easily derived from our results. In this work we have shown that by using powerful numerical approach and our collisional method, general model giving the depolarization of the ions can be obtained to be exploited for solar applications.

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1. Introduction

The transitions between levels of solar ions caused by anisotropic scattering of the incident radiation induce population imbalances and quantum coherences among the Zeeman sublevels. Population imbalances and quantum coherences are usually called *atomic polarization*. The second solar spectrum (SSS), which is the spectrum of the linear polarization observed near the limb of the Sun, is the observational signature of the atomic polarization. The term SSS was coined by [Ivanov \(1991\)](#). It is also usually referred to as spectrum of the scattering polarization since it is due to coherent scattering processes (e.g. [Trujillo Bueno, 2001](#)).

The SSS is modified by solar magnetic fields via the Hanle effect. Such a modification allows diagnostics of the magnetic fields. In fact, Hanle effect diagnostics of hidden, mixed-polarity magnetic fields at sub-telescopic scales require confronting the discrepancy between the polarization calculated in the absence of magnetic fields and the observed linear scattering polarization (e.g. [Stenflo \(1982\)](#); [Landi Degl'Innocenti \(1983\)](#); [Sahal-Bréchet et al. 1986](#); [Stenflo \(2004\)](#); [Trujillo Bueno et al. \(2004\)](#); [Derouich et al. \(2006\)](#); [Faurobert et al. \(2009\)](#)). Reliable diagnostics consists in solving numerically the coupled set of equations of the radiative transfer and the statistical equilibrium of a multilevel atomic system taking into account radiative and collisional processes. The collisional rates, which are often poorly known, are a fundamental ingredient for realistic diagnostics. Sometimes the information encoded in accurate solar spectropolarimetric observations would be

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inaccessible if the effect of the collisions is unknown (e.g. Derouich et al. (2006, 2007)). There is a need for theory and numerical modeling of collisional depolarization of spectral lines by nearby hydrogen atoms. We notice that the collisions with hydrogen are dominant because it is the most abundant atom in the solar photosphere where the SSS is formed.

In this context, we aim to generalize our numerical modeling of Derouich et al. (2004) to provide collisional data for any ionic level. The paper is organized as follows. Section 2 gives a brief review of the theoretical background. In Section 3, we formulate the problem. Section 4 explains the basic definitions and notations, describes the collisional data employed in the context of this work, and provides the results for simple atoms without hyperfine structure. Simple atoms with hyperfine structure and complex atoms are presented in Sections 5 and 6. Finally, the conclusion of the paper is presented in Section 7.

2. Brief theoretical background

In real plasmas like the solar atmosphere, emitting ions suffer the effects of collisions with nearby abundant particles. To correctly extract informations contained in the solar observations would be inaccessible, the effect of the collisions must be taken into account. During the 2000s, Derouich, Sahal-Br echot and Barklem (DSB) developed a semi-classical theory allowing precise and quick calculations of the depolarization and polarization transfer rates by collisions with neutral hydrogen (see for example Derouich et al. (2003a, b); (2005a, b); Derouich (2004); Derouich and Barklem (2007)). The DSB approach is based on the Anstee-Barklem-O'Mara (ABO) theory concerned with collisional line broadening by neutral hydrogen (Anstee, 1992; Anstee and O'Mara, 1991; 1995; Anstee et al., 1997; Barklem, 1998; Barklem and O'Mara, 1997; Barklem et al., 1998).

An important result which justifies the use of the DSB semi-classical approach is that the collisional depolarization and polarization transfer probabilities depend exclusively on the intermediate range of the interatomic separations. We have shown that a modification of the interaction potential values by a Gaussian magnification factor, for the close or long-range regions of the interaction, does not practically change the values of the calculated collisional probabilities (Derouich et al., 2003a, 2004). In fact, we have found that a significant effect on the collisional depolarization and polarization transfer probabilities takes place only in the intermediate range of the interatomic separations. The sophisticated quantum chemistry approach is different to our semi-classical approach only in the short-range regions of the interactions. Since close interaction regions do not influence the values of the depolarization rates, we obtain good results compared to the available quantum chemistry ones ($\sim 10\%$ of accuracy).

In addition, the semi-classical approach is very useful for heavy and/or complex atoms/ions like Fe I, Ti I, NdII, EuII, CeII, ZrII, etc., whose collisional rates cannot be presently obtained via quantum chemistry methods. The spectral lines of such atoms/ions show significant polarization peaks in many spectral lines (see the atlases by Gandorfer (2000, 2002a, 2005).)

Although the fact that this theory is of semi-classical nature, the close coupling is taken into account and the time-dependent Schr odinger equations is solved.

3. Formulation of the problem

For neutral atoms, the DSB and ABO theories give general results for neutral atoms however they lose their generality in the case of ionized atoms. This is because, for all neutral atoms, the Uns old energy E_p can be replaced by a constant value $E_p =$

$-4/9$ atomic units (see, e.g., Anstee 1992, Barklem & O'Mara 1998; Derouich et al. (2003a)).

On the contrary, while ABO and DSB theories can be applied for any singly ionized atom, the calculation of the parameter E_p is required for each level which implies that the results are specific for each level of a particular ion. The interaction energy associated to the interaction of a singly ionized atom with a hydrogen atom in its ground state is given by Eq. (4) of Derouich et al. (2004). After some derivations and by using the Uns old approximation, the expression of the interaction potential becomes dependent on the parameter E_p as shown by Eq. (9) of Derouich et al. (2004). The variation of the depolarization rates as a function of E_p is given by Derouich et al. (2004) who concluded that one has to determine E_p before going to the calculation of the depolarization rates. This limitation substantially restrict the generalization of the results of Derouich et al. (2004). In fact, two steps are needed in the calculation of the depolarization rates for the levels of ions

1. Step 1: one must determine E_p directly for each state of each ion via the expression:

$$E_p = -\frac{2 \langle p_2^2 \rangle}{C_6}, \quad (1)$$

where $\langle p_2^2 \rangle$ is the mean square distance between the optical electron and the perturbed ion core,

$$\langle p_2^2 \rangle = \frac{n^{*2}}{2Z^2} [5n^{*2} + 1 - 3l(l+1)]. \quad (2)$$

$l=1$ is the orbital momentum for p -states, $Z=2$ for singly ionized atoms and n^* is the effective quantum number (see Derouich et al. (2004). C_6 is the Van der Waals coefficient given by the standard relationship (see for instance Goodisman (1973) and Derouich et al. (2004))

2. Step 2: Then, the value of E_p is included in the expression of the interaction energy. After that, the probabilities of collisions are obtained by solving the semi-classical differential coupled equations which are derived from the time-dependent Schr odinger equation (Derouich et al., 2003a). To obtain the depolarization rates, one thus must perform the integration of the probabilities of collisions over the impact-parameter b and over a Maxwell distribution of velocities $f(v)$ for a temperature T of the medium.

In practice, solar physicists can calculate the value of E_p (step 1) but it might be quite complicated for them to determine the depolarization rates by using the collision theory (step 2). The main goal of this work is to overcome numerically the difficulty pointed out in the step 2 to give the possibility of the determination of the depolarization rates by completing only step 1.

4. Definitions, notations and numerical results

4.1. Definitions and notations

We denote the atomic levels by (αJ) where J is the total angular momentum of the level and α represents the other quantum numbers necessary to define the electronic level of the ion. The atomic states (αJ) are described by the tensorial components $\rho_q^k(\alpha J)$ of the atomic density matrix. The number k is the tensorial order where $0 \leq k \leq 2J$ and $-k \leq q \leq k$ quantifies the coherences between the levels and the sublevels (e.g. Fano 1963; Omont (1977); Sahal-Br echot (1977); Landi Degl'Innocenti and Landolfi (2004)).

In the case of interactions of singly ionized ions with neutral hydrogen, the inelastic and super-elastic collisions between two different electronic levels are negligible. The indice α is omitted from now on for the sake of brevity. We apply the semi-classical

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