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Multipole rates for atomic polarization studies: the case of complex atoms in non-spherically symmetric states colliding with atomic hydrogen

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Abstract. Interpretation of linearly polarized parameters of the spectral lines of the second solar spectrum permits to obtain information about the magnetic field vector of the medium where the spectral lines are formed, provided suitable theoretical and numerical methods be applied to extract the physical information. This linear polarization is modified by the magnetic field and by collisions. In this context, with a few approximations, we provide in the present paper general and simple formulae giving the coefficients of the atomic master equation (depolarization, polarization transfer, population transfer and relaxation coefficients) for the case of an atom in any (but not spherically symmetric) level, perturbed by collisions with hydrogen atoms. It would be possible to apply this method for fast calculation of multipole rates for any level having an external shell $l \neq 0$.

Key words. Collision processes – Line: formation – Polarization – Sun: photosphere – Sun: magnetic fields

1. Introduction

The interaction of an atom with anisotropic unpolarized radiation can create atomic linear polarization. The populations of the Zeeman sublevels are not only not in LTE, but quantum coherences between the Zeeman sublevels can appear too. A linearly polarized spectrum is observed close to the solar limb (the so-called "second solar spectrum"), the anisotropy of the absorbed photospheric radiation field being due to limb darkening. Under the physical conditions of the solar photosphere and the low chromosphere, isotropic collisions between the atom and the neutral hydrogen atoms of the surrounding medium can partially or completely destroy the linear polarization of the levels. Therefore these collisions are of crucial importance to understand the underlying physics that governs light emission and absorption at the solar photosphere and low chromosphere levels. Hence, they must be taken into account in the analysis of the linear polariza-

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tion of the spectral lines. In the present paper, we will consider the case of complex atoms and we will only study collisional transitions between levels of the same configuration, with a few assumptions which are described in the next Section. Then, with these basic assumptions, we will find that the formulae giving the depolarization and polarization transfer coefficients due to collisions with neutral hydrogen for $l \neq 0$ levels of complex atoms can be expressed as a linear combination of the k-pole depolarization and elastic collisional rate coefficients obtained for simple atoms. It would be possible to apply this method for fast calculation of multipole rates for any level having an external shell $l \neq 0$. We will use the theory of the density-matrix and the theory of collisions and we will work in the T^k_q irreducible tensorial operators representation.

2. Basic assumptions and notations

First, we only consider the case of an atomic configuration having no equivalent electrons in the external shell nl, with $l \geq 1$.

Second, we will assume that the rest of the configuration (the core) remains frozen, and thus we will study only elastic collisions and inelastic collisions that induce transitions between the levels of the external shell. In fact, transitions between levels belonging to different configurations are negligible for collisions with neutral hydrogen in the solar atmosphere.

Third, we will neglect the nuclear spin (if it exists) and also the electronic spin for treating the collision problem. In fact, it is well known that internal-energy differences which correspond to frequency separations that are small compared to the inverse duration of a collision do not affect the scattering process. The time needed for a precession of the electronic (resp. nuclear) spin is mostly (resp. always) much longer than the collision time, so that the spins can be considered as fixed during the collision time. This is true in all cases for the hyperfine splitting and in most cases for fine structure splitting at the temperatures of interest in the solar atmosphere (Derouich et al. 2003a) for the case $l \neq 0$. Consequently we will limit the hydrogen-atom interaction to its electrostatic part.

The case $l = 0$ needs the spin to be taken into account during the collision. This is due to the fact that the electrostatic interaction potential is then spherically symmetric and cannot yield depolarization. That case has been treated in a preceding paper (Derouich et al. 2005b) and is beyond the scope of the present paper.

In the present paper, since we will study the case $l \neq 0$, where the electrostatic interaction potential is no longer spherically symmetric, depolarization and polarization transfer can be obtained. Furthermore, since collisional transitions between levels belonging to different configurations are negligible, this will permit us to use the so-called ABO approach to the interaction potential.

In the ABO approximation suitable for neutrals, the interaction between the valence electron of the studied atom and the hydrogen atom which remains in its ground state is limited to its electrostatic part. It is derived the from time-independent second-order perturbation theory without exchange, allowing the Lindholm-Foley average over m states to be removed. Whereas the Van der Waals potential underestimates the line broadening by typically a factor two or more, the ABO method created and developed by Anstee & O'Mara (1991, 1995), Anstee et al. (1997), Barklem & O'Mara (1997), Barklem & O'Mara (1998), give good results for solar line widths. The method has been extended by Derouich et al. (2003a,b, 2004) to depolarization rates, and gives also a rather good agreement (10%) with the results obtained from quantum chemistry calculations.

The impact approximation is well satisfied for isotropic collisions between neutral hydrogen atoms and emitting/absorbing atoms in the solar photosphere. So, we will consider binary collisions between the atom and an hydrogen atom in its ground state.The collisional rates are simply obtained by multiplying the rates for a binary collision by the hydrogen density. The scattering S-matrix is obtained by solving the semi-classical collisional coupled differential equations.

We use the standard atomic spectroscopic notations in *LS* coupling and we consider neutral atoms having no equivalent electrons in the external shell *nl* of the studied configuration $\gamma(S_C L_C)nl$. The labels n and l represent the principal and orbital angular momentum quantum numbers of the external shell, respectively. $\gamma S_C L_C$, or ($\gamma\ ^{2S_C+1}L_C$) represents the core that will be considered as frozen and thus not affected during the collision. γ is an abbreviation for the configuration of the core, L_C its total orbital angular momentum quantum number and S_C its total spin. The level J is defined as follows:

$\gamma(S_C L_C)nlSLJ$,

For simplicity, we will also use the following notations :

$\gamma(S_C L_C)nlSLJ = \beta SLJ = \alpha J.$

3. Density-matrix formalism and definitions of the multipole rates probabilities

We refer to Sahal-Bréchot (1977) for the formalism applied to astrophysical applications. Omont (1977) and Nienhuis (1976) developed also the same formalism, particularly for the two-level atom with hyperfine structure and Zeeman and level-crossing coherences. Sahal-Bréchot (1977) did not include coherences. In fact, due to the isotropy of the collisional processes, the rate constants obtained in the irreducible tensorial operators T^k_q basis are q-independent and only the $q = 0$ need to be calculated. Thus the formalism of Sahal-Bréchot (1977) is sufficient. For Sahal-Bréchot (1977) and Landi Degl'Innocenti & Landolfi (2004), relaxation denotes the deexcitation of a given level towards the other ones (especially destruction or relaxation rate of population). The elastic collisional processes, which do not modify the population of a given level J, are denoted as depolarization processes. The other terms of the multipole elements that couple the levels are also denoted as transfer rates (population transfer, alignment transfer, and so on). We will use this vocabulary in the present paper.

We start from the so-called master equation for the atom, or evolution equation of the atomic density-matrix, which becomes the so-called system of statistical equilibrium equations at the stationary state. We will limit it to the contribution of collisions in the following, which is of interest in the present paper. It can be written as follows :

$$\begin{aligned}\left(\frac{\mathrm{d}\,{}^{\alpha J}\rho^k_q}{\mathrm{d}t}\right)_{coll} &= -D^k(\alpha J)\,{}^{\alpha J}\rho^k_q \\ &- \sum_{\alpha' J' \neq \alpha J} \sqrt{\tfrac{2J'+1}{2J+1}}\, D^0(\alpha J \to \alpha' J')\,{}^{\alpha J}\rho^k_q \\ &+ \sum_{\alpha' J' \neq \alpha J} D^k(\alpha' J' \to \alpha J)\,{}^{\alpha' J'}\rho^k_q\,,\end{aligned} \tag{1}$$

where for $\alpha J \neq \alpha' J'$, if $\alpha = \alpha'$ one must have $J \neq J'$, and if $\alpha \neq \alpha'$ one can have $J = J'$.

1. $D^k(\alpha J)$ is the so-called depolarization rate due to elastic collisions and is a part of the coefficient of destruction of the k-pole component ${}^{\alpha J}\rho^k_q$ of the atomic density matrix. $D^0(\alpha J) = 0$.
2. $\sum_{\alpha' J' \neq \alpha J} \sqrt{\frac{2J'+1}{2J+1}}\, D^0(\alpha J \to \alpha' J')$ is the relaxation part of the coefficient of destruction of the k-pole component ${}^{\alpha J}\rho^k_q$ of the atomic density matrix and is the same for all k-values. We have:

$$\sqrt{\frac{2J'+1}{2J+1}}\, D^0(\alpha J \to \alpha' J') = C(\alpha J \to \alpha' J')\,, \tag{2}$$

where $C(\alpha J \to \alpha' J')$ is the usual inelastic collisional rate correponding to the transition ($\alpha J \to \alpha' J'$ between the levels (in excitation or deexcitation). Thus the relaxation coefficient of ${}^{\alpha J}\rho^k_q$ due to collisions can be written as:

$$\sum_{\alpha' J' \neq \alpha J} \sqrt{\frac{2J'+1}{2J+1}}\, D^0(\alpha J \to \alpha' J') = \sum_{\alpha' J' \neq \alpha J} C(\alpha J \to \alpha' J')\,. \tag{3}$$

3. $D^k(\alpha J \to \alpha' J')$ is the k-pole transfer rate from level $\alpha' J'$ to level αJ. $D^0(\alpha J \to \alpha' J')$ is the population transfer rate, $D^1(\alpha J \to \alpha' J')$ the orientation transfer rate, $D^2(\alpha J \to \alpha' J')$ the alignment transfer rate, and so on.

4. Expression of the multipole rate as a function of the rates between Zeeman sublevels

In this section, we shall express the depolarization rate $D^k(\alpha J)$, the relaxation part of the coefficient of destruction of the k-pole component, and the k-pole transfer rates $D^k(\alpha J \rightarrow \alpha' J')$ as a function of the rates between Zeeman sublevels $C(\alpha J M \rightarrow \alpha' J' M')$. We start from expressions (19) and (20) of Sahal-Bréchot (1977).

The off-diagonal elements are given by:

$$D^k(\alpha J \rightarrow \alpha' J') = \sum_{M M'} (2k+1) \times (-1)^{J+J'-(M+M')} \times \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix} \begin{pmatrix} J' & k & J' \\ -M' & 0 & M' \end{pmatrix} \times C(\alpha J M \rightarrow \alpha' J' M'). \tag{4}$$

The diagonal element of the master equation can be written as:

$$\begin{aligned} D^k(\alpha J) + \sum_{\alpha' J' \neq \alpha J} C(\alpha J \rightarrow \alpha' J') = \\ - \sum_{\substack{M \\ M' \neq M}} (2k+1)\,(-1)^{M-M'} \times \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix} \begin{pmatrix} J & k & J \\ -M' & 0 & M' \end{pmatrix} \times C(\alpha J M \rightarrow \alpha J M') + \\ \sum_{\substack{M \\ \alpha' J' M' \\ \text{and } M \neq M' \\ \text{if } \alpha J = \alpha' J'}} (2k+1) \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix}^2 \times C(\alpha J M \rightarrow \alpha' J' M'). \end{aligned} \tag{5}$$

An alternate expression for the diagonal element and which will be used in the following sections is :

$$\begin{aligned} D'^k(\alpha J) + \sum_{\alpha' J'} C(\alpha J \rightarrow \alpha' J') = \\ - \sum_{M M'} (2k+1)\,(-1)^{M-M'} \times \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix} \begin{pmatrix} J & k & J \\ -M' & 0 & M' \end{pmatrix} \times C(\alpha J M \rightarrow \alpha J M') + \\ \sum_{M \alpha' J' M'} (2k+1) \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix}^2 \times C(\alpha J M \rightarrow \alpha' J' M'). \end{aligned} \tag{6}$$

The collisional rates between Zeeman sublevels are obtained in the standard atomic representation $\alpha J M$ of the laboratory (or fixed) reference frame. The impact and semi-classical approximation (straight path trajectory for the hydrogen atom perturber) being valid, the rates are obtained at the hydrogen density N_H and at the temperature T through an integration over the distribution of relative velocities $f(v)$ and over the impact parameter b of the probability transition $\langle P(\alpha J M \rightarrow \alpha' J' M', v, b)\rangle_{Ang\,Av}$ averaged over all directions of relative velocities (angular average, notation $\langle\rangle_{Ang\,Av}$). We refer to previous papers (Derouich et al. 2003a,b, 2004, 2005a,b) for details:

$$C(\alpha J M \rightarrow \alpha' J' M') = N_H \int_0^\infty v\, f(v)\, \mathrm{d}v \int_0^\infty 2\pi b\, \mathrm{d}b \times \langle P(\alpha J M \rightarrow \alpha' J' M', v, b)\rangle_{Ang\,Av}\ , \tag{7}$$

and

$$\langle P(\alpha J M \rightarrow \alpha' J' M', v, b)\rangle_{Ang\,Av} = \oint \frac{\mathrm{d}\Omega}{4\pi} P(\alpha J M \rightarrow \alpha' J' M', v, b, \Omega). \tag{8}$$

The angular average is given by Masnou-Seeuws & Roueff (1972):

$$\begin{aligned} \langle P\,(\alpha J M \rightarrow \alpha' J' M')\rangle_{Ang\,Av} = \\ \sum_{m m' n n'} \sum_{K=|J-J'|}^{J+J'} (2K+1) \sum_x \begin{pmatrix} J & J' & K \\ M & M' & x \end{pmatrix} \\ \times \sum_k \begin{pmatrix} J & J' & K \\ m & n' & k \end{pmatrix} \begin{pmatrix} J & J' & K \\ n & m' & k \end{pmatrix} \\ \times \langle \alpha J m | \, T \, | \alpha' J' m' \rangle \langle \alpha J n | \, T \, | \alpha' J' n' \rangle^* . \end{aligned} \tag{9}$$

S is the scattering collisional matrix for an impact parameter b, and a relative velocity v, and we will work with the so-called transtion matrix $T = 1 - S$. The S-matrix can be calculated in any reference frame, in particular in the so-called collision frame (or atomic frame), (see Derouich et al. 2003a,and references therein).

5. Calculations: electronic spin neglected and frozen core + Racah Algebra

Dropping the question of the nuclear spin for the moment, we will successively neglect the electronic spin during the collision and then we will assume that the core is frozen.

1. First step : we neglect the fine structure during the collision:

We have $\boldsymbol{S}+\boldsymbol{L}=\boldsymbol{J}$, and $M_S+M_L=M_J$.
We decouple the standard basis:

$$|\alpha J M_J\rangle = \sum_{M_S M_L} \sqrt{2J+1}\times \begin{pmatrix} S & L & J \\ M_S & M_L & -M_J \end{pmatrix} \times(-1)^{S-L+M_J}\,|S\,M_S\rangle\,|\beta L M_L\rangle\,, \tag{10}$$

If the fine structure is neglected (the total electronic spin S has no time to rotate) the S-matrix (or T-matrix) is diagonal in S and does not depend on M_S :

$$\left\langle \alpha J M_J\,|T|\,\alpha' J' M'_J\right\rangle = \sum_{M_S M'_S M_L M'_L} \sqrt{(2J+1)(2J'+1)}\times (-1)^{L-L'+M_J-M'_J}\times \begin{pmatrix} S & L & J \\ M_S & M_L & -M_J \end{pmatrix}\begin{pmatrix} S & L' & J' \\ M'_S & M'_L & -M'_J \end{pmatrix}\times \delta(M_S,M'_S)\ \langle\beta L M_L|\,T\,\left|\beta L' M'_L\right\rangle \tag{11}$$

2. Second step: we assume the core as frozen: We have
$\boldsymbol{L}=\boldsymbol{L_C}+\boldsymbol{l}$, $M_L=M_{L_C}+m_l$
and we ignore the spin $\boldsymbol{S}=\boldsymbol{S_C}+\boldsymbol{s}$, with $\boldsymbol{s}=\mathbf{1/2}$.
We decouple the basis $\beta L M_L$ and we perform the same reasoning by considering that the S-matrix (or T-matrix) is diagonal in L_C and does not depend on M_{L_C}. So we replace J by L, J' by L', L and L' by l, and S by L_C in (11). We obtain the result :

$$\left\langle \beta L M_L\,|T|\,\beta L' M'_L\right\rangle = \sum_{M_{L_C} M'_{L_C} m_l m'_l} \sqrt{(2L+1)(2L'+1)}\times (-1)^{l-l'+M_L-M'_L}\times \begin{pmatrix} L_C & l & L \\ M_{L_C} & m_l & -M_L \end{pmatrix}\begin{pmatrix} L_C & l & L' \\ M'_{L_C} & m'_l & -M'_L \end{pmatrix}\times \delta(M_{L_C},M'_{L_C})\ \langle\gamma\, n l m_l|\,T\,\left|\gamma\, n l m'_l\right\rangle\ . \tag{12}$$

We now enter expressions (11) and (12) into (4) and (6) and reduce all the sums of products of "3j" symbols by using the standard formulae of Racah Algebra. Cf. Brink & Satchler (1968) for instance. "9j" symbols appear. We will not detail the calculations and only give the results.

6. Results

The formulae are gathered below :

1. Coefficient of the off-diagonal element of the master equation:

$$D^k(\alpha J\to\alpha' J') = (2J+1)(2J'+1)\times \sum_{k_L}(2k_L+1)\,D^{k_L}(\beta S\,L\to\beta S\,L')\times \sum_{k_S}(2k_S+1) \times\begin{Bmatrix} L & S & J \\ L & S & J \\ k_L & k_S & k \end{Bmatrix}\begin{Bmatrix} L' & S & J' \\ L' & S & J' \\ k_L & k_S & k \end{Bmatrix}, \tag{13}$$

$$D^{k_L}(\beta S\,L\to\beta S\,L') = (2L+1)(2L'+1)\times \sum_{k_1}(2k_l+1)\,D^{k_l}(\gamma nl)\sum_{k_{L_C}}(2k_{L_C}+1) \times\begin{Bmatrix} l & L_C & L \\ l & L_C & L \\ k_l & k_{L_C} & k \end{Bmatrix}\begin{Bmatrix} l & L_C & L' \\ l & L_C & L' \\ k_l & k_{L_C} & k_L \end{Bmatrix}, \tag{14}$$

$$D^{k_l}(\gamma nl) = N_H\times \int_0^\infty v\,f(v)\,\mathrm{d}v\int_0^\infty 2\pi b\,\mathrm{d}b\times \sum_{\mu\mu'\nu\nu'}\langle\gamma nl\,\mu\,|T|\,\gamma nl\,\mu'\rangle\,\langle\gamma nl\,\nu\,|T|\,\gamma nl\,\nu'\rangle^* \times\sum_x(-1)^{\nu-\nu'} \times\begin{pmatrix} l & l & k_l \\ \nu & -\mu & x \end{pmatrix}\begin{pmatrix} l & l & k_l \\ \nu' & -\mu' & x \end{pmatrix}. \tag{15}$$

2. Coefficient of the diagonal element of the master equation:

$$\sum_{\alpha' J'\neq\alpha J} C(\alpha J\to\alpha' J')\ +\ D^k(\alpha J) = C(\gamma nl\leftrightarrow\gamma nl)\ - (2J+1)^2\sum_{k_L}(2k_L+1)\,D^{k_L}(\beta S\,L)\times \sum_{k_S}(2k_S+1) \times\begin{Bmatrix} L & S & J \\ L & S & J \\ k_L & k_S & k \end{Bmatrix}\begin{Bmatrix} L & S & J \\ L & S & J \\ k_L & k_S & k \end{Bmatrix}, \tag{16}$$

with

$$D^{k_L}(\beta S\,L) = (2L+1)^2\sum_{k_1}(2k_l+1)\,D^{k_l}(\gamma nl)\times \sum_{k_{L_C}}(2k_{L_C}+1) \times\begin{Bmatrix} l & L_C & L \\ l & L_C & L \\ k_l & k_{L_C} & k \end{Bmatrix}\begin{Bmatrix} l & L_C & L \\ l & L_C & L \\ k_l & k_{L_C} & k_L \end{Bmatrix}. \tag{17}$$

We recall that this diagonal coefficient is, according to our definitions, the sum of the depolarization (due to elastic collisions) and of the relaxation (due to inelastic collisions) coefficients. However, care must be taken since this total diagonal coefficient is called the depolarization coefficient by some authors.

Thus, by neglecting the spin during the collision process and by assuming the core as frozen, we have shown that the collisional coefficients can be expressed as a linear combination of all the $D^{k_l}(\gamma nl)$ collisional rates given by (15). These rates are the total ($k_l = 0$) elastic collisional rate and the collisional depolarization rates ($k_l \geq 1$) of the $\gamma\, nl$ external shell, the shell being treated as the one of a simple atom. The core being frozen and the spin being neglected, there is neither depolarization associated to the spin nor to the core L_C of the complex atom, and the collisional depolarization reflects that of the external shell n with the valence electron l. These rates can be calculated by means of the method developed by (Derouich et al. 2003a,b, 2004) by solving the semi-classical differential coupled equations leading to the S-matrix by using the ABO potential for simple atoms, using the effective quantum number n^* of the γnl shell.

7. Case of hyperfine structure

If there is a hyperfine structure, by neglecting the nuclear spin during the collision, we can apply the preceding method by replacing J by F, S by I, L by J and so on. This only adds a further layer to the preceding formulae.

8. Applications and conclusion

All these rates can be provided through tables, by describing the nl shell by an effective quantum number n^*. The tables given in (Derouich et al. 2003a,b, 2004) only concern linear depolarization rates ($k = 2$, destruction of alignment) for nl, with $l = 1, 2, 3$. For the present purpose, these tables must be complemented by the total elastic rates ($k = 0$) and by the other k-pole rates of interest ($1 \leq k \leq 2l$). They will be provided in a following paper. After that, by interpolation in the tables, we will test the precision of the method by comparing the obtained results with those of (Derouich et al. 2005a). Then, if the present method is sufficiently accurate, it will be possible to apply it to fast calculation of all the multipole rates for any level and between any levels of an external shell $l \geq 1$ of any complex atom of the second solar spectrum.

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