RADIATIVE TRANSFER MODELING OF THE ENIGMATIC SCATTERING POLARIZATION IN THE SOLAR Na I D\textsubscript{1} LINE

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ABSTRACT

The modeling of the peculiar scattering polarization signals observed in some diagnostically important solar resonance lines requires the consideration of the detailed spectral structure of the incident radiation field as well as the possibility of ground level polarization, along with the atom’s hyperfine structure and quantum interference between hyperfine $F$-levels pertaining either to the same fine structure $J$-level, or to different $J$-levels of the same term. Here we present a theoretical and numerical approach suitable for solving this complex non-LTE radiative transfer problem. This approach is based on the density-matrix metalevel theory (where each level is viewed as a continuous distribution of sublevels) and on accurate formal solvers of the transfer equations and efficient iterative methods. We show an application to the D-lines of Na, with emphasis on the enigmatic D\textsubscript{1} line, pointing out the observable signatures of the various physical mechanisms considered. We demonstrate that the linear polarization observed in the core of the D\textsubscript{1} line may be explained by the effect that one gets when the detailed spectral structure of the anisotropic radiation responsible for the optical pumping is taken into account. This physical ingredient is capable of introducing significant scattering polarization in the core of the Na I D\textsubscript{1} line without the need for ground-level polarization.

Key words: atomic processes – line: formation – polarization – radiative transfer – scattering – stars: atmospheres

1. INTRODUCTION

For nearly two decades, the modeling of the scattering polarization signals observed by Stenflo & Keller (1997) in the core of the Na I and Ba II D\textsubscript{1} lines has represented one of the most challenging problems in the field of theoretical spectropolarimetry (see also Stenflo et al. 2000). Given that these spectral lines are produced by atomic transitions between an upper level and a lower level with total angular momentum $J = 1/2$ (i.e., atomic levels that cannot carry atomic alignment), they were initially considered to be intrinsically unpolarizable lines. On the other hand, the only stable isotope of sodium ($^{23}$Na) and two of the seven stable isotopes of barium ($^{135}$Ba and $^{137}$Ba, with relative abundances of about 7\% and 11\%, respectively) have nuclear spins $I = 3/2$. In these isotopes, the upper and lower levels of the D\textsubscript{1} line split into two hyperfine structure (HFS) levels with total (electronic plus nuclear) angular momenta $F = 1$ and $F = 2$. Therefore, the main problem is identifying a physical mechanism through which atomic alignment can be induced in the $F$-levels of the D\textsubscript{1} line.

According to the theory of spectral line polarization described in Landi Degl’Innocenti & Landolfi (2004), the mere absorption of anisotropic radiation is not sufficient to induce atomic alignment in the upper $F$-levels of the D\textsubscript{1} line, unless the lower $F$-levels are also polarized. As shown in Section 2 of Belluzzi & Trujillo Bueno (2013), this is ultimately due to the hypothesis, required by the theory of Landi Degl’Innocenti & Landolfi (2004), that the incident radiation field is flat (i.e., independent of frequency) across the spectral interval spanned by the HFS components of the D\textsubscript{1} line (flat-spectrum approximation). This assumption, on the other hand, does not appear to be particularly unsuitable in the solar case, since the frequency separation among the various HFS components of the D\textsubscript{1} line is significantly smaller than the Doppler width of the spectral line.

By generalizing the idea of “internal levels” (or “metalevels”) to the polarized case, Landi Degl’Innocenti et al. (1997) developed a theoretical approach that does not require the flat-spectrum condition to be satisfied, and that is suitable for treating coherent scattering processes in the presence of pumping radiation fields with an arbitrary spectral structure. Working within the framework of this theory, and assuming that the anisotropy degree of the incident radiation is constant with frequency, Landi Degl’Innocenti (1998, 1999) showed that a conspicuous polarization signal, similar to the observed one, can be produced in the core of the Na I D\textsubscript{1} line, provided that a substantial amount of atomic polarization is present in the lower level (the ground level of sodium). This result, on the other hand, leads to a sort of paradox since the required atomic polarization in the long-lived ground level of sodium is incompatible with the presence in the lower solar chromosphere of inclined magnetic fields sensibly stronger than 0.01 G (see Landi Degl’Innocenti 1998), which seems to contradict the results obtained from other types of observations (e.g., Bianda et al. 1998; Stenflo et al. 1998). Moreover, through a calculation based on Quantum Chemistry, Kerkeni & Bommier (2002) argued that the effect of depolarizing collisions is sufficiently strong to destroy the required atomic polarization in the ground level of sodium.

In the work of Landi Degl’Innocenti (1998), lower level polarization was included in the problem as a free parameter. The physical mechanism through which atomic polarization can be induced in the ground level of sodium via the D\textsubscript{2} line transition, and then transferred to the upper $F$-levels of the D\textsubscript{1} line (the repopulation pumping mechanism), was pointed out by Trujillo Bueno et al. (2002), who in addition investigated the sensitivity of the atomic polarization of the sodium HFS levels to the presence of magnetic...
fields (see also Casini et al. 2002). These works, which were carried out within the framework of the theory of polarization described in Landi Degl’Innocenti & Landolfi (2004), neglecting depolarizing collisions, showed the actual possibility of inducing a significant amount of atomic polarization in the ground level of sodium, but also confirmed its incompatibility with the estimated intensities and geometries of the magnetic fields of the lower chromosphere.

The “enigma” of the D1 lines remained substantially unchanged until the recent identification by Belluzzi & Trujillo Bueno (2013) and by Del Pino Alemán et al. (2014) of two mechanisms that can introduce scattering polarization in the core of such lines, without requiring the presence of atomic polarization in the ground levels of sodium and barium. The idea at the basis of the mechanism identified by Belluzzi & Trujillo Bueno (2013) is that if the incident radiation field (and, in particular, its anisotropy degree) varies across the HFS multiplet, so that the various HFS components are affected by different pumping radiations, then atomic polarization can be induced in the upper F-levels of the D1 line, and the emitted radiation can in general be polarized, also in the absence of atomic polarization in the lower F-levels. Belluzzi & Trujillo Bueno (2013) modeled the D1 lines of Na i and Ba ii by solving the full non-LTE radiative transfer (RT) problem in one-dimensional semi-empirical models of the solar atmosphere, according to the partial frequency redistribution (PRD) approach described in Belluzzi & Trujillo Bueno (2014). Through the R_{J} part of their redistribution matrix, which describes coherent scattering processes according to the metalevel approach, they took into account the detailed spectral structure of the pumping radiation, finding that the small differences among the radiation fields experienced by the various HFS components of the D1 line are actually sufficient to produce appreciable scattering polarization signals in the core of these lines.

The signal obtained by Belluzzi & Trujillo Bueno (2013) in the core of the Na i D1 line is, however, sensibly weaker than the one observed by Stenflo & Keller (1997), but it is similar to that shown in the right panel of Figure 2 of Trujillo Bueno (2009), resulting from the observations by Trujillo Bueno et al. (2001). On the other hand, two physical ingredients, which were taken into account by Landi Degl’Innocenti (1998), have been neglected by Belluzzi & Trujillo Bueno (2013): quantum interference between HFS magnetic sublevels pertaining to different J-levels, and the possibility that a given amount of atomic polarization is present in the lower F-levels. It is well known that interference between the upper J-levels of the D1 and D2 lines plays a very important role in the generation of the scattering polarization pattern observed in these lines (see Stenflo 1980; Landi Degl’Innocenti 1998; Landi Degl’Innocenti & Landolfi 2004), while recent RT calculations seem to indicate that in the atmospheric region where the core of the sodium D-lines is formed depolarizing collisions might not completely destroy lower level polarization as previously thought.

In the first part of this paper, we derive a redistribution matrix suitable for describing coherent scattering in the atom rest frame (with Doppler redistribution in the observer’s frame), accounting for lower level polarization, interference between HFS magnetic sublevels pertaining to the upper J-levels of D1 and D2, and inelastic collisions with electrons. In the second part, we describe the numerical method of solution of the ensuing non-LTE problem, and we present a series of results obtained by treating lower level polarization as a free parameter of the problem (it will not be calculated self-consistently when solving the non-LTE problem).

As previously mentioned, another mechanism that may explain the physical origin of the signals observed by Stenflo & Keller (1997) and Stenflo et al. (2000) in the core of the Na i and Ba ii D1 lines, without requiring the presence of lower level polarization, has been recently identified by Del Pino Alemán et al. (2014). In their work, the authors show that measurable Q/I signals can be produced in the core of intrinsically unpolarizable lines through the redistribution of the spectral line radiation due to the non-coherence of the continuum scattering. Although this mechanism (which strongly depends on the assumed model atmosphere) may well coexist with the previous one, it will be neglected in this investigation.

Finally, we point out that the enigmatic polarization signals observed in the solar D1 line have led to the realization of a laboratory experiment on scattering polarization by the potassium atom, which has the same D1 quantum structure as sodium (Thalmann et al. 2006, 2009). This experiment, performed by pumping the potassium atoms through a tunable laser, has shown an unexpected phenomenology that cannot be interpreted by means of the standard Kramers–Heisenberg equation. Stenflo (2015) has recently suggested an interpretation of these results based on quantum interference between the sublevels of the ground state of potassium. It will be of interest to investigate whether this physical ingredient may also play a role in the solar case, but this lies outside the scope of the present paper. This kind of interference is thus neglected in the present work.

2. FORMULATION OF THE PROBLEM

We consider a two-term atom with HFS, in the absence of magnetic fields. Under the assumption of L–S coupling, the atomic Hamiltonian has eigenvectors of the form |βLSJFM⟩, where β, L, and S indicate the electronic configuration, the orbital angular momentum, and the electronic spin, respectively, I is the nuclear spin, J is the total electronic angular momentum, F is the total (electronic plus nuclear) angular momentum, and M is its projection along the quantization axis. We recall that each term is composed of (L + S – |L – S| + 1) fine structure (FS) J-levels, while each J-level splits into (J + I – |J – I| + 1) HFS F-levels. In each term, we thus have

$$\sum_{J,L=|L-S|}^{L+S} \sum_{F=|J-I|}^{J+I} (2F+1) = (2L+1)(2S+1)(2I+1),$$

(1)

magnetic sublevels.

In the standard representation, the atomic model under consideration is described by the density matrix elements

$$\langle \rho | JFJM', J'F'M' \rangle \equiv \langle \beta LSJFM | \hat{\rho} | \beta LSJ'F'M' \rangle,$$

(2)

where $\hat{\rho}$ is the density operator. As is clear from Equation (2), this atomic model accounts for quantum interference between pairs of HFS magnetic sublevels belonging either to the same F-level or to different F-levels pertaining either to the same J-level or to
different \( J \)-levels within the same term. In the following, we will work with the irreducible spherical components of the density matrix (or spherical statistical tensors) defined by (see Equation (11b) of Casini & Manso Sainz 2005)

\[
\beta_{\text{LSI}} K \rho_{K}^{Q}(JF, J'F') = \sum_{MM} (-1)^{F-M} \sqrt{2K+1} \begin{pmatrix} F & F' & K \\ M & -M' & -Q \end{pmatrix} \beta_{\text{LSI}} \rho(JFM, J'FM').
\]

Equation (3) shows that in a two-term (or multi-term) atom with HFS, besides the 0-rank elements \( \beta_{\text{LSI}} K \rho_{0}^{Q}(JF, JF) \), which are proportional to the statistical weights: is not calculated through a self-consistent solution of the statistical equilibrium equations and of the total population, we have

the overall population of the lower term, we have

\[
\frac{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J'_{F} I'_{F})}{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F})} = \delta_{I_{F} I'} \delta_{F_{F} F'} \delta_{Q_{0}} \beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F}).
\]

where the label \( \ell \) indicates that the corresponding quantity refers to the lower term, or to one of its FS or HFS levels (accordingly, quantities of the same \( \ell \)-level will be labeled with the letter \( u \)). Furthermore, we assume that the populations of the various HFS \( \ell \)-levels of the lower term, \( N(J_{F}, I_{F}) \), are proportional to the statistical weights:

\[
N(J_{F}, I_{F}) = \frac{N(L_{F})}{(2L_{F} + 1)(2S + 1)(2I + 1)} (2F_{I} + 1),
\]

with \( N(L_{F}) \) the overall population of the lower term. Indicating with \( N_{T} \) the total population, we have

\[
\frac{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F})}{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F})} = \frac{N(L_{F})}{N_{T}} \sqrt{2F_{I} + 1} \frac{N(L_{F})}{N_{T}} \frac{2L_{F} + 1}{(2L_{F} + 1)(2S + 1)(2I + 1)}. \]

Introducing the quantity

\[
\sigma_{K}^{Q}(J_{F}, I_{F}) = \frac{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F})}{\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J_{F} I_{F})} \frac{N(L_{F})}{N_{T}} \frac{2F_{I} + 1}{(2L_{F} + 1)(2S + 1)(2I + 1)} \sigma_{0}^{Q}(J_{F}, I_{F}).
\]

we can finally write

\[
\beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J'_{F} I'_{F}) = \delta_{I_{F} I', F_{F} F'} \delta_{Q_{0}} \frac{N(L_{F})}{N_{T}} \frac{2F_{I} + 1}{(2L_{F} + 1)(2S + 1)(2I + 1)} \sigma_{0}^{K}(J_{F}, I_{F}).
\]

In this work, the quantity \( \sigma_{0}^{K}(J_{F}, I_{F}) \) is not calculated through a self-consistent solution of the statistical equilibrium equations and of the RT equations, but it is set as a free parameter of the problem.

We account for inelastic collisions with electrons, inducing transitions between the upper and the lower term. On the other hand, we neglect “weakly inelastic” collisions inducing transitions between different FS or HFS levels pertaining to the same term, as well as elastic collisions with neutral perturbers. Finally, we assume that the magnetic sublevels of the lower term are infinitely sharp. In the atom rest frame, this last set of hypotheses implies coherence in frequency for Rayleigh scattering, and the usual energy conservation relationship between the frequencies of the incoming and outgoing photons for Raman scattering. Stimulated emission is neglected.

3. THE ABSORPTION AND EMISSION COEFFICIENTS

The expression of the absorption coefficient for a two-term atom with HFS, accounting for lower term polarization and for the presence of an arbitrary magnetic field, is given by Equation (33a) of Casini & Manso Sainz (2005). With the help of Equation (2.34) of Landi Degl’Innocenti & Landolfi (2004), it can be shown that, in the absence of magnetic fields, it takes the simpler form

\[
\eta_{0}(\nu, \bar{\Omega}) = \frac{\hbar \nu}{4\pi N_{T}} B(L_{F} \rightarrow L_{u}) \sum_{KQ} \sum_{J_{F} I_{F} J_{F} I_{F}} \sum_{J_{u} I_{u}} (-1)^{1+K+J} \left\{ \begin{array}{ccc} J_{u} & J_{F} & J_{F} \\ L_{u} & L_{F} & L_{F} \end{array} \right\} \left\{ \begin{array}{ccc} J_{u} & J_{F} & J_{F} \\ I_{u} & I_{F} & I_{F} \end{array} \right\} \left\{ \begin{array}{ccc} J_{u} & L_{u} & L_{u} \\ J_{u} & J_{u} & J_{u} \end{array} \right\} \left\{ \begin{array}{ccc} 1 & 1 & 1 \\ F_{u} & F_{u} & F_{u} \end{array} \right\} \\
\times \sqrt{\left( 2 \begin{array}{ccc} J_{F} & J_{F} & J_{F} \\ L_{F} & L_{F} & L_{F} \end{array} \right) \left( 2F_{I} + 1 \right) \left( 2I + 1 \right) \left( 2L_{F} + 1 \right)} \left\{ \begin{array}{ccc} J_{u} & J_{F} & J_{F} \\ I_{u} & I_{F} & I_{F} \end{array} \right\} \left\{ \begin{array}{ccc} L_{u} & L_{u} & L_{u} \\ J_{u} & J_{u} & J_{u} \end{array} \right\} \left\{ \begin{array}{ccc} F_{u} & F_{u} & F_{u} \end{array} \right\} \\
\times \Re \left\{ \begin{array}{ccc} T_{0}^{\bar{\Omega}}(\nu, \bar{\Omega}) \beta_{\text{LSI}} K \rho_{Q}^{K}(J_{F} I_{F}, J'_{F} I'_{F}) \Phi(\nu_{J_{u} I_{F} L_{F} F_{F}} - \nu) \right\}. \]

\[\text{Note that in the recent modeling of polarized scattering by tunable laser light on potassium gas in the laboratory, quantum coherence in the lower term was identified as the source of the observed D}_{1} \text{ polarization (Stenflo 2015). It will be of interest to investigate whether this coherence may play a significant role also in the solar case, where the pumping radiation is broadband and not nearly monochromatic and highly polarized (as in a tunable laser). In this work, we demonstrate that it is possible to obtain significant solar D}_{1} \text{ polarization by neglecting them.}\]
with \( i = 0, 1, 2, 3 \) representing Stokes \( I, Q, U, \) and \( V \), respectively, and where \( B(L_\ell \rightarrow L_u) \) is the Einstein coefficient for absorption from the lower to the upper term and \( T^K_{\Omega_0}(i, \Omega) \) is the geometrical tensor introduced by Landi Degl’Innocenti (1983). The complex profile \( \Phi(\nu_0 - \nu) \) is defined by

\[
\Phi(\nu_0 - \nu) = \phi(\nu_0 - \nu) + i \psi(\nu_0 - \nu),
\]

with \( \phi(\nu_0 - \nu) \) the Lorentzian profile and \( \psi(\nu_0 - \nu) \) the associated dispersion profile.

Assuming that no interference is present in the lower term, so that the spherical statistical tensors of this term are given by Equation (4), then Equation (2) of Landi Degl’Innocenti (1999) is easily recovered. Substituting Equation (8) into (9), we have

\[
\eta_i(\nu, \Omega) = k_L \sum_K T^K_{\Omega_0}(i, \Omega) \alpha^K_0(\nu),
\]

with

\[
\alpha^K_0(\nu) = \frac{1}{(2S + 1)(2I + 1)} \sum_{b,s} \sum_{i,j} (-1)^{i + K - E_b - E_i} \sqrt{3} (2L_u + 1)(2L_\ell + 1)(2J_{lower} + 1)(2J_{upper} + 1)(2F_u + 1)(2F_\ell + 1)^{3/2} \times \left\{ J_u \begin{array}{cc} J_u & J_u' \end{array} \right\} \left\{ I_u \begin{array}{cc} I_u & I_u' \end{array} \right\} \times \left\{ \begin{array}{cc} J_{lower} & J_{lower}' \end{array} \right\} \left\{ \begin{array}{cc} J_{upper} & J_{upper}' \end{array} \right\} K \begin{array}{cc} K & K \end{array} \times \left\{ \delta(\nu_- - \nu) \right\} \left\{ \Phi(\nu_0 - \nu) \right\},
\]

and where we have introduced the frequency-integrated absorption coefficient

\[
k_L = \frac{4\pi}{h} N(L_\ell) B(L_\ell \rightarrow L_u).
\]

The expression of the emission coefficient for a two-term atom with HFS, in the absence of magnetic fields, neglecting any kind of collisions, assuming that no interference is present in the lower term, and under the assumption that the magnetic sublevels of the lower term are infinitely sharp, has been derived by Landi Degl’Innocenti (1999), working within the framework of the metalevel approach of Landi Degl’Innocenti et al. (1997). This expression, which is given by Equation (1) of Landi Degl’Innocenti (1999), can be rewritten in the equivalent form

\[
\varphi_0(\nu, \Omega) = \frac{4\pi}{h} N_0 B(L_\ell \rightarrow L_u) C^{\infty}(2L_u + 1)(2L_\ell + 1) \sum_{b,s} \sum_{i,j} \sum_{K} \sum_{K'} (-1)^{i + K - E_b - E_i} \sqrt{3} (2L_u + 1)(2L_\ell + 1)(2J_{lower} + 1)(2J_{upper} + 1)(2F_u + 1)(2F_\ell + 1)^{3/2} \times \left\{ J_u \begin{array}{cc} J_u & J_u' \end{array} \right\} \left\{ I_u \begin{array}{cc} I_u & I_u' \end{array} \right\} \times \left\{ \begin{array}{cc} J_{lower} & J_{lower}' \end{array} \right\} \left\{ \begin{array}{cc} J_{upper} & J_{upper}' \end{array} \right\} K \begin{array}{cc} K & K \end{array} \times \left\{ \delta(\nu_- - \nu) \right\} \left\{ \Phi(\nu_0 - \nu) \right\},
\]

where \( A(L_u \rightarrow L_\ell) \) is the Einstein coefficient for spontaneous emission from the upper to the lower term, while \( \nu_{ab} \) is the frequency separation between levels \( a \) and \( b \). The tensor \( J^K_{\Omega_0}(\nu') \) describing the incident radiation field is given by (see Equation (5.157) of Landi Degl’Innocenti & Landolfi 2004)

\[
J^K_{\Omega_0}(\nu') = \frac{2\pi}{4\pi} \sum_{j=0}^{3} T^K_{\Omega_0}(j, \Omega) I_j(\nu', \Omega'),
\]

where \( I_j(\nu', \Omega') \) represents the four Stokes parameters.

In order to take the effect of inelastic collisions with electrons into account, we proceed by analogy with the complete frequency redistribution (CRD) case. The expression of the emission coefficient for a two-term atom with HFS, in the limit of CRD, taking such collisions into account, has been derived by Belluzzi et al. (2015), working within the framework of the theory of Landi Degl’Innocenti & Landolfi (2004). By analogy with Equation (37) of Belluzzi et al. (2015), we thus include the effect of inelastic
collisions by modifying Equation (14) as follows

\[ \varepsilon_i(\nu, \tilde{\Omega}) = \frac{h\nu}{4\pi} N_T B(L_\ell \rightarrow L_u) (2L_u + 1)(2L_\ell + 1) \sum_{J_{\ell} J_u' F_{\ell} F_u'} T(L_u L_\ell S I, J_u J_u' J_{\ell} J_{\ell}' F_u F_u' F_{\ell} F_{\ell}') \]

\[ \times \frac{1}{2} \left[ \Phi(\nu J_u F_u E_u - \nu) + \Phi(\nu J_u' F_u' E_u' - \nu) \right] \sum_{K_1 K_2} \left( \sum_{K_{\ell} K_u} \left( \sum_{K_{\ell} K_u} (-1)^{1 + K_{\ell} + F_{\ell} + K} \sqrt{3} \right) \left( K_{\ell} K_u \right) \left( J_{\ell} J_{\ell}' F_{\ell} F_{\ell}' \right) + \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) \right] \]  

\[ \times \left\{ F_u' F_{\ell}' 1 \left( F_u F_{\ell} K \right) \right\} T_{0}^{\tilde{\Omega}}(i, \tilde{\Omega}) \beta_{\ell}^{\text{Se}} \rho_0 K (J_{\ell} F_{\ell}', J_{\ell}' F_{\ell}') \]  

where, in order to simplify the notation, we have introduced the quantity

\[ \Upsilon(L_u L_\ell S I, J_u J_u' J_{\ell} J_{\ell}' F_u F_u' F_{\ell} F_{\ell}') = (2L_u + 1)(2L_{\ell} + 1)(2L_{\ell} + 1)(2L_u + 1)(2F_u + 1)(2F_{\ell} + 1)(2F_{\ell} + 1) \]

\[ \times \left\{ L_u L_\ell 1 \left( L_u L_\ell 1 \right) \right\} \left\{ L_{\ell} J_\ell S 1 \right\} \left\{ J_u J_{\ell} S 1 \right\} \left\{ J_{\ell} J_{\ell}' S 1 \right\} \left\{ J_u J_u' 1 \right\} \left\{ J_{\ell} J_{\ell}' 1 \right\} \left\{ F_u F_u' 1 \right\} \left\{ F_{\ell} F_{\ell}' 1 \right\} \left\{ F_u F_{\ell} K \right\} \]

As in the CRD case, the quantity \( \epsilon' \) is defined by

\[ \epsilon' = \frac{C_\ell (L_u \rightarrow L_\ell)}{A(L_u \rightarrow L_\ell)} \]  

where \( C_\ell (L_u \rightarrow L_\ell) \) is the inelastic collision rate for the transition from the upper to the lower term (see Equation (21) of Belluzzi et al. 2015, and the discussion therein). The term \( \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) \), which represents the contribution to the emission coefficient brought by collisionally excited atoms, is given by (see Equation (37) of Belluzzi et al. 2015)

\[ \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) = \frac{h\nu}{4\pi} N_T B(L_\ell \rightarrow L_u) (2L_u + 1)(2L_\ell + 1) \epsilon' B_T(\nu_0) \sum_{J_{\ell} J_u' F_{\ell} F_u'} \Upsilon(L_u L_\ell S I, J_u J_u' J_{\ell} J_{\ell}' F_u F_u' F_{\ell} F_{\ell}') \]

\[ \times \frac{1}{2} \left[ \Phi(\nu J_u F_u E_u - \nu) + \Phi(\nu J_u' F_u' E_u' - \nu) \right] \sum_{K_1 K_2} \left( \sum_{K_{\ell} K_u} \left( \sum_{K_{\ell} K_u} (-1)^{1 + K_{\ell} + F_{\ell} + K} \sqrt{3} \right) \left( K_{\ell} K_u \right) \left( J_{\ell} J_{\ell}' F_{\ell} F_{\ell}' \right) + \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) \right] \]

\[ \times \left\{ F_u' F_{\ell}' 1 \left( F_u F_{\ell} K \right) \right\} T_{0}^{\tilde{\Omega}}(i, \tilde{\Omega}) \beta_{\ell}^{\text{Se}} \rho_0 K (J_{\ell} F_{\ell}', J_{\ell}' F_{\ell}') \]  

where \( B_T(\nu_0) \) is the Planck function in the Wien limit (consistent with our assumption of neglecting stimulated emission), at the frequency \( \nu_0 = (E(L_u) - E(L_\ell))/h \), with \( E(L_u) \) and \( E(L_\ell) \) as the energies of the centers of gravity of the upper and lower term, respectively, and \( h \) the Planck constant.

**4. THE R_H REDISTRIBUTION MATRIX**

Recalling the definition of the radiation field tensor (see Equation (15)), the emission coefficient of Equation (16) can be expressed in terms of a suitable redistribution matrix \( R_H \) following the terminology introduced by Hummer 1962. Following the convention according to which unprimed quantities refer to the scattered radiation while primed quantities refer to the incident radiation, we can write

\[ \varepsilon_i(\nu, \tilde{\Omega}) = \int d\nu' \int \frac{dS'}{4\pi} \sum_{j=0}^{3} R_H(\nu', \tilde{\Omega}'; \nu, \tilde{\Omega}) f_j(\nu', \tilde{\Omega}') + \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) \]  

with

\[ R_H(\nu', \tilde{\Omega}'; \nu, \tilde{\Omega}) = \frac{h\nu}{4\pi} N_T B(L_\ell \rightarrow L_u) (2L_u + 1)(2L_\ell + 1) \sum_{J_{\ell} J_u' F_{\ell} F_u'} \Upsilon(L_u L_\ell S I, J_u J_u' J_{\ell} J_{\ell}' F_u F_u' F_{\ell} F_{\ell}') \]

\[ \times \frac{1}{2} \left[ \Phi(\nu J_u F_u E_u - \nu) + \Phi(\nu J_u' F_u' E_u' - \nu) \right] \sum_{K_1 K_2} \left( \sum_{K_{\ell} K_u} \left( \sum_{K_{\ell} K_u} (-1)^{1 + K_{\ell} + F_{\ell} + K} \sqrt{3} \right) \left( K_{\ell} K_u \right) \left( J_{\ell} J_{\ell}' F_{\ell} F_{\ell}' \right) + \varepsilon_i^{\text{coll}}(\nu, \tilde{\Omega}) \right] \]

\[ \times \left\{ F_u' F_{\ell}' 1 \left( F_u F_{\ell} K \right) \right\} T_{0}^{\tilde{\Omega}}(i, \tilde{\Omega}) T_{0}^{\tilde{\Omega}'}(j, \tilde{\Omega}') \beta_{\ell}^{\text{Se}} \rho_0 K (J_{\ell} F_{\ell}', J_{\ell}' F_{\ell}') \]  

\[ \left( K F_u F_{\ell} 1 \left( -Q -Q \right) \right) \left\{ K K_{\ell} K_{\ell}' 0 \right\} T_{0}^{\tilde{\Omega}'}(i, \tilde{\Omega}) T_{0}^{\tilde{\Omega}}(j, \tilde{\Omega}') \beta_{\ell}^{\text{Se}} \rho_0 K (J_{\ell} F_{\ell}', J_{\ell}' F_{\ell}') \]

[Equation 21]
The $R_{\|}$ redistribution matrix derived above is valid in the atom rest frame. In order to find the corresponding expression in the observer’s frame, one has to take the Doppler effect into account for the given velocity distribution of the atoms. The derivation is similar to that outlined in Belluzzi & Trujillo Bueno (2014) and will not be given here. Assuming that the atoms have a Maxwellian distribution of velocities, characterized by the temperature $T$, it can be demonstrated that the expression of the $R_{\|}$ redistribution matrix in the observer’s frame is obtained by performing the following substitution in Equation (21)

$$\frac{1}{2} \left[ \Phi(\nu, E_{fi}) - \nu \right] + \frac{1}{2} \left[ \Phi(\nu', E_{fi}') - \nu' \right] \delta(\nu - \nu' - \nu_{ij} - \nu_{ik}) \rightarrow \frac{1}{1 + \epsilon' + 2\pi i\nu_{ij} E_{fi}/A(L_u \rightarrow L_f)} \frac{1}{1 + \epsilon' + 2\pi i\nu_{ij}' E_{fi}'/A(L_u \rightarrow L_f)}$$

where $\Delta\nu_D$ is the Doppler width in frequency units and $\theta$ is the scattering angle. The complex profile $W(\alpha, \beta)$ is defined as

$$W(\alpha, \beta) = H(\alpha, \beta) + i L(\alpha, \beta),$$

where $H$ and $L$ are the Voigt and Faraday–Voigt functions, respectively. The damping parameter $a$ is given by

$$a = \frac{\Gamma}{4\pi \Delta\nu_D},$$

where $\Gamma$ is the broadening constant of the upper level (we recall that the lower level is assumed to be infinitely sharp). We assume that the various HFS levels of the upper term are characterized by the same broadening constant. In the applications shown in Section 7, $\Gamma$ is calculated including the contributions due to radiative and collisional decays from the upper to the lower term, and the contribution of elastic collisions:

$$\Gamma = \Gamma_R + \Gamma_I + \Gamma_E = A(L_u \rightarrow L_f) + C_{el}(L_u \rightarrow L_f) + Q_{el},$$

with $Q_{el}$ the rate of elastic collisions. The reduced frequencies $x_{ab}$ and $x'_{ab}$ are given by

$$x_{ab} = \frac{\nu_{ab} - \nu}{\Delta\nu_D}, \quad \text{and} \quad x'_{ab} = \frac{\nu_{ab} - \nu'}{\Delta\nu_D}.$$

In the observer’s frame, the collisional term $\epsilon_i^{\text{coll}}(\nu, \tilde{\Omega})$ and the absorption coefficient $\eta_i(\nu, \tilde{\Omega})$ are still given by Equations (19) and (11), respectively, with the only difference being that the Lorentzian and the associated dispersion profiles entering the definition of the complex profile $\Phi(\nu_0 - \nu)$ (see Equation (10)) are now the Voigt and the Faraday–Voigt profiles, respectively.

The numerical calculation of the $R_{\|}$ redistribution matrix of Equation (21) is rather demanding since the angular and frequency dependencies cannot be factorized as in the atom rest frame. For this reason, it is customary to work with an approximate expression, obtained by averaging the frequency-dependent terms of the redistribution matrix over all the possible propagation directions $\tilde{\Omega}'$ and $\tilde{\Omega}$ of the incoming and outgoing photons (see Rees & Saliba 1982). Observing that this average can be easily reduced to an integral over the scattering angle $\theta$, the “angle-averaged” observer’s frame expression of the redistribution matrix is obtained by performing the following substitution in Equation (21)

$$\frac{1}{2} \left[ \Phi(\nu, E_{fi}) - \nu \right] + \frac{1}{2} \left[ \Phi(\nu', E_{fi}') - \nu' \right] \delta(\nu - \nu' - \nu_{ij} - \nu_{ik}) \rightarrow \frac{1}{1 + \epsilon' + 2\pi i\nu_{ij} E_{fi}/A(L_u \rightarrow L_f)} \frac{1}{1 + \epsilon' + 2\pi i\nu_{ij}' E_{fi}'/A(L_u \rightarrow L_f)}$$

where $\Delta\nu_D$ is the Doppler width in frequency units and $\theta$ is the scattering angle. The complex profile $W(\alpha, \beta)$ is defined as

$$W(\alpha, \beta) = H(\alpha, \beta) + i L(\alpha, \beta),$$

where $H$ and $L$ are the Voigt and Faraday–Voigt functions, respectively. The damping parameter $a$ is given by

$$a = \frac{\Gamma}{4\pi \Delta\nu_D},$$

where $\Gamma$ is the broadening constant of the upper level (we recall that the lower level is assumed to be infinitely sharp). We assume that the various HFS levels of the upper term are characterized by the same broadening constant. In the applications shown in Section 7, $\Gamma$ is calculated including the contributions due to radiative and collisional decays from the upper to the lower term, and the contribution of elastic collisions:

$$\Gamma = \Gamma_R + \Gamma_I + \Gamma_E = A(L_u \rightarrow L_f) + C_{el}(L_u \rightarrow L_f) + Q_{el},$$

with $Q_{el}$ the rate of elastic collisions. The reduced frequencies $x_{ab}$ and $x'_{ab}$ are given by

$$x_{ab} = \frac{\nu_{ab} - \nu}{\Delta\nu_D}, \quad \text{and} \quad x'_{ab} = \frac{\nu_{ab} - \nu'}{\Delta\nu_D}.$$

Using Equation (8), we obtain the following final expression of the angle-averaged redistribution matrix

$$[R_{\| - AA}(\nu', \tilde{\Omega}'; \nu, \tilde{\Omega})]_{ij} = k_{L} \sum_{KQ} T_{Q}^{K}(i, \tilde{\Omega}) \sum_{KQ} T_{Q}^{K}(j, \tilde{\Omega}) R_{\| - AA}(KQ, KQ, \nu', \nu),$$

We recall that elastic collisions play three different, although intimately related, roles: they contribute to the broadening of the spectral lines, they redistribute the photon frequency during the scattering process, and they relax atomic polarization. In this work, we heuristically take the first effect into account through the damping parameter $a$, but we neglect the second and third ones.
with
\[
\begin{align*}
\epsilon_{\text{ii}}(\nu, \tilde{\Omega}) &= k_\ell \sum_{k} T_{0}^{K}(i, \tilde{\Omega}) B_{T}(\nu_{0}) \beta_{0}^{K}(\nu), \\
\beta_{0}^{K}(\nu) &= \frac{(2L_{u} + 1)}{(2S + 1)(2I + 1)} \sum_{k} \sum_{J_{u}'J_{l}'F_{u}'F_{l}'} (\frac{2F_{l}'^{2} + 1}{2} \mathcal{T} - \nu_{0}^2) \\
&\times \frac{1}{1 + \epsilon' + 2\pi i \nu_{l}J_{u}'J_{l}'F_{u}'F_{l}' / A(L_{u} \rightarrow L_{l})} \int_{0}^{\pi} d\theta \left\{ \exp \left( -\frac{(\nu' - \nu - \nu_{l}J_{u}'J_{l}'F_{u}'F_{l}')^2}{2 \Delta \nu D \sin \theta / 2} \right) \right\} \\
&\times \frac{1}{2} \left[ W \left( \frac{a}{\cos \theta / 2}, \frac{x_{l}J_{u}'J_{l}'F_{u}'F_{l}'}{2 \cos \theta / 2} \right) + W \left( \frac{a}{\cos \theta / 2}, \frac{x_{u}J_{u}'J_{l}'F_{u}'F_{l}'}{2 \cos \theta / 2} \right) \right] \\
&\times \sum_{K} (-1)^{1 + K_{l} + K_{u}} 3^{2}(2K_{u} + 1)(2K_{l} + 1) \left\{ K_{u} F_{u} F_{u}' F_{u}' \right\} \left\{ K_{l} K_{l} F_{l} F_{l}' \right\} \sigma_{0}^{K}(J_{l}', F_{l}').
\end{align*}
\]
with

$$J^K_Q(\nu) = \sum_{K,Q} \int d\nu' J^K_Q(\nu') r_{\nu-\nu'}(KQ, K_rQ_r; \nu', \nu). \quad (36)$$

We consider the contribution of a coherent polarized continuum. Neglecting dichroism (which is a very good approximation in the visible part of the solar spectrum), the continuum total absorption coefficient (opacity) is given by

$$\eta_i^c(\nu) = \left[ k_c(\nu) + \sigma(\nu) \right] \delta_{0i}, \quad (37)$$

where $k_c(\nu)$ is the continuum true absorption coefficient and $\sigma(\nu)$ is the continuum scattering coefficient. The continuum emission coefficient is given by

$$\varepsilon_i^c(\nu, \tilde{\Omega}) = \sigma(\nu) \sum_{KQ} T^KQ_0(i, \tilde{\Omega}) (-1)^{0j} J^K_Q(\nu) + \varepsilon_{0i}^c(\nu) \delta_{0i}. \quad (38)$$

The first term in the right-hand side of Equation (38) represents the contribution to the continuum emission coefficient coming from coherent scattering processes (Rayleigh and Thomson scattering), the second term represents the thermal contribution (which does not contribute to the polarization of the continuum). Under the assumption that the continuum is in LTE, $\varepsilon_{0i}^c(\nu) = k_c(\nu) B_T(\nu)$.

As is clear from Equation (32), when dichroism is taken into account (i.e., when $\eta_1$ is non-zero), the RT equations for the Stokes parameters $I_0$ and $I_1$ are coupled to each other. However, they can be easily decoupled by introducing the quantities

$$I_0(\nu, \tilde{\Omega}) = \tilde{I}_0(\nu, \tilde{\Omega}) + \tilde{I}_1(\nu, \tilde{\Omega}), \quad \tilde{I}_1(\nu, \tilde{\Omega}) = I_0(\nu, \tilde{\Omega}) - \tilde{I}_0(\nu, \tilde{\Omega}). \quad (39)$$

Indeed, from Equations (32) and (39), it can be easily shown that the RT equations for $\tilde{I}_j(\nu, \tilde{\Omega}) (j = 0, 1)$ are given by

$$\frac{d}{ds} \tilde{I}_j(\nu, \tilde{\Omega}) = -\tilde{\eta}_j(\nu, \tilde{\Omega}) \tilde{I}_j(\nu, \tilde{\Omega}) + \tilde{\varepsilon}_j(\nu, \tilde{\Omega}), \quad (40)$$

with

$$\tilde{\varepsilon}_j(\nu, \tilde{\Omega}) = \varepsilon_0(\nu, \tilde{\Omega}) + (-1)^j \varepsilon_1(\nu, \tilde{\Omega}), \quad (41)$$

$$\tilde{\eta}_j(\nu, \tilde{\Omega}) = \eta_0(\nu, \tilde{\Omega}) + (-1)^j \eta_1(\nu, \tilde{\Omega}). \quad (42)$$

The Stokes parameters $I_0$ and $I_1$ can be easily obtained from the new quantities through the relations

$$I_0(\nu, \tilde{\Omega}) = \frac{1}{2} \left[ \tilde{I}_0(\nu, \tilde{\Omega}) + \tilde{I}_1(\nu, \tilde{\Omega}) \right], \quad I_1(\nu, \tilde{\Omega}) = \frac{1}{2} \left[ \tilde{I}_0(\nu, \tilde{\Omega}) - \tilde{I}_1(\nu, \tilde{\Omega}) \right]. \quad (43)$$

It can be easily shown that the quantities $\tilde{\eta}_j^c(\nu, \tilde{\Omega})$, and $\tilde{\varepsilon}_j^c(\nu, \tilde{\Omega})$ are given by Equations (11) and (35), respectively, provided that the geometrical tensor $T^KQ_{0i}(i, \tilde{\Omega})$ appearing in such equations is substituted by

$$\tilde{T}^KQ_{0j}(j, \tilde{\Omega}) = T^KQ_{00}(0, \tilde{\Omega}) + (-1)^j T^KQ_{01}(1, \tilde{\Omega}) \quad j = 0, 1. \quad (44)$$

On the other hand, we have

$$\tilde{\eta}_j^c(\nu) = \eta_0^c(\nu) = k_c(\nu) + \sigma(\nu) \quad j = 0, 1, \quad (45)$$

and

$$\tilde{\varepsilon}_j^c(\nu, \tilde{\Omega}) = \sigma(\nu) \sum_{KQ} \tilde{T}^KQ_{0j}(j, \tilde{\Omega}) (-1)^{0j} J^K_Q(\nu) + \varepsilon_{0j}^c(\nu) \quad j = 0, 1. \quad (46)$$

In terms of the new quantities $\tilde{I}_j(\nu, \tilde{\Omega})$ and $\tilde{T}^KQ_{0j}(j, \tilde{\Omega})$, the radiation field tensor is given by

$$J^K_Q(\nu) = \int \frac{d\Omega}{4\pi} \sum_{j=0}^1 \tilde{T}^KQ_{0j}(j, \tilde{\Omega}) \tilde{I}_j(\nu, \tilde{\Omega}) = \frac{1}{2} \int \frac{d\Omega}{4\pi} \sum_{j=0}^1 \tilde{T}^KQ_{0j}(j, \tilde{\Omega}) \tilde{I}_j(\nu, \tilde{\Omega}). \quad (47)$$

Introducing the optical depth $\tilde{\tau}_j(\nu, \tilde{\Omega})$ defined by

$$d\tilde{\tau}_j(\nu, \tilde{\Omega}) = -\tilde{\eta}_j(\nu, \tilde{\Omega}) ds, \quad (48)$$

and the source function

$$\tilde{S}_j(\nu, \tilde{\Omega}) = \frac{\tilde{\varepsilon}_j(\nu, \tilde{\Omega})}{\tilde{\eta}_j(\nu, \tilde{\Omega})}, \quad (49)$$

it can be easily shown that $\tilde{T}^KQ_{0j}(j, \tilde{\Omega})$ and $\tilde{I}_j(\nu, \tilde{\Omega})$ are coupled to each other. However, they can be easily decoupled by introducing the quantities

$$I_0(\nu, \tilde{\Omega}) = \tilde{I}_0(\nu, \tilde{\Omega}) + \tilde{I}_1(\nu, \tilde{\Omega}), \quad \tilde{I}_1(\nu, \tilde{\Omega}) = I_0(\nu, \tilde{\Omega}) - \tilde{I}_0(\nu, \tilde{\Omega}). \quad (39)$$
the RT equation for the quantities \( \hat{I} \) takes the form

\[
\frac{d}{d\tau_j} \hat{I}_j (\nu, \vec{\Omega}) = \hat{I}_j (\nu, \vec{\Omega}) - \hat{S}_j (\nu, \vec{\Omega}).
\]  

(50)

The source function \( \hat{S}_j (\nu, \vec{\Omega}) \) can be conveniently written in the form

\[
\hat{S}_j (\nu, \vec{\Omega}) = \frac{k_L}{\delta_j (\nu, \vec{\Omega})} \sum_{\mathcal{Q} \Omega} \hat{J}_\mathcal{Q}^j (j, \vec{\Omega}) \hat{S}_\mathcal{Q}^j (\nu),
\]

with

\[
\hat{S}_\mathcal{Q}^j (\nu) = \hat{J}_\mathcal{Q}^j (\nu) + \delta_{\mathcal{Q}0} B_T (\nu_0) \beta_\mathcal{Q}^j (\nu) + \delta_{\mathcal{Q}0} \delta_{\nu_0} \frac{\varepsilon_{\nu h} (\nu)}{k_L}.
\]

(52)

The quantity \( \hat{J}_\mathcal{Q}^j (\nu) \) is given by

\[
\hat{J}_\mathcal{Q}^j (\nu) = \hat{J}_\mathcal{Q}^j (\nu) + s(\nu) (-1)^\mathcal{Q} \hat{J}_\mathcal{Q}^j (\nu) = \sum_{K,Q} \int d\nu' \hat{J}_\mathcal{Q}^j (\nu') \psi_{KQ,KQ} (\nu', \nu),
\]

with \( s(\nu) = \sigma (\nu)/k_L \), and

\[
\psi_{KQ,KQ} (\nu', \nu) = \left[ \rho_{I\Pi AA} (KQ, KQ; \nu', \nu) + \delta_{K,K} \delta_{Q,-Q} \delta (\nu - \nu') s(\nu) (-1)^\mathcal{Q} \right].
\]

(54)

6. ITERATIVE SOLUTION OF THE NON-LTE PROBLEM

The calculation of \( \hat{J}_0^0 (\nu) \) and \( \hat{J}_0^2 (\nu) \) at each height in the atmosphere requires the knowledge of the quantities \( \hat{I}_j (\nu, \vec{\Omega}) \) along the various directions of the chosen angular quadrature, as obtained from the solution of Equation (50). The formal solution of this equation is given by

\[
\hat{I}_j (\nu, \mu; O) = \hat{I}_j (\nu, \mu; M) e^{-\Delta \hat{I}_j (\nu, \mu)} + \int_0^{\Delta \hat{I}_j (\nu, \mu)} \hat{S}_j (\nu, \mu; t) e^{t^*} dt,
\]

where \( O \) is a given height point in the considered discretization of the atmosphere, and \( M \) is the corresponding “upwind” point. As far as the dependence on the propagation direction is concerned, we have taken into account that, due to the cylindrical symmetry of the problem, the various quantities only depend on \( \mu = \cos \theta \), where \( \theta \) is the angle between the vertical and the propagation direction. The quantity \( \Delta \hat{I}_j (\nu, \mu) \) is the optical distance between \( O \) and \( M \), at frequency \( \nu \), along the direction specified by \( \mu \). We evaluate the integral in the right-hand side of Equation (55) by means of the short-characteristic method (see Kunasz & Auer 1988). Indicating the values of \( \hat{I}_j \) and \( \hat{S}_j \) at the various points of the spatial grid through the elements of column vectors, the formal solution of the RT equation can be written in the form

\[
\hat{I}_j (\nu, \mu; \ell) = \sum_{m=1}^N \Lambda_{\ell, m} \hat{S}_j (\nu, \mu; m) + \hat{I}_j (\nu, \mu; \ell),
\]

(56)

where \( \ell, m = 1, ..., N \), where \( N \) is the number of grid points, \( \hat{I}_j (\nu, \mu; \ell) \) is the value of the transmitted \( \hat{I}_j (\nu, \mu) \) at point \( \ell \) due to the radiation incident at the boundary, and \( \Lambda_{\ell, m} \) are the elements of an \( N \times N \) operator.

Substituting Equation (56) into (47) the operations required for the numerical calculation of \( \hat{J}_0^K (\nu) \) at point \( \ell \) can be indicated as follows:

\[
\hat{J}_0^K (\nu; \ell) = \sum_{m=1}^N \sum_{K'=1}^K \Lambda_{K0,K'0} (\nu; \ell, m) \hat{S}_0^{K'} (\nu, m) + T_0^K (\nu; \ell),
\]

(57)

where we have explicitly indicated the dependence on the height point in the atmosphere of the various physical quantities previously introduced. The \( \Lambda \) operators and the \( T_0^K \) tensor are given by

\[
\Lambda_{K0,K'0} (\nu; \ell, m) = \frac{1}{2} \int \frac{d\vec{\Omega}}{4\pi} \sum_{j=0}^1 \Lambda_{\ell, m} (\nu, \mu; \ell, \vec{\Omega}) \frac{k_L (m)}{\delta_j (\nu, \mu; m)} \hat{T}_0^K (j, \vec{\Omega}) \hat{T}_0^K (j, \vec{\Omega}).
\]

(58)

\[
T_0^K (\nu; \ell) = \frac{1}{2} \int \frac{d\vec{\Omega}}{4\pi} \sum_{j=0}^1 \hat{T}_0^K (j, \vec{\Omega}) \hat{I}_j (\nu, \mu; \ell).
\]

(59)

The equations for \( S_0^0 \) and \( S_0^2 \) resulting from the substitution of Equation (57) into (52) (through Equation (53)) represent the fundamental equations for the non-LTE problem under consideration. It is well known that the most suitable approach for the numerical solution of this set of equations is through iterative methods. In this work, we apply the Jacobian-based iterative method.

Let \( \hat{S}_0^{\text{old}} \) and \( \hat{S}_0^{\text{old}} \) be given estimates of the unknowns at the various points of the grid. At any grid point \( \ell \), we calculate \( \hat{J}_0^0 \) and \( \hat{J}_0^2 \) through Equation (57) by using such “old” values of the source function at all the grid points, except at point \( \ell \) where the new
estimates, $S_0^{\text{old}}$ and $S_0^{\text{old}}$, are implicitly (their value being still unknown) used:

$$J^K_0 (\nu; \ell) = J^K_0 (\nu; \ell)^{\text{old}} + \sum_K \Lambda_{K0,K'0} (\nu; \ell) \Delta S^K_0 (\nu; \ell),$$

with

$$\Delta S^K_0 (\nu; \ell) = S^K_0 (\nu; \ell)^{\text{new}} - S^K_0 (\nu; \ell)^{\text{old}},$$

and where $J^K_0 (\nu; \ell)^{\text{old}}$ and $J^K_0 (\nu; \ell)^{\text{old}}$ are the values of $J^K_0$ and $J^K_0$ that are obtained from a formal solution of the RT equation, carried out using the “old” estimates $S_0^{\text{old}}$ and $S_0^{\text{old}}$. The following step is to calculate $J^K_0 (\nu; \ell)$ through Equation (53):

$$J^K_0 (\nu; \ell) = J^K_0 (\nu; \ell)^{\text{old}} + \sum_{K,K'} \int d\nu' \psi_{K0,K',0} (\nu'; \nu, \ell) \Lambda_{K0,K',0} (\nu'; \ell) \Delta S^K_0 (\nu'; \ell).$$

The new values of the source function are finally obtained by substituting Equation (62) into (52):

$$\Delta S^K_0 (\nu; \ell) = \sum_{K,K'} \int d\nu' \psi_{K0,K',0} (\nu'; \nu, \ell) \Lambda_{K0,K',0} (\nu'; \ell) \Delta S^K_0 (\nu'; \ell) + R^K_0 (\nu; \ell),$$

with

$$R^K_0 (\nu; \ell) = J^K_0 (\nu; \ell)^{\text{old}} + B_T (\nu; \ell) \beta^K_0 (\nu; \ell) + \delta_{\text{th}} (\nu; \ell) \frac{\delta_{\text{th}} (\nu; \ell)}{k_L (\ell)} - S^K_0 (\nu; \ell)^{\text{old}}.$$  

The Jacobi-based method that we apply in this work is obtained by setting $\Lambda_{K0,K'0} = \Lambda_{00,00} = \delta_{K0}$ (see Trujillo Bueno & Manso Sainz 1999, for a detailed discussion on the role of the various $\Lambda$-operators). Introducing the ensuing expressions into Equation (52), we obtain

$$\Delta S^K_0 (\nu; \ell) = \int d\nu' \psi_{00,00} (\nu'; \nu, \ell) \Lambda_{00,00} (\nu'; \ell) \Delta S^K_0 (\nu'; \ell) + R^K_0 (\nu; \ell),$$

$$\Delta S^K_0 (\nu; \ell) = \int d\nu' \psi_{20,00} (\nu'; \nu, \ell) \Lambda_{00,00} (\nu'; \ell) \Delta S^K_0 (\nu'; \ell) + R^K_0 (\nu; \ell).$$

We calculate the new estimate of $S_0^0$ by solving Equation (65) through the so-called “Frequency-by-frequency” method.
7. RESULTS

In this section, we present and discuss the scattering polarization profiles of the Na I D1 line resulting from the numerical solution of the non-LTE problem described in the previous sections, in two semi-empirical models of the solar atmosphere. In particular, we show how the $Q/I$ signal produced in the core of the D1 line by the mechanism pointed out by Belluzzi & Trujillo Bueno (2013) is affected by quantum interference between the upper $J$-levels of D1 and D2, and by the presence of an increasing amount of atomic polarization in the ground level of sodium. Although our work is focused on the D1 line, we also present and discuss the polarization profiles of the D2 line, which is naturally included in our calculations.

7.1. Sensitivity to the Atmospheric Model (No Lower Level Polarization)

Figure 1 shows the $Q/I$ profiles calculated in model C of Fontenla et al. (1993; hereafter, FAL-C), and in model $M_{CO}$ (also known as FAL-X) of Avrett (1995), assuming that there is no atomic polarization in the lower levels. As far as the D2 line is concerned, the theoretical profile shows the typical triplet peak structure that is observed in this line. The central peak of the calculated profile has a small but appreciable sub-structure, which is sensibly reduced once the $I$ and $Q$ profiles are convolved with a Gaussian, so to take the spectral smearing due to the finite bandwidth of the instrument into account. While in the observed profiles the central peak is higher than the wing peaks, in our theoretical profile the three peaks have approximately the same amplitude. Although the presence of lower level polarization produces an increase of the amplitude of the central peak (see Section 7.2), we believe that the main reason for this disagreement with the observations has to be sought in the assumption of purely coherent scattering in the atom rest frame. Indeed, calculations carried out within the framework of the PRD approach of Bommier (1997), considering a simpler two-level model atom, show that the $R_{III}$ part of the redistribution matrix, which describes the contribution of scattering processes in the limit of CRD, produces a decrease of the amplitude of the wing peaks, leaving almost unaffected the central one. This is not surprising since the central peak forms much higher in the atmosphere, where the impact of collisions capable of redistributing the photon frequency during the scattering process is negligible. We finally observe that the two peaks in the wings of the line do not have the same amplitude, the red one being slightly smaller than the blue one. This is due to the effect of $J$-state interference, and it is in agreement with the observed profiles.

Moving toward longer wavelengths, the theoretical profile reproduces the sign reversal that is observed between D1 and D2 very well, as well as the general pattern that is observed in the wings of the D1 line. We recall that these are the typical signatures of $J$-state interference (see Stenflo 1980; Landi Degl’Innocenti & Landolfi 2004; Belluzzi & Trujillo Bueno 2011), which are fully accounted for.
for in our theoretical approach. In the core of the D$_1$ line, we obtain a clear $Q/I$ signal, with positive and negative peaks leading to an almost null integrated polarization signal. The positive peak is slightly blueshifted with respect to line center (where the signal is zero), while the negative one is slightly redshifted. A small negative dip can also be recognized between the positive peak and the negative minimum of the J-state interference pattern. Remarkably, this signal is not due either to lower level polarization or to the presence of a magnetic field (both ingredients have been neglected in the calculations of Figure 1), but it is produced by the physical mechanism identified and discussed by Belluzzi & Trujillo Bueno (2013). It is important to note that this signal appears in the core of the D$_1$ line, where the assumption of purely coherent scattering in the atom rest frame is a good approximation and the contribution of R$_{II}$ (not included in this work) can be safely neglected. The amplitude of the positive and negative peaks is quite sensitive to the atmospheric model. In particular, in agreement with the results of Belluzzi & Trujillo Bueno (2013), the peaks obtained in FAL-X are almost two times larger than those calculated in FAL-C. Nonetheless, the amplitude of our theoretical profiles remains sensibly

Figure 3. Panel (a): plot of $\sigma^2_0(F_2=2)$ as a function of optical depth (along the line of sight, at the center frequency of D$_2$) in the FAL-X model, for three different values of the parameter $a(F_2=2)$. The values of the parameters $a$ and $b$ in the three cases considered are indicated in the figure. Panel (b): fractional linear polarization profiles of the D$_2$ line, calculated for the three different parametrizations of lower level polarization shown in panel (a). The profile with the solid line corresponds to the case of no lower level polarization (it coincides with the dotted profile in panel (b) of Figure 1), and it is included for reference. All of the profiles have been calculated in the FAL-X model, for $\mu = 0.1$. Panel (c): same as panel (b), but for the D$_1$ line.

Figure 4. Left panel: center-to-limb variation of the D$_2$ line $Q/I$ profile calculated in the FAL-X atmospheric model, in the absence of atomic polarization in the lower level. The values of $\mu$ corresponding to the various profiles are indicated in the right panel. Right panel: same as the left panel, but for the D$_1$ line.
smaller than that of the signal observed by Stenflo & Keller (1997), although it is in agreement with other observations (e.g., Trujillo Bueno et al. 2001).

The presence of non-zero signals in the core of the Na I D₁ line has been confirmed by recent observations carried out with the Zürich Imaging Polarimeter at the Istituto Ricerche Solari Locarno (such observations will be published in a forthcoming paper). These signals, which show conspicuous variations along the slit, are much more similar to our theoretical profiles than to the large signal observed by Stenflo & Keller (1997). As it will be shown below, the presence of ad-hoc amounts of atomic polarization in the ground level of sodium allows us to significantly increase the amplitude of our theoretical profiles. On the other hand, the physical mechanism pointed out by Belluzzi & Trujillo Bueno (2013), possibly together with the presence of some lower level polarization, appears to be perfectly suitable for explaining the Q/I signals revealed by recent observations.

### 7.2. The Impact of Lower Level Polarization

We now include a given amount of atomic polarization in the lower F-levels, parametrizing the quantity \( \sigma_0^2 \) defined in Equation (7) according to the following expression

\[
\sigma_0^2(F_i, h) = \frac{a(F_i)}{1 + b(F_i) \tau_{\text{opt}}(h)},
\]

where \( h \) is the geometrical height in the atmosphere, and \( \tau_{\text{opt}} \) is the optical depth along the vertical, at the line center frequency of the D₂ line. The parameter \( a \) represents the value of \( \sigma_0^2 \) at the top of the atmosphere, while \( b \) sets its scale height. A similar parametrization of lower level polarization was used by Landi Degl’Innocenti (1998).

Figure 2 shows the Q/I profiles of the D₁ and D₂ lines calculated in the FAL-X model, for different values of the parameter \( b(F_i) \), keeping fixed the parameter \( a(F_i) \). We set \( b(F_i = 1) = b(F_i = 2) \), and \( a(F_i = 2) = 2a(F_i = 1) \) (we recall that a ratio of about 2 between the atomic polarization of the levels \( F_i = 2 \) and \( F_i = 1 \) was also considered by Landi Degl’Innocenti (1998), in order to obtain his best fit to the observed profiles). In the D₂ line, lower level polarization produces an appreciable increase of the amplitude of the central peak, and a slight modification of its sub-structure. On the other hand, the two peaks in the wings, as well as the dips between the central and wing peaks are unchanged. As expected, the increase of the central peak is larger for smaller values of the parameter \( b \), that is, when the value of \( \sigma_0^2 \) starts decreasing below the height of formation of the line.

In the D₁ line, the presence of atomic polarization in the lower F-levels produces an increase of the amplitude of the Q/I signal. Although both the positive and negative peaks are increased, the variation is sensibly larger in the negative one. Interestingly, the small negative structure in the blue wing is not affected by lower level polarization. Contrary to the D₂ line, the impact of lower level polarization is almost negligible for \( b = 10 \), while for \( b = 0.1 \), the profile starts being very similar to the one calculated by Landi Degl’Innocenti (1998).

Figure 3 shows the Q/I profiles of the D₁ and D₂ lines calculated in the FAL-X model, for different values of the parameter \( a(F_i = 2), \) assuming \( a(F_i = 1) = 0.01 \) and \( b(F_i = 1) = b(F_i = 2) = 0.1 \). The amplitudes of the central peak of D₂, and of the positive and negative peaks of the Q/I signal of D₁ increase proportionally to the atomic polarization of the lower level \( F_i = 2 \). As in the previous case, the variation of the signal amplitude in the D₁ line is larger in the negative peak than in the positive one. Interestingly, the sub-structure of the central peak of D₂ becomes more asymmetric when increasingly different amounts of atomic polarization in the lower levels \( F_i = 1 \) and \( F_i = 2 \) are considered.

### 7.3. Center-to-limb Variation

Moving from the limb to disk center, the amplitude of the central peak and of the wing peaks of the D₂ line Q/I profile gradually decreases (see left panel of Figure 4). The value of the two dips between the central peak and the wing peaks changes from positive to negative while going from \( \mu = 0.1 \) to \( \mu = 0.2 \). It reaches a (negative) minimum around \( \mu = 0.4 \), and it finally starts decreasing (in absolute value), going to zero, for larger values of \( \mu \). The figure shows the Q/I profiles up to \( \mu = 0.6 \). For larger \( \mu \)-values the whole profile goes gradually to zero without changing its shape and sign.

As far as the D₁ line is concerned, it can be observed that the amplitude of both the positive and negative peaks gradually decreases going from the limb to disk center (see the right panel of Figure 4). The small negative dip in the blue wing of the line remains almost unchanged going from \( \mu = 0.1 \) to \( \mu = 0.4 \), and only for higher values of \( \mu \) its amplitude starts decreasing. Interestingly, in the red wing of the line, where, for \( \mu = 0.1 \), a small and almost flat positive feature is obtained, going to \( \mu = 0.2 \) we find another small, but appreciable, negative dip. This dip does not change appreciably going from \( \mu = 0.2 \) to \( \mu = 0.6 \). As for the case of the D₂ line, for values of \( \mu \) larger than 0.6 (not shown in the figure), the whole Q/I profile of the D₁ line goes gradually to zero without changing its shape and sign.

### 8. CONCLUDING COMMENTS

The modeling of the linear polarization produced by resonance scattering in the solar atmosphere is a complex RT problem, especially when strong spectral lines resulting from HFS multiplets are considered. This is because there are, in general, several mechanisms and physical ingredients that need to be taken into account for explaining the observed spectral line polarization: frequency correlations between the incoming and outgoing photons along with the spectral structure of the incident radiation field, ground-level polarization, and quantum interference among FS and HFS levels. In this work, we have developed a theoretical and numerical approach suitable for solving the non-LTE RT problem for polarized radiation, taking the above-mentioned ingredients into account.
The theoretical approach is based on the density-matrix metalevel theory proposed by Landi Degl’Innocenti et al. (1997), according to which each atomic level is considered as a continuous distribution of sublevels. We consider a two-term atomic model with HFS, with prescribed atomic polarization in the $F$-levels of the ground level, and we focus on the limit of coherent scattering in the atomic rest frame, taking into account the effects of Doppler redistribution in the observer’s frame. Moreover, in addition to the radiative transitions we include excitations and de-excitations due to inelastic collisions with electrons, as explained in Belluzzi et al. (2015). As far as elastic collisions with neutral hydrogen atoms are concerned, in this first step, we have neglected them, except for their line broadening effect (see footnote 8). With these assumptions, RT applications aimed at modeling the fractional scattering polarization observed in strong resonance lines are expected to be appropriate concerning the core of the lines. The numerical approach is a careful generalization of the methods explained in Belluzzi & Trujillo Bueno (2014).

A detailed application to the D-lines of Na I, with emphasis on the enigmatic D$_1$ line, has allowed us to analyze the observable signatures of all the above-mentioned physical mechanisms. In agreement with Belluzzi & Trujillo Bueno (2013), we conclude that the enigmatic linear polarization observed in the core of the sodium D$_1$ line may be explained by the effect that one gets when taking properly into account the detailed spectral structure of the incident solar D$_1$-line radiation over the small frequency interval spanned by the HFS transitions. Interestingly, this key mechanism is capable of introducing significant scattering polarization in the core of the Na D$_1$ line without the need for ground-level polarization.

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