FREQUENCY REDISTRIBUTION FUNCTION FOR THE POLARIZED TWO-TERM ATOM*

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ABSTRACT

We present a generalized frequency redistribution function for the polarized two-term atom in an arbitrary magnetic field. This result is derived within a new formulation of the quantum problem of coherent scattering of polarized radiation by atoms in the collisionless regime. The general theory, which is based on a diagrammatic treatment of the atom–photon interaction, is still a work in progress. However, the results anticipated here are relevant enough for the study of the magnetism of the solar chromosphere and of interest for astrophysics in general.

Key words: atomic processes – line: formation – polarization – Sun: magnetic fields

1. INTRODUCTION

The diagnosis of magnetic fields in astrophysical plasmas relies on the measurement and interpretation of the polarization signature of the magnetic fields in spectral lines. The physical conditions of these plasmas vary greatly depending on the type of astronomical objects considered. Consequently a variety of simultaneous, and sometimes competing, effects—radiative, collisional, and from plasma electric and magnetic fields—need to be taken into consideration in the modeling of the observed radiation.

In dense plasmas, such as those characteristic of stellar atmospheres, strong gradients of temperature and density, as well as of magnetic and velocity fields, often occur (e.g., due to atmosphere stratification under the effect of gravitation and pressure gradients, or because of the presence of convective motions and dynamo actions), which need to be taken into account in modeling the transport of polarized radiation through the plasma. This is certainly the case for the strongest absorption lines of the solar spectrum, giving rise to a great diversity of line profile shapes and degrees of polarization, especially when observed with high temporal and spatial resolution (e.g., Belluzzi & Landolfi 2009).

Besides these non-local, radiative transfer effects, the particular excitation conditions of a magnetized plasma away from local thermodynamic equilibrium often represents a challenging problem for the description of the interaction between matter and polarized radiation. Apart from the well-studied Zeeman effect, subtle quantum processes associated with the polarized state of the atoms are often at play in stellar atmospheres, such as the Hanle effect, or other quantum effects associated with level-crossing physics. While these processes offer an opportunity for highly refined diagnostics of magnetized plasmas, they also present theoretical and computational difficulties that have commonly prevented their full exploitation in the astrophysical context.

Modeling of partial redistribution of the photon’s frequency in the scattering of polarized radiation is perhaps one of the most difficult problems to treat at the fundamental level, as this generally requires to describe the interaction of radiation with matter beyond the lowest order of approximation, which is instead adequate in the case of absorption and emission lines that are formed under conditions of complete frequency redistribution. For example, when isotropic plasma collisions are effective at destroying the coherence of multi-photon interactions, the scattering of radiation can safely be described as the incoherent succession of single-photon absorption and emission. It can also be shown that irradiation of the atom by a spectrally flat radiation allows a description of the scattering process that is phenomenologically identical to that provided by such two-step, single-photon processes of absorption and incoherent re-emission (e.g., Heitler 1954, Section 20; see also Sakurai 1967, Section 2.6; and Section 6 of this paper). Therefore, the regime for which the frequency coherence effects characteristic of radiation scattering are instead important is typically one of low plasma densities (i.e., low collisional rates) and highly spectrally modulated radiation, such as that emerging from stellar atmospheres in correspondence of very deep absorption lines.

This paper introduces a general frequency redistribution function for the polarized two-term atom, and then considers particular cases of it, which are relevant to the investigation of strong resonance lines in the solar spectrum, for which partial redistribution effects are deemed to be important. However, the results presented here are also valid in the case of subordinate lines, when both the upper and lower terms are radiatively broadened by spontaneous de-excitation. This study is based on a novel formalism (R. Casini et al., in preparation) that, within the framework of non-relativistic quantum electrodynamics, describes the time evolution of the atomic system and the radiation field in terms of propagators. This formalism relies on a diagrammatic representation of the atom–photon interaction, which allows to correctly identify and enumerate the types of processes that contribute to the scattering of polarized radiation. At the lowest order of interaction, it reproduces the theory of polarized line formation for complete redistribution of frequency (Landi Degl’Innocenti & Landolfi 2004).

Over the past four decades, several authors have addressed the problem of partial redistribution in polarized spectral lines. We will not provide a detailed account of the progress in this area, but we limit ourselves to simply tracing the main lines of work. Notable are the works of Omont et al. (1972, 1973), and of Heinz el and collaborators (e.g., Heintzel 1981; Heinz el & Hubeny 1982; Hubeny 1982), all of which derive essentially from the seminal work of Fiutak & Van Kranendonk (1962), who had extended the

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impact theory of pressure broadening developed by Anderson (1949; see also Baranger 1958) to second order, in order to study the line shape of molecular Raman scattering. Fiutak & Van Kranendonk (1962) assumed the diagonality of the density matrix of the initial (lower) state, as did the subsequent works that were based on the same formalism. This assumption corresponds to the hypothesis of non-coherent lower term (see Section 3). More recently, Stenflo (1994) followed a heuristic approach built upon the Kramers–Heisenberg scattering amplitude in order to derive a semi-classical theory of partial redistribution, which has enabled the derivation of redistribution functions similar to those presented in this paper (see, e.g., Smitha et al. 2013), again for atoms with non-coherent lower term.

Other works have approached the general problem of spectral line formation, investigating frequency redistribution effects in the statistical equilibrium of the atom and in the transport of polarized radiation through an absorptive and scattering medium. Lamb & Ter Haar (1971) followed an approach based on Heitler (1954), which allowed for the presence of atomic coherence (i.e., non-diagonal density matrix) in the lower term. Remarkably their work led to results for the scattering redistribution function that are in full agreement with ours. Cooper et al. (1982) investigated the redistribution problem relying on the quantum-regression theorem (e.g., Louisell 1973), and derived results that agree with those of Omont et al. (1972), Landi Degl’Innocenti et al. (1997) extended the first-order theory of polarized line formation of Landi Degl’Innocenti (1983) to include partial redistribution effects in a two-term atom. This was done by describing the atomic states in terms of energy metalevels (or energy sub-states; Woolley & Stibbs 1953), and proposing a heuristic generalization of the atomic density matrix based upon the “metalevel” idea. Their formalism naturally reproduces the results of the first-order theory of polarized line formation, in the limit of complete redistribution (e.g., for a flat-spectrum illumination of the atom), and it was applied successfully to the problem of the scattering polarization in the NaI D-doublet (Landi Degl’Innocenti 1998). Finally, Bommier (1997a, 1997b) formally extended the line formation theory of Landi Degl’Innocenti (1983) to higher orders of perturbation, at the same time relying also on the results of Baranger (1958) to describe relaxation effects on the atomic system from the interaction with a thermal bath of colliding perturbers. The redistribution function for the two-level atom with unpolarized lower level derived from that theory was shown to be in agreement with the results of Omont et al. (1972, 1973), and of the heuristic approaches of Stenflo (1994) and Landi Degl’Innocenti et al. (1997) in the absence of collisions.

In this paper, we introduce in Section 2 some fundamental theoretical results that lie at the basis of our treatment of partial frequency redistribution of polarized radiation. In Section 3, we re-derive several special forms of the redistribution function known from the past literature, and also present a generalization of those previous results that allows for atomic coherence in the lower term. In Section 4, we briefly discuss the definition of the radiative lifetimes of atomic states perturbed by the presence of external fields. This is an important clarification for the applicability of the results here presented. (As usual, collisional widths can be added to the natural widths of the atomic level in a phenomenological way, in the limit of the impact approximation; see, e.g., Anderson 1949; Lamb & Ter Haar 1971.) In Section 5, we specialize the equation of radiative transfer with partial redistribution to the general case of a polarized two-term atom with hyperfine structure. The cases of simpler atomic structures can be obtained from this more general case, and as an illustration we re-derive the expression of the scattering emissivity for the two-term atom with unpolarized lower levels and in the limit of zero magnetic field, which has been derived previously through the metalevel approach (Landi Degl’Innocenti et al. 1997). Finally, in Section 6, we verify that the generalized radiative transfer equation with the inclusion of coherent scattering satisfies the fundamental condition that the energy flux of the radiation through a closed surface containing the scatterer must be zero, in the absence of collisions.

2. THEORY

We consider a two-term atom with upper levels \{u, u', u'', \ldots \} and lower levels \{l, l', l'', \ldots \}. These levels represent the energy eigenstates of the atomic Hamiltonian in the presence of the external fields. In general, we allow for these levels to be arbitrarily polarized, and therefore we assume the existence of atomic coherence among the levels, described by the (complex) non-diagonal elements of the atomic density matrix, such as \( \rho_{uu'} \) and \( \rho_{ll'} \). We want to study the scattering of polarized radiation by an ensemble of such atoms, the radiation being described by an arbitrary incident beam of wave vector \( \mathbf{k} \) and polarization state \( (\lambda, \mu) \), and an emerging beam of given wave vector \( \mathbf{k}' \) and polarization state \( (\lambda', \mu') \). In particular, we want to focus on the coherent part of the evolution equation of the radiation field, where the upper levels \( u, u' \) enter only as virtual states. This part only appears when we push the development of the formal theory to include multi-photon effects (e.g., Bommier 1997a).

We thus find that the equation for the transport of polarized radiation for the two-term atom, expressed in the atomic reference frame, can be written in the form

\[
\frac{d}{dt} I_{\lambda'\mu'}(k') = - \sum_{\lambda\mu} \kappa_{\lambda\mu}^{(1)}(k') I_{\lambda\mu}(k') + \epsilon_{\lambda'\mu'}^{(1)}(k') + \epsilon_{\lambda'\mu'}^{(2)}(k').
\]

(1)

The first-order terms, \( \epsilon_{\lambda'\mu'}^{(1)}(k') \) and \( \kappa_{\lambda\mu}^{(1)}(k') \), whose explicit expressions we omit for the moment (see Section 5), describe, respectively, the emission of radiation of wave vector \( k' \) and polarization state \( (\lambda', \mu') \) due to the spontaneous de-excitation of the atom from all possible states \( \rho_{uu'} \), and the absorption rate of the incident radiation propagating along the same vector \( k' \) (but in all possible polarization states) when the atom is in any of the possible states \( \rho_{ll'} \). We neglect, here and in the following, any contribution of stimulated emission to the expression of \( \kappa_{\lambda\mu}^{(1)}(k') \). We make this choice in order to facilitate comparison of our results with those in the former literature on the subject of partial redistribution. The second-order term \( \epsilon_{\lambda'\mu'}^{(2)}(k') \) describes instead the scattering of radiation by the atom from all possible lower states \( \rho_{ll'} \), via all possible intermediate (virtual) levels \( u, u' \), and final levels \( l'' \).

Thus, the first-order terms in Equation (1) account for the transfer of radiation along the direction \( k' \), while the second-order term describes the phenomenon of coherent scattering. We note that we use here the term “coherent” in the broader sense of “memory
preserving," rather than in the usual restricted sense of "frequency preserving." This seems to be a better interpretation in light of the theoretical development that led to Equation (1) (R. Casini et al., in preparation).

The coherent-scattering term has the following expression:

\[
\varepsilon^{(2)}_{\lambda',\mu'}(k') \equiv \frac{1}{R^3} \sum_{\ell'} \sum_{\mu} \sum_{\alpha} \sum_{\beta} Q_{\alpha\beta}^{*}(\lambda', k') Q_{\mu}(\lambda, k) \langle \mu | I_{\lambda} | \lambda' \rangle,
\]

where \( V \) is the volume of the quantization box. The "vertex" form factor, \( Q_{ab}(\lambda, k) \), in the electric-dipole approximation, is given by (e.g., Landi Degl’Innocenti & Landolfi 2004)

\[
Q_{ab}(\lambda, k) = \sqrt{\frac{2\pi e^2 \hbar}{V}} \omega_k \sum_q (-1)^q \langle r_q | ab | e_{kq} \rangle - q,
\]

where we adopted the spherical-tensor representation of the electric-dipole and polarization unit vectors, \( r \) and \( e_{kq} \), respectively.

Finally, the complex line profiles \( \Psi_{ab,cde}^{h,k,l} \) are given by

\[
\Psi_{ab,cde}^{h,k,l} = \frac{-i}{(\omega_{ac} \pm \omega_h \pm \omega_k \pm \omega_l \pm i\epsilon_a + i\epsilon_c)(\omega_{ad} \pm \omega_h \pm \omega_k \pm \omega_l \pm i\epsilon_a + i\epsilon_c)}
\]

\[
\times \left( \frac{\omega_{ac} \pm \omega_h \pm \omega_k \pm \omega_l \pm i\epsilon_a + i\epsilon_c}{\omega_{ad} \pm \omega_h \pm \omega_k \pm \omega_l \pm i\epsilon_a + i\epsilon_c} \right) \frac{-i}{\omega_{cd} \pm \omega_k \pm \omega_l \pm i\epsilon_c + i\epsilon_d}.
\]

For notational convenience, we introduced the Bohr frequency, \( \omega_{pq} = \omega_p - \omega_q \), for any two levels \( p \) and \( q \). The quantity \( \epsilon_p \) represents the width of the level \( p \). In Equation (2), \( \Psi \) indicates complex conjugation of the profile \( \Psi \).

Both Equations (2) and (5) are derived from first principles. The supporting theory, which is still work in progress, follows a diagrammatic approach to the derivation of the evolution equation for a general atomic system interacting with a polarized radiation field. This approach leads to the same perturbation series for the evolution equation of the coupled system atom+radiation as that of Bommier (1997a), and the initial conditions for the system’s density matrix are also handled in a similar way. Somewhat surprisingly, the fundamental results that we derive separately for the statistical equilibrium of the atomic system and for the transport of polarized radiation do not agree with the work of Bommier (1997a, 1997b), although both approaches lead to the same redistribution function for the two-level atom with unpolarized lower level and in the absence of collisions.

It is worth briefly addressing the notation adopted for the profiles \( \Psi_{ab,cde}^{h,k,l} \). The subscripts identify the atomic levels involved in a transition, while the superscripts represent the frequencies of the corresponding emitted (+) and absorbed (−) photons. These profiles originate in our theory from the formal product of a first-order Feynman diagram with a second-order diagram. The two diagrams are distinguished by the comma separators in both the subscript and superscript lists. The time ordering of these Feynman diagrams must be respected, respectively, to the upper and lower terms of the model atom, and so the intermediate transition through the virtual state \( r \) is
constrained by the set of selection rules that apply to the $p-q$ transition. This typically results in a very low rate for the two-photon emission process. An instructive example is that of the Ly$\alpha$ transition of hydrogen, between the atomic terms of principal quantum numbers $n = 2$ and $n = 1$. The Ly$\alpha$ emission is dominated by the electric-dipole transition from $2P_{1/2,3/2}$ to $1S_{1/2}$, with a lifetime $\approx 1.6 \times 10^{-9}$ s. The transition between $2S_{1/2}$ and $1S_{1/2}$ is forbidden to the lowest order of approximation, but it can occur via two-photon emission, corresponding to the last diagram of Figure 1, through a virtual state $r$ belonging to a $n P_{j}$ term. Such transition has indeed been observed in the laboratory, and it is responsible for a measurable lifting of the metastability of the $1S_{1/2}$ state, with a lifetime $\approx 0.14$ s (Bethe & Salpeter 1957). However, its contribution compared to the dominant term of Ly$\alpha$ is completely negligible for any practical application to the polarized line diagnostics of astrophysical plasmas.

In the general case of a multi-term atom, there are additional terms that must be considered, which originate from different combinations of Feynman diagrams (involving up to third-order processes, to the degree of approximation of the theory). For the two-term atom, and neglecting stimulation effects, the profiles of Equation (5) are the only ones bringing a contribution to the polarized line diagnostics of astrophysical plasmas.

After a rather involved algebraic manipulation, the sum of complex profiles in Equation (2) is shown to be proportional to the following redistribution function:

$$\mathcal{R}(\Omega_{ul}, \Omega_{ul'}; \Omega_{ll'}, \Omega_{ll''}; \omega_{l}, \omega_{l'}) \equiv (\epsilon_{ul} + i\omega_{ul})(\Psi_{ul'}^{+}k^{+}k' - k^{+}k' + \Psi_{ul'}^{-}k^{+}k' - k' + k - k')$$

$$= \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})} \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})}$$

$$+ \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})} \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})}$$

$$+ \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})} \frac{2\epsilon_f(\epsilon_{ul'} + io_{ul'})}{(\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})}$$

$$\times \epsilon_{ul'} + i\omega_{ul'} + i(\omega_{ul'} + \omega_{ul''}) \times (\omega_{ul} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{ul} - \omega_{ul'} - i\epsilon_{ul'})$$

where we introduced the sum of the level widths, $\epsilon_{ul} = \epsilon_u + \epsilon_l$, and in the argument list of the function $\mathcal{R}$ we adopted the shorthand notation $\Omega_{ul} = \omega_{ul} - i\epsilon_{ul}$ to indicate the complex energy of the level $\alpha$, including its width.

Equation (6) is one of the preliminary results of our theory of partial redistribution with polarization. Another result suggests that, in the absence of collisions (i.e., at zero temperature), the process that populates the upper term by radiative absorption is inhibited in the limit of infinitely sharp lower levels (s.l.l.s.). In this limit, the first-order contribution to the emissivity in Equation (1) vanishes, and all radiation processes contributing to the emergent radiation depend exclusively on the population distribution and coherence within the lower term. The self-consistency of this last result has not yet been fully demonstrated, and for this reason we cannot provide here a rigorous proof of the phenomenon of inhibition of one-photon absorption in the limit of infinitely s.l.l.s.. However, such picture is supported also by the following intuitive physical argument. Since the ideal limit of s.l.l.s. is equivalent to that of infinite lifetime of the same levels, any measurement aimed at determining the population distribution of the atomic system would always find the system in the lower state. In other words, any radiative transition involving the upper levels can only be virtual, without actually populating the upper state (in the sense specified above). Thus the corresponding contribution to the emitted radiation must be fully accounted for by the coherent-scattering emissivity given in Equation (2), in which only the density matrix of the lower state explicitly appears.

Equation (6) represents the most general form of redistribution function for a two-term atom with polarized levels that are partially degenerate or non degenerate. It includes, as particular cases, the redistribution functions for the two- and three-level atoms that have formerly been described in the literature (see Section 3). While it is possible to cast $\mathcal{R}(\Omega_{ul}, \Omega_{ul'}; \Omega_{ll'}, \Omega_{ll''}; \omega_{l}, \omega_{l'})$ in

Figure 1. Feynman diagrams representing the first-order (i.e., single photon) processes of absorption and emission (top row), and the second-order (i.e., two-photon) processes describing scattering, two-photon absorption, and two-photon emission (bottom row). The central diagram in the bottom row represents the lowest-order radiative correction to the atomic propagator. Its main effect is that of “dressing” a given atomic state with a finite lifetime associated with spontaneous de-excitation.
form of the redistribution function, we observe that the diagonality condition
small radiative level widths. In this limit of s.l.s.,
(i.e., for zero magnetic field), so that
\[\Omega_u = \Omega_u',\ \text{and } \Omega_l = \Omega_l' = \Omega_l'.\]
From Equation (6), we immediately find

\[R_0(\Omega_u; \Omega_l'; \omega_k, \omega_k') = \frac{4\epsilon_f^2}{\epsilon_k^2 + \epsilon_{rl}^2} \left(\frac{4\epsilon_f}{\epsilon_k^2}ight) \left(\frac{4\epsilon_r^2}{\epsilon_k^2}ight)\]

\[+ \frac{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}ight] + \left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

\[+ \frac{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right]
+ \left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

(7)

which is identical to the redistribution function derived by Woolley & Stibbs (1953, see their Equation (VIII.3.33); see also Omont et al. 1972; Mihalas 1978) using a metalevel model of the atomic system.

The case of a three-level, “A-type” atomic system (see, e.g., Lamb & Ter Haar 1971, Figure 2) with fully degenerate sublevels, is obtained by letting \(\Omega_u = \Omega_u',\ \text{and } \Omega_l = \Omega_l' \neq \Omega_l'\) in Equation (6), which gives at once

\[R_1(\Omega_u; \Omega_l; \Omega_l'; \omega_k, \omega_k') = \frac{4\epsilon_f^2}{\epsilon_k^2 + \epsilon_{rl}^2} \left(\frac{4\epsilon_f}{\epsilon_k^2}ight) \left(\frac{4\epsilon_r^2}{\epsilon_k^2}\right)\]

\[+ \frac{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

\[+ \frac{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

(8)

This problem, which describes, for example, the Raman scattering in subordinate lines, has also been previously considered in the literature, e.g., by Hubeny (1982, Equation (3.2); see also Woolley & Stibbs 1953; Weisskopf 1933).

Of more general interest is the redistribution function for a two-term atom with non-degenerate levels, and completely relaxed atomic coherence in the lower term (non-coherent lower term; n.c.l.t.). Such a model can describe the formation of many resonance lines observed in the quiet-Sun atmosphere, in a regime of magnetic strengths such that the Hanle effect of the lower levels is saturated, but not so large as to induce level-crossing interference in the lower term. For example, the formation of the Na\(\text{i}\) D1–D2 doublet at 2,859 nm falls into this category, for 0.1 G \(\lesssim B \lesssim 300\) G (Trujillo Bueno et al. 2002; Casini et al. 2002). In order to derive this form of the redistribution function, we observe that the diagonality condition \(\rho_{ll'} = 0\) for the case of n.c.l.t. implies \(\Omega_l = \Omega_l'\) in Equation (6). We thus obtain

\[R(\Omega_u, \Omega_u'; \Omega_l, \Omega_l'; \omega_k, \omega_k')_{n.c.l.t.} = \frac{4\epsilon_f^2}{\epsilon_k^2 + \epsilon_{rl}^2} \left(\frac{4\epsilon_f}{\epsilon_k^2}\right) \left(\frac{4\epsilon_r^2}{\epsilon_k^2}\right)\]

\[+ \frac{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

\[+ \frac{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

\[+ \frac{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2}{\left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

\[\times \frac{2\epsilon_f^2 + 2\epsilon_r^2}{\epsilon_k^2 + \epsilon_{rl}^2} \left[\frac{4\epsilon_r^2}{\epsilon_k^2}\right] + \left(\omega_k - \omega_{ul} + \omega_{ul}\right)^2 + \epsilon_{ul}^2\]

(9)

Often the initial and final levels of the scattering process, \(l\) and \(l'\), represent metastable states, and hence are characterized by very small radiative level widths. In this limit of s.l.s., \(\epsilon_f, \epsilon_r \rightarrow 0\), the first and fourth contributions in Equation (9) vanish, and the redistribution function tends to the well-known result (e.g., Landi Degl’Innocenti et al. 1997)

\[R_2(\Omega_u, \Omega_u'; \Omega_l, \Omega_l'; \omega_k, \omega_k') = \frac{2\pi}{\epsilon_k^2 + \epsilon_{rl}^2} \delta(\omega_k - \omega_k + \omega_{ll'}) \frac{\delta(\omega_k - \omega_k + \omega_{ll'})}{\epsilon_k^2 + \epsilon_{rl}^2},\]

(10)

where we also considered that \(\omega_k' + \omega_{ll'} = \omega_k + \omega_l\) (because of the Dirac-\(\delta\) function) in order to combine the two non-vanishing contributions of Equation (9).
A more general case is that of infinitely s.l.ls. with the possibility of atomic coherence in the lower term. The derivation of the corresponding redistribution function from Equation (6) is not trivial. It is however easily accomplished if we first recast the general redistribution function of Equation (6) in the alternative but equivalent form

\[
\mathcal{R}(\Omega_u, \Omega_{u'}, \Omega_l, \Omega_{l'}, \omega_k, \omega_{k'}; \epsilon_{uw'} + i\omega_{uw'}) = \frac{i}{(\omega_k - \omega_{u'} + i\epsilon_u - i\epsilon_{u'})} \left( \frac{\epsilon_{uw'} + i\omega_{uw'}}{(\omega_{u'} - \omega_{u'} + i\epsilon_u - i\epsilon_{u'})} \right) \left( \frac{\epsilon_{uw'} + i\omega_{uw'}}{(\omega_{u'} - \omega_{u'} + i\epsilon_u - i\epsilon_{u'})} \right) \right]
\]

We also define the generalized function\(^6\)

\[
\zeta(x) \equiv \lim_{\sigma \to 0} \frac{i}{x + i\sigma} = \pi \delta(x) + i \text{PV} \frac{1}{x}.
\]

Then, in the limit of \(\epsilon_l, \epsilon_{l'}, \epsilon_{l''} \to 0\), the redistribution function for s.l.ls. follows at once from Equation (11):

\[
\mathcal{R}(\Omega_u, \Omega_{u'}, \Omega_l, \Omega_{l'}, \omega_k, \omega_{k'})_{\text{s.l.ls.}} = \left( \epsilon_{uw'} + i\omega_{uw'} \right) \left( \frac{\zeta(\omega_k - \omega_{u'} + \omega_{l'})}{(\omega_k - \omega_{u'} + i\epsilon_u - i\epsilon_{u'})} \right) \left( \frac{\zeta^*(\omega_k - \omega_{u'} + \omega_{l'})}{(\omega_k - \omega_{u'} + i\epsilon_u - i\epsilon_{u'})} \right) - \omega_{l'} \left[ \frac{1}{(\omega_k - \omega_{u'} + i\epsilon_u)(\omega_k - \omega_{u'} + i\epsilon_u)(\omega_k - \omega_{u'} + i\epsilon_u)} \right] \]  

We note that Equation (13) properly tends to the redistribution function \(\mathcal{R}_2\) of Equation (10) when \(\omega_{l'} \to 0\), since there is no contribution from the second square bracket in this case, and \(\zeta(x) + \zeta^*(x) = 2\pi \delta(x)\).

We conclude this section with the evaluation of the integral norm of the general redistribution function, Equation (6) or (11). By contour integration,\(^7\) we find

\[
\int_{-\infty}^{\infty} d\omega_k \mathcal{R}(\Omega_u, \Omega_{u'}, \Omega_l, \Omega_{l'}, \omega_k, \omega_{k'}) = 2\pi \left( \epsilon_{uw'} + i\omega_{uw'} + i(\omega_{uw'} + i\omega_{u'} + i\omega_{uw'}) \right)
\]

and from either of these two expressions it follows immediately that

\[
\int_{-\infty}^{\infty} d\omega_k \int_{-\infty}^{\infty} d\omega_{k'} \mathcal{R}(\Omega_u, \Omega_{u'}, \Omega_l, \Omega_{l'}, \omega_k, \omega_{k'}) = 4\pi^2
\]

The results expressed by Equations (14)–(16) differ from those derived in the theory of Bommier (1997a, 1997b), where the line shape function in the radiative transfer equation contributed by higher orders is shown to vanish, when integrated over the frequency of either the incoming or the outgoing photon. On the other hand, in Bommier’s formalism, the contribution of the first-order emissivity is always present, even when the lifetime of the lower term is assumed to be infinite and thus no upper-term excitation should be expected, based on the physical argument presented at the end of Section 2. Thus, in the work of Bommier (1997a), the redistribution function always results from the combination of both first- and second-order emissivity terms, even in the limit of infinitely s.l.ls. Accordingly, redistribution effects are accounted for through a modified emission coefficient where the distinction between true absorption and scattering is lost (see also Cooper et al. 1982). Despite this difference between our respective formalisms, in the collisionless regime and for an unpolarized lower term, we verified that the redistribution function \(\mathcal{R}(\Omega_u, \Omega_{u'}, \Omega_l, \Omega_{l'}, \omega_k, \omega_{k'})_{\text{s.l.ls.}}\) of Equation (9) coincides with that derived by Bommier (1997b, Equations (43)–(45); for this demonstration, all level widths in those formulas that correspond to our \(\epsilon_u\) must be replaced by \(\epsilon_{ul}\)).

The general redistribution function, Equation (6) or (11), with all the particular cases considered in this section, is expressed in the reference frame of the atom. In realistic applications to the plasma diagnostics of astrophysical objects, we must generalize this function to the laboratory frame, so to include the effects of Doppler broadening through the convolution of the atomic velocity distribution (typical, a Maxwellian). In order not to burden the presentation of the following discussion, we provide the details of such derivation in the Appendix.

---

\(^{6}\) This definition differs from the \(\zeta(x)\) function introduced by Heitler (1954) for the presence of \(i\) at the numerator.

\(^{7}\) Because \(\omega_{ul} \gg \epsilon_{ul}\), the frequency domain of integration \([0, +\infty)\) can always be extended backward to \(-\infty\) with no appreciable modification of the value of the integral.
4. INTERLUDE: THE PROBLEM OF RADIATIVE LIFETIMES

One critical question, in the application of Equations (2) and (6) (or (11)) to the study of partial redistribution effects in the presence of external fields, is the proper definition of the level widths, $\epsilon_i$, i.e., of the lifetimes of atomic states that are in general energetically perturbed by the presence of external fields. If we restrict our considerations to the case of a two-term atom with s.l.l.s., the problem of such definition concerns only the excited states $u$ and $u'$ (cf. Equation (13)). To the lowest order of approximation, their widths are determined exclusively by the external fields and by the process of spontaneous de-excitation (in particular, we are neglecting in this treatment the effects of stimulated emission). Within such an approximation, the complex frequencies $\Omega_i$ correspond to the eigenvalues of the non-Hermitian operator (e.g., Cohen-Tannoudji et al. 1992)

$$K_u = \mathcal{P}_u H_A \mathcal{P}_u - \ii \hbar \Gamma_u,$$

where $H_A$ is the Hamiltonian of the atomic system in the presence of the external fields, $\mathcal{P}_u$ is the projection operator over the subspace of the states $u$ of that Hamiltonian, and finally

$$\Gamma_u = \frac{2}{3 \hbar c^3} \alpha_{ul}^3 \sum_q \mathcal{P}_u r_q \mathcal{P}_l r_q^\dagger \mathcal{P}_u,$$

where evidently $\mathcal{P}_l$ is the projection operator over the subspace of the lower terms, which is radiatively connected to the subspace of the excited states $u$.

We note how in Equation (18) we have assumed that the energy separation between the levels of the upper and lower terms can be approximated by a single value $\alpha_{ul}$. This is an adequate approximation in most cases of interest for magnetic studies of the solar atmosphere, where the field strengths at play, and the fine structure (FS) of the atomic terms, are such that the associated energy separations of the levels are much smaller than $\alpha_{ul}$. Correspondingly, level mixing and quantum interference are also triggered between relatively close levels, such that the energy span of the atomic terms (intended here as the sets of the interfering atomic levels) is much smaller than their average separation $\alpha_{ul}$. Under this approximation, and in the presence of a magnetic field, it is possible to show that the damping matrix $\Gamma_u$ is diagonal on the basis of the eigenvectors of $H_A$ (e.g., Rose & Caravallino 1961). In this case, $K_u$ is also diagonal on the same basis. Thus, the level widths for radiative de-excitation correspond to the diagonal elements of the damping matrix $\Gamma_u$.

The use of Equation (18) for determining the line shape of the scattered radiation is adequate when the frequency of the emitted photon is near the atomic resonance. On the other hand, away from the resonance condition (e.g., in the case of Rayleigh scattering of a photon), one retrieves the usual form of the damping matrix as given by Equation (18). In the presence of a magnetic field, it is possible to “dress” a metastable lower term, and determine thus its radiative lifetime for transitions toward the upper level. Nonetheless, the limitations of our current theory of radiation scattering in the absence of collisions, no new contributions can arise that are not already covered by the conventional theory of radiative lifetimes.

5. THE TWO-TERM ATOM WITH HYPERFINE STRUCTURE

Standard manipulations (e.g., Landi Degl’Innocenti & Landolfi 2004) allow us to express Equation (1) by means of the irreducible spherical tensor formalism, and the emerging polarized radiation $I_{\lambda, \mu}(\mathbf{k})$ in terms of the corresponding Stokes vector,

$$\frac{1}{c} \frac{d}{dt} S_i(\omega_k, \mathbf{k}') = -\sum_j \kappa_{ij}(\omega_k, \mathbf{k}') S_j(\omega_k, \mathbf{k}') + \epsilon_i^{(1)}(\omega_k, \mathbf{k}') + \epsilon_i^{(2)}(\omega_k, \mathbf{k}'), \quad (i = 0, 1, 2, 3),$$

where

$$\epsilon_i^{(2)}(\omega_k, \mathbf{k}') = \frac{4}{3 \hbar c^3} N \alpha_{ik}^4 \sum_{p'} \rho_{pq} \sum_{q'} \sum_{p''} (-1)^{p'+p''} (r_q)_{ul}^* (r_q')_{ul'} (r_p)_{ul'} (r_{p'})_{ul}^* \times \sum_{K\bar{K}} \sum_{K'} \sum_{K_0} \sqrt{(2K+1)(2K'+1)} \left( \begin{array}{ccc} 1 & 1 & K \\ -q & \bar{q} & -\bar{Q} \end{array} \right) \left( \begin{array}{ccc} 1 & 0 & K' \\ -p & p' & -Q \end{array} \right) T_{K\bar{K}0}^{K'}(i, \mathbf{k}') \times \int_0^\infty d\omega_k \left( \Psi_{ul,\mathbf{k}}^* \Psi_{ul',\mathbf{k}'} \right) J_0^K(\omega_k), \quad (i = 0, 1, 2, 3).$$
The geometric tensors \( T^K_Q \) were introduced by Landi Degl’Innocenti (1984), and are conveniently tabulated by Bommier (1997b; see also Landi Degl’Innocenti & Landolfi 2004). The radiation tensors \( J^K_Q(\omega_K) \) are defined in terms of the incident Stokes vector as follows:

\[
J^K_Q(\omega_K) = \oint d\hat{k} \frac{d\dot{k}}{4\pi} \sum_{j=0}^{3} T^K_Q(j, \hat{k}) S_j(\omega_K, \hat{k}).
\]  

(21)

It is instructive to compare the form of Equation (19) with the usual expression of the radiative transfer equation for unpolarized light (e.g., Mihalas 1978; Shu 1991) including the contribution from non-monochromatic scattering, as it becomes evident when we specialize Equation (21) to that case (i.e., see also Landi Degl’Innocenti & Landolfi 2004). The radiation tensors \( J^K_Q(\omega_K) \) include also the non-monochromatic scattering, which is the projection of the total angular momentum \( z \) axis (\( z \)), then the atomic states involved in Equation (19) are of the form

\[
|\alpha I \mu M \rangle = \sum_{JF} C^{JF}_{\mu}(\alpha I M) |\alpha I J F M \rangle,
\]

with the orthogonality conditions

\[
\sum_{JF} C^{JF}_{\mu}(\alpha I M) C^{JF}_{\mu'}(\alpha I M) = \delta_{\mu \mu'}, \quad \sum_{\mu} C^{JF}_{\mu}(\alpha I M) C^{JF'}_{\mu}(\alpha I M) = \delta_{JJ'}\delta_{FF'}.
\]  

(23)

The density matrix element for the lower state, \( \rho_{\mu\mu'} \), can be written in terms of the irreducible spherical tensor components of the statistical operator,

\[
\rho_{\mu\mu'} \equiv \langle \alpha I \mu_1 M_1 | \rho | \alpha I \mu'_1 M'_1 \rangle = \sum_{JF} \sum_{J_{\mu}\mu_1 F_{\mu} J_{\mu}'\mu'_1} C^{J_{\mu}F_{\mu}}_{\mu}(\alpha I M_1) C^{J_{\mu}'F_{\mu}'}_{\mu'}(\alpha I M'_1) \times \sum_{K_{\mu},Q_{\mu}} (-1)^{F_{\mu}-M_{\mu}} \sqrt{2K_{\mu}+1} \left( \begin{array}{ccc} -J_1 & F_{\mu} & K_{\mu} \\ M_{\mu} & -M_{\mu}' & Q_{\mu} \end{array} \right) \frac{1}{\sqrt{2J_{\mu}+1}} (J_{\mu} F_{\mu} J_{\mu}' F_{\mu}').
\]

(24)

Finally, using the Wigner–Eckart theorem and its corollaries (e.g., Brink & Satchler 1993), we derive the following expression of the dipole matrix element:

\[
(r_\mu)_{\mu\mu'} \equiv \langle \alpha_a I \mu_1 M_a | r_\mu | \alpha_a I \mu_1 M_1 \rangle = \sum_{J_{\mu} F_{\mu} J_{\mu}' F_{\mu}'} C^{J_{\mu}F_{\mu}}_{\mu}(\alpha_a I M_a) C^{J_{\mu}'F_{\mu}'}_{\mu'}(\alpha_a I M_1) \sqrt{(2J_{\mu}+1)(2F_{\mu}+1)(2F_{\mu}'+1)} \langle \alpha_a M_a || r || \alpha_a J_1 \rangle \times \sum_{J_{\mu} F_{\mu} J_{\mu}' F_{\mu}'} (-1)^{J_{\mu}-M_{\mu}} \left( \begin{array}{ccc} F_{\mu} & F_1 & 1 \\ -M_{\mu} & J_{\mu} & J_{\mu}' \end{array} \right) \left( \begin{array}{ccc} F_{\mu}' & F_1 & 1 \\ J_{\mu}' & J_{\mu} & 1 \end{array} \right).
\]  

(25)
To proceed further, we will assume that the two-term atom is adequately described within the LS-coupling scheme, so that \( \alpha \equiv \beta \), where \( \beta \) identifies a particular LS term of the atom. We then can write additionally
\[
\langle \alpha_u J_{\alpha u} \parallel r \parallel \alpha_l J_l \rangle = (-1)^{J_u+J_{\alpha u}+J_l} (2J_u + 1)(2J_l + 1) \left \{ \frac{J_u}{L_u} \frac{J_l}{L_l} \frac{1}{S} \right \} \langle \beta_u L_u \parallel r \parallel \beta_l L_l \rangle.
\]
(26)
The reduced matrix element in the last line can be expressed in terms of the Einstein \( B_{\alpha u} \) coefficient for absorption from the lower to the upper term of the atom,
\[
B_{\alpha u} = \frac{16\pi^3}{3} \frac{\varepsilon_0^2}{\hbar C} \frac{2L_u + 1}{2L_l + 1} | \langle \beta_u L_u \parallel r \parallel \beta_l L_l \rangle |^2,
\]
or alternatively through the Einstein coefficient for spontaneous emission (see Equation (18)),
\[
A_{\alpha l} = \frac{4\varepsilon_0^2}{3\hbar C^3} \alpha_{\alpha l}^3 | \langle \beta_u L_u \parallel r \parallel \beta_l L_l \rangle |^2 = \frac{4\varepsilon_0^2}{3\hbar C^3} \alpha_{\alpha l}^3 \sum_{ql} |(r_{q\alpha})_{ul}|^2.
\]
(28)
It is relevant at this point to follow up on the discussion presented at the end of Section 4, with regard to the proper expression that must be adopted for the natural width of the excited state \( u \), under excitation conditions that are away from the atomic resonance. Because of the conclusions of that discussion, we note that we cannot make the usual identification \( A_{\alpha l} = 2\epsilon_u \), which is adequate only near the atomic resonance, and we must adopt instead for \( \epsilon_u \) the more general expression
\[
\epsilon_u \equiv \epsilon_u (\omega_k) = \frac{1}{2} A_{\alpha l} \frac{\omega_{\alpha l}^3}{\omega_{\alpha l}^3}.
\]
(29)
This result will be used in Section 6. It is worth noting that Heitler (1954) proposed that one should rather use
\[
\epsilon_u \equiv \epsilon_u (\omega_k) = \frac{1}{2} A_{\alpha l} \frac{\omega_{\alpha l}^3}{\omega_{\alpha l}^3}.
\]
However, Power (1964) pointed out that such alternative expression of the line width is a consequence of adopting the \( p \cdot A \) form for the atom–photon interaction Hamiltonian (velocity gauge), rather than the dipolar form \( d \cdot E \) (length gauge; see footnote at p. 116 of Power 1964). Since in this paper we consistently use the electric-dipole interaction Hamiltonian in the length gauge, Equation (29) represents the appropriate form of the line width that must be adopted in our treatment of radiation scattering.

Using Equations (21)–(25), Equation (20) becomes
\[
\epsilon_i^{(2)} (\omega_k, \hat{k}) = \frac{3}{16\pi^3} \frac{N \hbar}{\omega_{\alpha l}^3} \Pi_{L_u L_l} A_{\alpha l} B_{\alpha u}
\]
\[
\times \left \{ \begin{array}{c}
J_u \ J'_u \ J''_u \ J_l \ J'_l \ J''_l \\
F_u \ F'_u \ F''_u \ F_l \ F'_l \ F''_l
\end{array} \right \} \left \{ \begin{array}{c}
J_u \ J'_u \ J''_u \ J_l \ J'_l \ J''_l \\
F_u \ F'_u \ F''_u \ F_l \ F'_l \ F''_l
\end{array} \right \}
\]
\[
\times \Pi_{J_u J'_u J''_u} \Pi_{J_l J'_l J''_l} \Pi_{F_u F'_u F''_u} \Pi_{F_l F'_l F''_l} \Pi_{F_u F'_u F''_u} \Pi_{F_l F'_l F''_l}
\]
\[
\times \sum_{\mu_u \mu_l} \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \sum_{\bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} C_{\mu_u}^{J_u F_u} (M_u) C_{\mu_l}^{J_l F_l} (M_l) C_{\bar{\mu}_{u \mu_u}}^{J'_u F'_u} (M_u) C_{\bar{\mu}_{l \mu_l}}^{J''_u F''_u} (M_u) C_{\bar{\mu}_{u \mu_u}}^{J'_l F'_l} (M_l) C_{\bar{\mu}_{l \mu_l}}^{J''_l F''_l} (M_l)
\]
\[
\times \left \{ \begin{array}{c}
F_u \\
-M_u \ M_l \ q \ p
\end{array} \right \} \left \{ \begin{array}{c}
F'_u \\
-M'_u \ M'_l \ q' \ p'
\end{array} \right \} \left \{ \begin{array}{c}
F''_u \\
-M''_u \ M''_l \ q'' \ p''
\end{array} \right \}
\]
\[
\times \Pi_{K'K'K} T_{\bar{Q} K' (i, \hat{k})}^{K} (\tilde{\hat{k}} \tilde{F}_l, \tilde{F}_u)
\]
\[
\times \int_0^\infty d\omega_k \langle \Psi_{u \mu_u}^{j \bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}} (\bar{\Psi}_{u \mu_u}^{j \bar{\mu}_{u \mu_u} \bar{\mu}_{l \mu_l}}) S_j (\omega_k, \hat{k}), \ (i = 0, 1, 2, 3).
\]
(30)
where for simplicity of notation we removed the information of the term from the density matrix element and from the argument of the projection coefficients $C_{\mu}^{JJ'}$ of the atomic eigenstates, as well as defining

$$\Pi_{ab\cdots} \equiv \sqrt{(2a + 1)(2b + 1)\cdots}.$$  \hspace{1cm} (31)

The quantities of the first order appearing in Equation (19), which represent single-photon absorption and spontaneous emission, for the case of the multi-term atom with hyperfine structure, have been given by Casini & Manso Sainz (2005; see their Equations (32a), (32b), (33a), and (33b)). For convenience, we reproduce those expressions using the same notation adopted in this paper:

$$\epsilon^{(1)}_{\ell}(\omega_k, \hat{k}) = \frac{\sqrt{3}}{8\pi^2} N h \omega_k \Pi_{la} A_{ul} \sum_{l_j l_j'} J_{l_j} J_{l_j'} \left\{ J_{l_j} \begin{pmatrix} J_{l_j'} & 1 \\ L_{l_j} & S \end{pmatrix} \right\} L_{l_j} \left\{ J_{l_j'} \begin{pmatrix} J_{l_j} & 1 \\ L_{l_j} & S \end{pmatrix} \right\} F_{u} \left\{ F_{l_j} \begin{pmatrix} F_{l_j'} & 1 \\ J_{l_j} & I \end{pmatrix} \right\} F_{l_j'},$$

$$\times \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'} C_{\mu u}^{l_j} C_{\mu u}^{l_j'} (M_{l_j}) C_{\mu u}^{l_j} C_{\mu u}^{l_j'} (M_{l_j'}) C_{\mu u}^{l_j} C_{\mu u}^{l_j'} (M_{l_j'}) C_{\mu u}^{l_j} C_{\mu u}^{l_j'} (M_{l_j'}) \times \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'} \sum_{l_j l_j'}$$

$$\times \Pi_{K K} T_{Q}^{K}(i, \hat{k}) \rho_{Q}^{K} (\hat{J}_{u}, \hat{J}_{l}) (\Phi_{u}^{K} + \Phi_{u}^{K}), \quad (i = 0, 1, 2, 3),$$

having also defined

$$\Phi_{ab}^{\pm} \equiv \frac{i}{\omega_a + \omega_b + \epsilon_{ba}},$$

where $|a\rangle$ and $|b\rangle$ are in general eigenstates of the atomic Hamiltonian including the contributions of the external fields. Again, we used the notation $\Phi$ to indicate the complex conjugate of the profile $\Phi$.

The magneto-optical coefficients $\rho_{i}(\omega_{k}, \hat{k})$, for $i = 1, 2, 3$ (see Equation (32a) of Casini & Manso Sainz 2005), are obtained from the expression of $\eta_{i}(\omega_{k}, \hat{k})$, Equation (33), through the following substitution,

$$(\Phi_{u}^{K} + \Phi_{u}^{K}) \rightarrow i(\Phi_{u}^{K} - \Phi_{u}^{K}).$$

The elements of the absorption matrix $\kappa_{ij}(\omega_{k}, \hat{k})$, which appear in Equation (19), are related to the coefficients $\eta_{i}(\omega_{k}, \hat{k})$ and $\rho_{i}(\omega_{k}, \hat{k})$ via the following relations

$$\kappa_{ii} \equiv \eta_{0}, \quad \kappa_{ik} = \kappa_{ki} = \eta_{i}, \quad (i = 0, 1, 2, 3),$$

$$\kappa_{ij} = \epsilon_{ijk} \rho_{k}, \quad (i, j, k = 1, 2, 3),$$

where $\epsilon_{ijk}$ is the fully antisymmetric Levi–Civita tensor.

As a special case, we consider the limit of zero magnetic field for Equations (30), (32), and (33). In that case, there is no dependence of the line profiles on the $\mu$-indices, and so we can use the orthogonality properties (23) to perform the trivial summations over those
indices. In addition, it is possible to sum over all magnetic quantum numbers, as well as over the indices \((q, q')\) and \((p, p')\). After some tedious Racah-algebra manipulations (e.g., Varshalovich et al. 1988), we find

\[
\epsilon_i^{(2)}(\omega_k, \mathbf{k'}) \bigg|_{B=0} = \frac{3}{16\pi^3} N_h \frac{\alpha_k^2}{\omega_0} \Pi_{\ell, J}^2 A_{\ell J} B_{\ell J} \sum_{J, J', J''} \sum_{J, J', J''} \sum_{F, F', F''} \sum_{F, F', F''} (-1)^{F_u + F'_u + 1}
\]

\[
\times \Pi_{J, J'} \Pi_{J, J''} \left[ \sum_{L, L_u} \sum_{L, L_u} \sum_{L, L_u} \right] \left[ \sum_{L, L_u} \sum_{L, L_u} \right]
\]

\[
\times \Pi_{F, F'} \Pi_{F, F''} \left[ \sum_{J, J'} \sum_{J, J''} \right]
\]

\[
\times \sum_{K, Q, K', Q', K''} \sum_{K, Q, K', Q', K''} (-1)^{K} \Pi_{K, K', K''} \left( \begin{array}{ccc}
K & K' & K'' \\
Q & Q' & Q''
\end{array} \right) \left[ \begin{array}{ccc}
K' & F_u & F'_u \\
F' & F'' & F''
\end{array} \right] \left[ \begin{array}{ccc}
K & K' & K'' \\
F_u & F'_u & F''
\end{array} \right], \quad (i = 0, 1, 2, 3),
\]

whereas the contributions of the first-order terms for this special case of vanishing magnetic fields are given by\(^8\)

\[
\epsilon_i^{(1)}(\omega_k, \mathbf{k'}) \bigg|_{B=0} = \frac{\sqrt{3}}{8\pi^2} N_h \frac{\alpha_k^2}{\omega_0} \Pi_{\ell, J}^2 A_{\ell J} \sum_{J, J', J''} \sum_{J, J', J''} \sum_{F, F', F''} \sum_{F, F', F''} (-1)^{J-J'+F+F'+1} \Pi_{J, J'} \Pi_{F, F'} \Pi_{J, J''} \Pi_{F, F'}
\]

\[
\times \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right]
\]

\[
\times \sum_{K, Q} \left[ \begin{array}{ccc}
K & F_u & F_u \\
F_u & F_u & F_u
\end{array} \right] T^K_{\ell} (i, \mathbf{k'}) \rho^K_{Q} (J_f, J'_f, F'_f) (\Phi^K_{\ell} + \Phi^K_{\ell}), \quad (i = 0, 1, 2, 3),
\]

In the absence of hyperfine structure \((I = 0)\), Equation (37) reduces to

\[
\epsilon_i^{(2)}(\omega_k, \mathbf{k'}) \bigg|_{B=0} = \frac{3}{16\pi^3} N_h \frac{\alpha_k^2}{\omega_0} \Pi_{\ell, J}^2 A_{\ell J} B_{\ell J} \sum_{J, J', J''} \sum_{J, J', J''} (-1)^{J-J'+F+F'+1} \Pi_{J, J'} \Pi_{J, J''} \Pi_{F, F'} \Pi_{F, F''}
\]

\[
\times \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right]
\]

\[
\times \sum_{K, Q} \left[ \begin{array}{ccc}
K & F_u & F_u \\
F_u & F_u & F_u
\end{array} \right] T^K_{\ell} (i, \mathbf{k'}) \rho^K_{Q} (J_f, J'_f, F'_f) (\Phi^K_{\ell} + \Phi^K_{\ell}), \quad (i = 0, 1, 2, 3),
\]

\[
\eta_i(\omega_k, \mathbf{k'}) \bigg|_{B=0} = \frac{\sqrt{3}}{8\pi^2} N_h \alpha_k \Pi_{\ell, J}^2 B_{\ell J} \sum_{J, J', J''} \sum_{J, J', J''} (-1)^{J-J'+F+F'+1} \Pi_{J, J'} \Pi_{J, J''} \Pi_{F, F'} \Pi_{F, F''}
\]

\[
\times \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right] \left[ \begin{array}{ccc}
J_u & J_u & J_u \\
F_u & F_u & F_u
\end{array} \right]
\]

\[
\times \sum_{K, Q} (-1)^{K} \left[ \begin{array}{ccc}
F & F & F
\end{array} \right] T^K_{\ell} (i, \mathbf{k'}) \rho^K_{Q} (J_f, J'_f, F'_f) (\Phi^K_{\ell} + \Phi^K_{\ell}), \quad (i = 0, 1, 2, 3).
\]

\[^{8}\text{We take here the opportunity to correct a statement given by Casini & Manso Sainz (2005). Equations (34) in that paper are only valid when both the fine and hyperfine structures of the levels—and not just the Zeeman splitting, as originally claimed in the paper—can also be neglected with respect to the width of the line profile. In particular, those equations hold for the frequency-integrated polarization. The case of zero magnetic field is instead properly represented by Equations (38) and (39) given here.}\]
and finally, in the additional case of unpolarized lower term (u.l.t.: \( K_l = 0, J_l = J_i \)),

\[
\frac{3}{16\pi^2} \frac{\hbar^2 \omega_i^2}{\omega_{ul}} \sum_{K_L} \frac{N_{e,K_L}^2}{\omega_{ul}^2} n_{ul} A_{ul} B_{ul}
\]

\[
\times \left\{ \begin{array}{c}
J_u & J_i & 1 \\
L_u & L_i & S
\end{array} \right\} \left\{ \begin{array}{c}
J_i' & J_l' & 1 \\
L_i' & L_l' & S
\end{array} \right\} \frac{1}{\sqrt{2 J_l + 1}} T_{Q0}(i, \hat{k}') \rho_0^0(J_l, J_i)
\]

\[
\sum_{j=0}^3 \oint d\hat{k} T_{i}^{K}(j, \hat{k}) \int_{0}^{\infty} d\omega_{k} R(\Omega_k, \Omega_{ul}; \Omega_l, \Omega_{ul}; \omega_k, \omega_{ul})_{n.c.l.t.} S_{j}(\omega_k, \hat{k}), \quad (i = 0, 1, 2, 3).
\]

where we recalled Equation (9), and renamed \( l' \) into \( l' \).

In the limit of s.l ls., this last expression can be compared with the one for the redistribution matrix derived for the same model atom by Landi Degl’Innocenti et al. (1997), using the metalevel approach to the description of the atomic density matrix. We note that the redistribution function \( R(\Omega_k, \Omega_{ul}; \Omega_l, \Omega_{ul}; \omega_k, \omega_{ul})_{n.c.l.t.} \) in the integral must be replaced by the function \( R_2 \) of Equation (10) for this comparison. Once this substitution is made, and taking into account the vanishing of the first-order emissivity in the limit of s.l ls., we can demonstrate the formal identity of Equation (41) with the result of that former derivation.

Similarly, imposing \( S = I = 0 \) in Equation (30), we can derive the coherent scattering emissivity for the two-level atom in the presence of a magnetic field. This also turns out to be identical with the analogous result derived by Landi Degl’Innocenti et al. (1997), in the limit of sharp and unpolarized lower level considered by those authors.

6. VERIFICATION OF THE ENERGY-BALANCE CONDITION FOR COHERENT SCATTERING

A fundamental property of the transport of radiation in a collisionless gas of atoms at the statistical equilibrium (i.e., under stationary conditions, such that the internal energy of the atomic ensemble does not change with time) is that the radiation’s energy flux through a closed surface containing the gas must be zero. It is thus important to verify that Equation (19)—which generalizes the usual radiative transfer equation for polarized radiation (e.g., Landi Degl’Innocenti & Landolfi 2004) via the inclusion of coherent scattering—satisfies such an fundamental energy-balance condition.

Because our present theory cannot account for the broadening of the lower levels due to photon absorption (see discussion at the end of Section 4), in order to guarantee the self-consistency of this verification, we only consider the case of infinitely s.l ls. It must be noted that this choice is consistent with the approximation of neglecting stimulated emission. In fact, if the incident radiation field is strong enough to induce any appreciable broadening of the lower levels, then one should also expect that stimulation effects will be comparatively important, and therefore should be included in the picture. This is certainly the case when the objective is to verify the energy balance among the various radiation processes.

As a consequence of the assumption of infinite lifetime of the lower level, we then must drop the contribution of the first-order emissivity to the radiative energy balance. Nonetheless, we will retain a finite width of the lower levels in the expressions of the line profiles, for the sake of this demonstration. This is because, in real cases, these levels may still be broadened by collisional processes, or by the possibility of spontaneous de-excitation toward other lower terms, in the case of subordinate lines in a multi-term atom.

The verification of the radiative balance condition in the collisionless regime can then be set up in general form starting from Equation (19). For simplicity, we assume that the incident radiation is unpolarized,

\[
S_{i}(\omega_k, \hat{k}) = \delta_{00} S_{0}(\omega_k, \hat{k}).
\]

We then can ignore the contribution from the absorption terms associated with the magneto-optical effects (see Equation (36)), and only need to consider the expression of the absorption coefficient adopting the same notations used in writing Equation (20),

\[
\eta_{a}(\omega_k', \hat{k}') = \frac{2\pi \epsilon_{0}^2}{\sqrt{3}} \frac{N_{e,K_L}}{\omega_{ul}} \sum_{i} \sum_{u} \sum_{q} \sum_{q'} (-1)^{q'+1} (r_{q,u}^{L+1} r_{q',u}^{L+1}) \times \frac{\sqrt{2K+1}}{K - Q} T_{Q0}(i, \hat{k}') (\Phi_{ul}^{(K)} + \Phi_{ul}^{(-K)}), \quad (i = 0, 1, 2, 3).
\]

Using the tabulated expressions for \( T_{i}^{K}(j, \hat{k}) \) (Bonnier 1997b; Landi Degl’Innocenti & Landolfi 2004), we can show that

\[
\oint d\hat{k} T_{i}^{K}(j, \hat{k}) = \delta_{i0} \delta_{K0} - \frac{1}{\sqrt{2 \delta_{i1} \delta_{K2}}},
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\[
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\]

Using the tabulated expressions for \( T_{i}^{K}(j, \hat{k}) \) (Bonnier 1997b; Landi Degl’Innocenti & Landolfi 2004), we can show that

\[
\oint d\hat{k} T_{i}^{K}(j, \hat{k}) = \delta_{i0} \delta_{K0} - \frac{1}{\sqrt{2 \delta_{i1} \delta_{K2}}},
\]
With the above assumptions, and for \( i = 0 \), from Equations (19), (20), (35), and (42), after some straightforward algebra, we find
\[
\oint \frac{d\hat{k}}{4\pi} \int_{-\infty}^{\infty} d\omega_k \frac{1}{c \, dt} S_0(\omega_k, \hat{k}) = -2\pi \frac{e^2}{\sqrt{\hbar c}} N' \sum_{\nu \nu'} \sum_{K Q} \sum_{q' q} (-1)^{q'+1} \Pi_K \left( \begin{array}{ccc} 1 & q' & K \\ q & 0 & -Q \end{array} \right) \oint \frac{d\hat{k}}{4\pi} T_Q^k(0, \hat{k}) \int_{-\infty}^{\infty} d\omega_k S_0(\omega_k, \hat{k})
\]
\[
\times \left\{ \sum_u (r_{qhu}(r_{q'})_{ul} \omega_k (\Phi_{ul}^{-k} + \Phi_{ul}^{k}) - \frac{2 e^2}{\hbar c} \sum_{u u'} (r_{qhu}(r_{q'})_{u'u} \sum_{pl'} (r_{pl'} su'(r_{pl'})^{u'u} - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega_k \omega_k^4 \left( \sum_{u u'} (\Psi_{ul}^{-k,k'-k} + \Psi_{ul}^{k,k'-k}) \right) \right) \right\}
\]
\[
= -2\pi \frac{e^2}{\sqrt{\hbar c}} N' \sum_{\nu \nu'} \sum_{K Q} \sum_{q' q} (-1)^{q'+1} \Pi_K \left( \begin{array}{ccc} 1 & q' & K \\ q & 0 & -Q \end{array} \right) \oint \frac{d\hat{k}}{4\pi} T_Q^k(0, \hat{k}) \int_{-\infty}^{\infty} d\omega_k S_0(\omega_k, \hat{k})
\]
\[
\times \left\{ \sum_u (r_{qhu}(r_{q'})_{ul} \omega_k (\Phi_{ul}^{-k} + \Phi_{ul}^{k}) - \frac{2 e^2}{\hbar c} \sum_{u u'} (r_{qhu}(r_{q'})_{u'u} \sum_{pl'} (r_{pl'} su'(r_{pl'})^{u'u} - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega_k \omega_k^4 \left( \sum_{u u'} (\Psi_{ul}^{-k,k'-k} + \Psi_{ul}^{k,k'-k}) \right) \right) \right\},
\]
(44)

where in the last equivalence we used the definition of \( \epsilon_u(\omega_k) \), Equations (28) and (29). In the following, we neglect the (weak) dependence of \( \epsilon_u(\omega_k) \) on the frequency of the scattered radiation, so that it can be taken outside the integral in the last line of Equation (44). This is justified by the fact that the redistribution function appearing in that integral effectively limits the frequency range around the resonance frequency \( \omega_{0k} \) that contributes to the finite value of the integral.

From Equation (6), and using the form of the redistribution function given in Equation (11), we see that the integration over \( \omega_{0k} \) in Equation (44) implies the evaluation of four divergent integrals. In order to accomplish this task, we apply a consistent cut-off procedure, which is derived from the usual Feynman’s regularization techniques of quantum field theory (e.g., Bogoliubov & Shirkov 1959). We thus find, once again extending the integration domain to \( -\infty \) (see Note 7),
\[
\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega_k \omega_k \left( \Psi_{ul,l'u'l}^{-k,k'-k} + \Psi_{ul,l'u'l}^{k,k'-k} \right) = \frac{\omega_k + \omega_{l'l'}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} - i \epsilon_{ul,l'u'l} \right) + \frac{\omega_k + \omega_{l'l'}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} + i \epsilon_{ul,l'u'l} \right)
\]
\[
+ \frac{\epsilon_{ul,l'u'l}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} - i \epsilon_{ul,l'u'l} \right) + \frac{\epsilon_{ul,l'u'l}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} + i \epsilon_{ul,l'u'l} \right)
\]
\[
+ \frac{\omega_k - \omega_{l'l'}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} - i \epsilon_{ul,l'u'l} \right) + \frac{\omega_k - \omega_{l'l'}}{\omega_k - \omega_{l'l'}} \left( \Omega_{ul,l'u'l} + i \epsilon_{ul,l'u'l} \right)
\]
(45)

We note that the dependence of this integral on \( \omega_{0l'} \) is confined to the numerator. We then introduce an approximation, which is to replace \( \omega_{0l'} \) in Equation (45) by some appropriate average \( \omega_l \). If we further assume that the conditions for the diagonality of the damping matrix \( \Gamma_u \) apply (see Section 4), we are then able to formally perform the summation over \( p \) and \( l' \) in Equation (44),
\[
\sum_{pl'} (r_{pl'} su'(r_{pl'})^{u'u} = \delta_{uu'} \sum_{pl'} |(r_{pl'})|^2.
\]
(46)

Under these assumptions, after some more tedious algebra, we obtain
\[
\frac{\epsilon_u}{\pi} \int_{-\infty}^{\infty} d\omega_k \omega_k \left( \Psi_{ul,l'u'l}^{-k,k'-k} + \Psi_{ul,l'u'l}^{k,k'-k} \right) = \frac{\epsilon_u + i (\omega_u - \omega_l)}{\omega_k - \omega_{l'l'}} + \frac{\epsilon_u - i (\omega_u - \omega_l)}{\omega_k - \omega_{l'l'}}
\]
\[
\approx \omega_k (\Phi_{ul}^{-k} + \Phi_{ul}^{k}).
\]
(47)

where, for the last approximation, we took into account the hypothesis of s.l.s., and recalled the definition of the profiles \( \Phi_{ul}^{\pm k} \), Equation (34). In particular, this approximation becomes exact in the absence of lower-level polarization, or if the magnetic field is zero. Using then the results of Equations (46) and (47), the quantity within curly braces in Equation (44) vanishes, thus verifying the expected condition of radiative balance in a collisionless gas of atoms.

It is important to note that the approximations involved in this verification are dominated by the assumption that the energy separation among the lower levels \([l, l', l'', \ldots]\) is much smaller than the frequency of the incident radiation, \( \omega_k \), so that the energy values of those levels can all be approximated by the average \( \omega_l \). In the presence of a magnetic field, the energy separation of the atomic levels is proportional to the Larmor frequency for the applied field, \( \omega_B \). For typical observing conditions in the solar atmosphere, the ratio of \( \omega_B/\omega_k \) is of the order of \( 10^{-4} \) or less (e.g., for \( \lambda \sim 1 \mu m \), and \( B \sim 10^3 G \), \( \omega_B/\omega_k \approx 5 \times 10^{-6} \)), so the above approximation is well justified. For transitions in complex atoms, the energy span of the various \( \omega_{0l'} \) may be dominated by the FS separation of the lower term, in which case the above approximation is justified if \( \omega_{PS}/\omega_k \ll 1 \). For example, in the case of the Hα line, \( \omega_{PS}/\omega_k \approx 2.4 \times 10^{-5} \).

To conclude this section, we formally demonstrate that the illumination of the atom by a spectrally flat radiation \( S_i(\omega_0, \hat{k}) \) produces a line profile that corresponds to the one obtained in the limit of complete redistribution (see, e.g., Heitler 1954, Section 20, or Sakurai...
Equations (20) and (21)), along with the integral norm of Equation (14), 1967, Section 2.6). In order to see this, we consider again the emissivity term associated with the coherent scattering of radiation (see Equations (20) and (21)), along with the integral norm of Equation (14),

\[
\epsilon^{(2)}_i(\omega_k, \hat{k})' \equiv \frac{4}{3} \frac{\hbar^2 c^3}{\epsilon^2_{0}} \omega_{0}^2 \sum_{l'l'} \mathbf{\rho}_{u'u''} \sum_{qq'} \sum_{pp'} (-1)^{q+q'} (r_{q})_{u}(r_{q'})_{u'} (r_{p})_{u'}^{-1} (r_{p'})_{u'}
\times \sum_{K Q} \sum_{K' Q'} \mathbf{\Pi}_{K K'} \left( \frac{1}{q'} - \frac{K}{Q} \right) \left( \frac{1}{p'} - \frac{K'}{Q'} \right) T^K_Q (i, \hat{k})
\times \frac{2\pi}{\epsilon_{uu'} + i\omega_{uu'}} \left( \Phi^{uK}_{uu'} + \Phi^{uK}_{uu'} \right) \oint \frac{d\hat{k}}{4\pi} \sum_{j=0}^{3} T^K_Q (j, \hat{k}) S_j (\omega_0, \hat{k})
\]

\[
= \frac{1}{2\pi^2 \sqrt{3}} \frac{\hbar^2 c^3}{\epsilon^2_{0}} \omega_{0}^2 \sum_{u'u''} \left\{ \frac{16\pi^3}{\sqrt{3}} \frac{\hbar^2 c}{\epsilon_{uu'} + i\omega_{uu'}} \sum_{l'l'} \sum_{qq'} \sum_{pp'} (-1)^{q+q'} (r_{q})_{u}(r_{q'})_{u'} (r_{p})_{u'}^{-1} (r_{p'})_{u'} \right\}
\times \sum_{K Q} \sum_{K' Q'} \mathbf{\Pi}_{K K'} \left( \frac{1}{q'} - \frac{K}{Q} \right) J^K_Q (\omega_0) \left\{ \sum_{l'} \sum_{p'} (-1)^{p'+1} (r_{p})_{u'} (r_{p'})_{u'}^{-1} \right\}
\times \sum_{K Q} \sum_{K' Q'} \mathbf{\Pi}_{K K'} \left( \frac{1}{p'} - \frac{K'}{Q'} \right) T^K_Q (i, \hat{k}) \left( \Phi^{uK}_{uu'} + \Phi^{uK}_{uu'} \right), \quad (i = 0, 1, 2, 3). \tag{48}
\]

On the other hand, using the same notation, the emissivity of the first order is given by

\[
\epsilon^{(1)}_i(\omega_k, \hat{k})' = \frac{1}{2\pi^2 \sqrt{3}} \frac{\hbar^2 c^3}{\epsilon^2_{0}} \omega_{0}^2 \sum_{u'u''} \mathbf{\rho}_{uu'} \sum_{l'} \sum_{pp'} (-1)^{p'+1} (r_{p})_{u'} (r_{p'})_{u'}^{-1}
\times \sum_{K Q} \sum_{K' Q'} \mathbf{\Pi}_{K K'} \left( \frac{1}{p'} - \frac{K'}{Q'} \right) T^K_Q (i, \hat{k}) \left( \Phi^{uK}_{uu'} + \Phi^{uK}_{uu'} \right), \quad (i = 0, 1, 2, 3). \tag{49}
\]

We then see that Equations (48) and (49) coincide in the case of spectrally flat illumination, once we identify the quantity within curly brackets in Equation (48) with the upper-term density matrix \( \mathbf{\rho}_{uu'} \) that appears in the expression of \( \epsilon^{(1)}_i(\omega_k, \hat{k})' \). In fact, this identification derives directly from the solution of the statistical equilibrium problem for the two-term atom illuminated by spectrally flat radiation (and neglecting stimulated emission), which is obtained within the lowest-order approximation of the theory of polarized line formation (Landi Degl’Innocenti & Landolfi 2004). In turn, this proves the validity of that former theory for the description of the scattering of polarized radiation in the limit of complete redistribution.

It is important to remark that the above result does not imply that the emitted radiation gets counted twice when we include the coherent-scattering term in the radiative transfer equation, as this would evidently violate energy conservation. We have previously noted that the excitation of \( \mathbf{\rho}_{uu'} \) is inhibited in the limit of infinitely slow, i.e., and therefore all the emitted radiation must come from the coherent-scattering term in that case. Then, if the illumination of the atom is spectrally flat, the above demonstration shows that the scattered radiation has exactly the same spectral structure as if the atom had absorbed and re-emitted incoherently the incident radiation (see Heitler 1954, Section 20).

7. CONCLUSION

We presented a general expression of the redistribution function for polarized radiation in the case of a transition between two atomic terms \( j \) and \( u \), which can both be partially degenerate and polarized, and subject to a magnetic field of arbitrary strength. In particular, this function applies to the description of resonance or subordinate lines of atoms with both fine and hyperfine structures. This function is derived from first principles, and it represents a preliminary result of a diagrammatic theory of scattering polarization that we have been developing, on and off, over the past decade. The full theory is still incomplete, lacking a self-consistent set of accompanying equations for the statistical equilibrium of the atomic system. Part of the problem is caused by a mild violation of the positivity condition for the atomic density matrix in the presence of magnetic fields. Following a revision of our diagrammatic approach, inspired by certain literature dealing with the problem of the treatment of the initial conditions in perturbative master equations (see, e.g., Whitney 2008 and references therein; a very clear discussion of this problem can also be found in a recent paper by Koller et al. 2010), we have identified new terms, previously unaccounted for, in the perturbative expansion of the evolution equation for the atomic density matrix. These terms are in the process of being evaluated, with the perspective that they should restore the self-consistency of the statistical-equilibrium problem.

Because of the approximations of the theory, we cannot rigorously model the radiative broadening of the atomic levels due to photon absorption. Therefore, in the absence of collisions, the lower term of an atomic transition remains infinitely sharp, and the scattered radiation only comes from the coherent contribution to the emissivity, Equation (2). However, we presented the general form of the redistribution function, Equation (6), where the widths of the lower levels appear explicitly. This function can then be applied to treat phenomenologically the frequency redistribution of radiation in the presence of collisional broadening.
Despite these formal difficulties, the results we presented are relevant enough for the spectro-polarimetric diagnostics of the upper layers of the Sun’s atmosphere, that we decided to propose them, already at this early stage, to the astrophysical community. In this paper, we limited ourselves to provide the algebraic formulas for the scattered radiation in a complex two-term atom with hyperfine structure, and in the presence of a magnetic field (relevant, for instance, to the case of the resonant Na I D-doublet, or of complex subordinate lines such as Hα). Numerical applications of this formalism will be considered in future papers.

Finally, it is important to note that the general redistribution function presented in this paper, Equation (6) or (11), coincides with a rarely quoted result by Lamb & Ter Haar (1971), which was derived through a completely different approach to the problem of resonance scattering (based on Heitler 1954). More precisely, these authors provided the expression of a “resonance matrix” for scattering (see their Equation (7.7)), which turns out to be equivalent to

\[
[(ε_{uu'} + iω_{uu'})(ε_{ll'} + iω_{ll'})]^{-1} \mathcal{R}(Ω_u, Ω_{u'}; Ω_l, Ω_{l'}; ω_k, ω_{l'})
\]

in our notation. This correspondence allows us to derive yet another form for the general redistribution function presented in this paper, which is fully equivalent to Equations (6) and (11),

\[
\mathcal{R}(Ω_u, Ω_{u'}; Ω_l, Ω_{l'}; ω_k, ω_{l'}) = \Phi_{lu}^{+k} \Phi_{l'u'}^{+k'} - \Phi_{lu}^{-k} \Phi_{l'u'}^{-k'} + \Phi_{lu}^{+k} \Phi_{l'u'}^{-k'} - \Phi_{lu}^{-k} \Phi_{l'u'}^{+k'} + \Phi_{lu}^{+k} \Phi_{l'u'}^{+k'} - \Phi_{lu}^{-k} \Phi_{l'u'}^{-k'}
\]

\[
= \Phi_{lu}^{+k} \Phi_{l'u'}^{+k'} + \Phi_{lu}^{+k} \Phi_{l'u'}^{-k'} + \Phi_{lu}^{-k} \Phi_{l'u'}^{-k'} + \Phi_{lu}^{-k} \Phi_{l'u'}^{+k'} + \Phi_{lu}^{+k} \Phi_{l'u'}^{+k'} + \Phi_{lu}^{-k} \Phi_{l'u'}^{-k'},
\]

(50)

where in the last line we used the conjugation property of the profiles \(\Phi_{ab}^{-k} = \Phi_{ba}^{+k}\) (see Equation (34)),

\[
\bar{\Phi}_{ab}^{-k} = \Phi_{ba}^{+k}.
\]

The equivalence between the general redistribution function presented in this paper and the form (50) derived by Lamb & Ter Haar (1971) gives us additional confidence of the solidity of our results and of the formalism on which they are based. It is regrettable that such a fundamental result of Lamb & Ter Haar (1971) has essentially gone unnoticed by the literature published over the past 40 years on the subject of partial redistribution for polarized radiation. We hope that our paper will at least succeed in bringing once again to the attention of the solar polarimetry community the beauty and relevance, still to this day, of that seminal work.

APPENDIX

FREQUENCY REDISTRIBUTION IN THE LABORATORY REFERENCE FRAME

In order to express the redistribution function \(\mathcal{R}(Ω_u, Ω_{u'}; Ω_l, Ω_{l'}; ω_k, ω_{l'})\) in the reference frame of the emitting plasma (the “laboratory” frame), it is convenient to start from the form (50).

Let \(ω_k\) and \(ω_{l'}\) be the angular frequencies in the laboratory reference frame, respectively, for the incident and scattered photons, corresponding to \(ω_k\) and \(ω_{l'}\) in the atomic rest frame. Then (Hummer 1962; Mihalas 1978),

\[
ω_k = \hat{ω}_k - Δω_T \mathbf{v} \cdot \mathbf{κ}, \quad ω_{l'} = \hat{ω}_{l'} - Δω_T \mathbf{v} \cdot \mathbf{κ}'.
\]

(51)

Here \(\mathbf{v}\) is the velocity of the scattering atom in the laboratory frame, expressed in units of the thermal velocity \(v_T = \sqrt{2k_BT/M}\), where \(k_B\) is the Boltzmann constant, \(T\) the temperature of the plasma, and \(M\) the mass of the atom. In turn, the Doppler width is given by \(Δω_T = ω_0v_T/c\), where \(ω_0\) is the “average” frequency of the atomic transition. In the following treatment, we ignore (as it is customarily done) the effects of the \(ω_0^2\) factor in the expression of the scattering emissivity (see Equation (20)).

To obtain the angle-dependent redistribution function in the laboratory frame, we must substitute Equation (A1) into Equation (50), and average the resulting expression over a Maxwellian distribution for the velocity of the scattering atom, which in the normalized units just introduced is simply given by

\[
P(\mathbf{v}) = π^{-3/2} \exp(-|\mathbf{v}|).\]

(52)

We introduce first a Cartesian system \(\{\mathbf{n}_i\}_{i=1,2,3}\) such that \(\mathbf{n}_1\) and \(\mathbf{n}_2\) are coplanar with \(\mathbf{κ}\) and \(\mathbf{κ}'\), and we indicate with \((p, q, r)\) the component vector of \(\mathbf{v}\) in this system. We define the scattering angle \(Θ\) such that \(\cos Θ = \mathbf{κ} \cdot \hat{κ}\), and for convenience we introduce the shorthand notations

\[
C_2 = \cos(Θ/2), \quad S_2 = \sin(Θ/2).
\]

(53)

We then choose \(\mathbf{n}_1\) as the bisector of the scattering angle, so that (e.g., Mihalas 1978)

\[
\mathbf{v} \cdot \mathbf{κ} = C_2p + S_2q, \quad \mathbf{v} \cdot \mathbf{κ}' = C_2p - S_2q.
\]

(54)
For simplicity we assume $\epsilon_{\alpha} = \epsilon_{\alpha'}$ and $\epsilon_{\beta} = \epsilon_{\beta'}$, so it is possible to introduce only two (dimensionless) damping parameters $a_{\alpha} = \epsilon_{\alpha}/\Delta \omega_T$. We note that this is a reasonable approximation in the case of a two-term atom. Finally, we introduce the normalized frequencies

$$v_{ab} = \frac{\hat{\omega}_b - \omega_{ab}}{\Delta \omega_T}, \quad w_{ab} = \frac{\hat{\omega}_b - \omega_{ab}}{\Delta \omega_T},$$

for any two levels $a$ and $b$.

After some tedious algebraic manipulation, and assuming $\Theta \neq 0, \pi$ (see McKenna 1980, for comments about those limiting cases), we find

$$R(\Omega_{\alpha}; \Omega_{\alpha'}; \Omega_{\beta}; \omega_{\beta}; \hat{\omega}_{\alpha}; \hat{\omega}_{\beta}; \Theta) = \frac{1}{2 \Delta \omega_T^2 C_2 S_2} \int_{-\infty}^{\infty} dq \ e^{-q^2} \times \left\{ \frac{W((\omega_{ab} - S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2)}{a_{\alpha}/S_2 - i\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q} + \frac{\bar{W}((\omega_{ab} - S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2)}{a_{\alpha}/S_2 + i\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q} \right\} + \left\{ \frac{W((\omega_{ab} + S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2)}{a_{\alpha}/S_2 + i\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q} + \frac{\bar{W}((\omega_{ab} + S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2)}{a_{\alpha}/S_2 - i\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q} \right\} - \frac{W((\omega_{ab} - S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2)}{i\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q},$$

where

$$W(v, a) = \frac{1}{\pi} \int_{-\infty}^{\infty} dp \ \frac{e^{-r^2}}{a + i(p - \nu)} = H(v, a) + iL(v, a),$$

with $H(v, a)$ and $L(v, a)$ being the Voigt and Faraday–Voigt functions (e.g., Landi Degl’Innocenti & Landolfi 2004), and we have indicated with $\bar{W}$ the complex conjugate of $W$. In the simplest case of a two-level atom with degenerate sublevels, Equation (A6) properly reduces to

$$R(\Omega_{\alpha}; \Omega_{\beta}; \hat{\omega}_{\alpha}; \hat{\omega}_{\beta}; \Theta) = \frac{1}{\Delta \omega_T^2 C_2 S_2^2} a_{\alpha} \int_{-\infty}^{\infty} dq \ \frac{e^{-q^2}}{(a_{\alpha}/S_2)^2 + \left[\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q\right]^2} \times \left\{ H((\omega_{ab} - S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2) + H((\omega_{ab} + S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2) \right\} + \frac{a_{\alpha}/S_2}{\frac{1}{2}(\omega_{ab} - \omega_{\alpha'})/S_2 - q} \left[ L((\omega_{ab} - S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2) - L((\omega_{ab} + S_2)q/C_2, (a_{\alpha} + a_{\beta})/C_2) \right],$$

which corresponds to Equation (21) of McKenna & Nelson (1986; see also Heinzel 1981).

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