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Abstract. The collisional width of a spectral line takes part in the frequency redistribution of the scattered radiation in the line. Within the impact approximation, collisional line broadening parameters (widths and shifts), depolarization and polarization transfer rates seem very similar: both include the effect of collisional transitions between the Zeeman sublevels of a given level, or between fine or hyperfine structure levels of a given term. However, there are important differences. On the one hand, for line broadening, the two levels connected by the radiative transition contribute to the broadening. There is also an interference term between the two levels of the line, which can be very important for collisions with neutral hydrogen. On the other hand, only one level or two close levels are concerned in the depolarization. Another difference lies in the fact that elastic cross-sections of the two levels contribute to the line broadening, whereas they do not contribute to the depolarization. The possibility to find some theoretical relationships concerning depolarization versus collisional broadening will be shown to be impossible. The perturbation expansion of the collisional S matrix and the Van der Waals interaction potential are recalled to be unsuitable, since all the derived parameters are too small (by approximately a factor 2). Finally, in the light of a very recent paper, numerical relationships between line widths and level depolarization rates will be quoted.

1. Introduction

This paper is a short review of the atomic physics of collisions and line broadening, which takes part in the spectroscopic and spectropolarimetric diagnostics of solar and stellar plasmas. It is especially geared towards scattering, the frequency redistribution of radiation, and atomic polarization, which can be modified by depolarization and polarization transfer by collisions. Atomic polarization can appear when the Zeeman sublevels are not in local thermodynamic equilibrium (LTE). This needs an anisotropic (or dissymmetric) radiation field or collisional excitation of the levels. Atomic polarization can be modified by a magnetic field (Hanle effect), by anisotropic velocity fields, multiple scattering, and isotropic collisions that tend to restore LTE. Spectropolarimetric diagnostics are based on the theory of the density matrix (Fano 1957, 1960; Blum 1981). It implies solving the statistical equilibrium equations, which correspond to the master equation of the atom at the stationary state. On the basis of the work on op-

tical pumping by Cohen-Tannoudji (1977) and earlier papers for the two-level atom, Bommier & Sahal-Bréchot (1978, 1991) extended the theory and solved the statistical equilibrium equations for the multi-level atom, and Bommier (1991) developed the theory for the transfer equation of polarized radiation. If there is coupling between the absorbed and emitted radiation, this calls for the theory of redistribution of radiation. This is considered in the following sections.

2. The basic theory and approximations leading to the line profile and the statistical equilibrium equations

In this section, we present the bases of the theory leading to the atomic master equation, which is necessary to derive the Stokes parameters of a radiation line. We begin from the very general formula by Baranger (1958a,b,c), for the intensity of a spectral line emitted between the levels i (initial level) and f (final level).

$$I(\omega) = \frac{4\omega^4}{3c^3} |\langle f | \boldsymbol{\mu} | i \rangle|^2 = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(\mathrm{i}\omega s)\, \Phi(s)\, \mathrm{d}s \ , \tag{1}$$

$$\Phi(s) = \mathrm{Tr}\,[\boldsymbol{\mu}\, T^*(s) \cdot \boldsymbol{\mu}\, T(s)\, \rho]. \tag{2}$$

In the above equations, ρ is the density matrix of the whole system consisting of the atoms and the perturbers (photons and colliders), $\boldsymbol{\mu}$ is the dipole moment, and $T(s)$ is the evolution operator of the full system. The above equation shows that the line profile $I(\omega)$ can be expressed as the Fourier transform of the autocorrelation function $\Phi(s)$ defined by Eq. (2), where "Tr" indicates the trace over the states of the full system. c is the velocity of the light. ω is the angular frequency of the radiation.

In order to derive the atomic master equation and the line profile, a number of key approximations are necessary:

– The *no-back-reaction approximation*, which assumes that the bath B is in a stationary state described by its unperturbed density matrix, i.e., that

$$\rho(t) = \rho_A(t) \otimes \rho_B \ .$$

– The *impact approximation*, which assumes that the interactions are separated in time such that the duration of a collision is much smaller than the mean interval between two collisions. The atom interacts also with one photon only at every time: the duration of an interaction, which is of the order of $1/\omega_{if}$, must be much smaller than the inverse of the natural lifetime. This is always valid when we do not consider the line profile.
– The *coarse-grained approximation*, which states that atom-photon and atom-collider interactions are decoupled. This is also called the *complete-collision approximation*, meaning that the collisional interaction has time to be completed before the emission of a photon. In other words, the collision must be considered as instantaneous in comparison with the time Γ^{-1} characteristic of the evolution of the excited state under the effect of the interaction with the radiation. This implies that the master equation cannot describe phenomena occuring during a collision.
– The *Markov approximation*, which states that the evolution of $\rho_A(t)$ does not depend on its past history but only on the present time t. This approximation leads to an infinitely narrow line profile (a δ-function), because the finite lifetime of the levels is ignored (Bommier & Sahal-Bréchot 1978, 1991, and references therein).

Going beyond the Markov approximation, the previous history of the system is taken into account, and the line profile and redistribution effects (coupling between the absorbed and the re-emitted photons) are naturally introduced (cf. Omont et al. 1972; Bommier 1997a,b, 2016). This implies that the atom-radiation interaction is no longer limited to the second order of perturbation theory, and consequently two photons can interact with the atomic system at the same time.

3. The frequency redistribution function

To simplify the discussion, we look into the treatment of Omont et al. (1972), especially their Eq. (60) and their Fig. 1, in the particular case where the initial (i) and final (f) levels are the same, denoted by $|1\rangle$, and the intermediate level e by $|2\rangle$. We indicate with $p(\omega_1, \omega_2)$ the joint probability for absorption of the incident radiation at the angular frequency ω_1 and re-emission at ω_2. The intensity of the re-emitted radiation $I(\omega_2)$ is proportional to

$$F(\omega_1, \omega_2) = A f(\omega_1)\, p(\omega_1, \omega_2)\ , \tag{3}$$

where

$$A = 4\pi^2\, |\langle 1|\boldsymbol{\mu}_1\,|2\rangle|^2\, |\langle 1|\boldsymbol{\mu}_2\,|2\rangle|^2\, \rho_{11}/\Gamma_2\ .$$

A contains the matrix elements of the dipole atomic moment $\boldsymbol{\mu}$ for the absorption and re-emission processes, the atomic density matrix ρ_{11} of the level $|1\rangle$, and the natural width Γ_2 of the level $|2\rangle$, which corresponds to the radiative decay rate A_{21} of the level due to spontaneous emission.

In Eq. (3), $f(\omega)$ represents the absorption or emission profile due to collisions and radiation (Omont et al. 1972, see their Eq. (54)). This is a Lorentzian, because of the assumption of the impact and complete-collision approximations, and also because the line is assumed by Omont et al. (1972) to be "isolated" (see below, and Baranger 1958b,c):

$$f(\omega) = \frac{\gamma_{21}/\pi}{(\omega - \omega_0 - \Delta_{21})^2 + \gamma_{21}^2}, \tag{4}$$

where $\gamma_{21} = (\Gamma_1 + \Gamma_2)/2 + \gamma_{21}^c$ and Δ_{21} are the line width and shift, respectively, and γ_{21}^c is the collisional half-width at half-maximum (HWHM) of the line. By neglecting the collisional and radiative lifetimes of level $|1\rangle$ ($\Gamma_1 = \gamma_1^c = 0$), Omont et al. (1972) obtain

$$p(\omega_1, \omega_2) = \left(\frac{\Gamma_2}{2\,\gamma_{21}}\right)\left[\delta(\omega_1 - \omega_2) + \left(\frac{2\,\gamma_{21} - \gamma_2}{\gamma_2}\right) f(\omega_2)\right], \tag{5}$$

where $\gamma_2 = \Gamma_2 + \gamma_2^c$, γ_2^c being the inelastic collisional decay of level $|2\rangle$ (i.e., the inverse of its collisional lifetime). Equation (5) is valid if there are neither fine structure transitions within the level $|1\rangle$, nor collisional transitions $|1\rangle \rightarrow |2\rangle$. The first parenthesis is the branching ratio. In the square brackets, the first term describes the coherent redistribution of radiation (Rayleigh scattering), whereas the second is the incoherent contribution, which is null if there are no collisions. In the following section, we consider the different collision terms of Eq. (5).

4. The inelastic collision frequency for level $|2\rangle$

We consider the collisional transitions between fine structure levels originating from level $|2\rangle$, i.e., $\alpha_2 J_2 \rightarrow \alpha_2 J_2'$, where α is the set of all quantum numbers other than J defining a level. We use the semi-classical picture where the collider is assumed to move along a classical path, characterized by its velocity v and impact parameter b. This is valid for collisions with hydrogen (the main collider) in the solar and stellar atmospheres. So, the trace over the density matrix of the colliders is equal to

$$\mathrm{Tr}_P = N_P \int_0^\infty \mathrm{d}v\, v\, f(v) \int_0^\infty \mathrm{d}b\, 2\pi\, b \oint \frac{\mathrm{d}\Omega}{4\pi} \,,$$

where $N_P = N_\mathrm{H}$. Since the impact approximation is valid, cross-sections σ integrated over the distribution function of velocities v appear. The angular average is an integration over all the directions of the isotropic colliders and is equivalent to summing over the final states $|J_2' M_2'\rangle$ and averaging over the initial states $|J_2 M_2\rangle$,

$$\gamma_2^{(c)} = C_2 = \sum_{J_2' \neq J_2} C(\alpha_2 J_2 \rightarrow \alpha_2 J_2') = N_\mathrm{H} \int \mathrm{d}v\, v\, f(v)\, \sigma(\alpha_2 J_2 \rightarrow \alpha_2 J_2', v) \,, \qquad (6)$$

$$\sigma(\alpha_2 J_2 \rightarrow \alpha_2 J_2', v) = \int \mathrm{d}b\, 2\pi\, b\, \frac{1}{2J_2+1} \sum_{M_2, M_2'} |\langle \alpha_2 J_2 M_2 | T(v,b) | \alpha_2 J_2' M_2' \rangle|^2 \,, \qquad (7)$$

where $T = 1 - S$ is the collisional transition matrix, and S is the collision scattering matrix, which is symmetric and unitary, $S^\dagger S = S^* S = 1$, and $T^* T = 2\,\mathrm{Re}(T)$.

5. The collisional line broadening

We consider a dipolar radiative transition between two levels i and f, with atomic configurations $(\alpha_i J_i)$ and $(\alpha_f J_f)$, respectively. In Eq. (53) of Omont et al. (1972), $(\alpha_i J_i)$ corresponds to $i = |2\rangle$, and $(\alpha_f J_f)$ to $f = |1\rangle$. Using the impact and complete collision approximations, and assuming there is no overlap between close levels (case of isolated lines, Baranger 1958c), the collisional profile is Lorentzian, characterized by a shift d, and a HWHM w. This is the so-called Baranger's formula for an isolated line:

$$w + \mathrm{i}\, d = N_P \int_0^\infty \mathrm{d}v\, v\, f(v) \int_0^\infty \mathrm{d}b\, 2\pi\, b \left\langle 1 - S_{ii}(v,b) S_{ff}^*(v,b) \right\rangle_{angle.avg.} \qquad (8)$$

Here, $\langle \cdots \rangle_{angle.avg.}$ is the angular average, $d = \Delta_{21}$, and $w = \gamma_{21}^c$.

Using the T matrix, and applying $T^* T = 2\,\mathrm{Re}(T)$, the real part of Eq. (8) reads:

$$w = \frac{1}{2} N_P \int_0^\infty \mathrm{d}v\, v\, f(v) \int_0^\infty \mathrm{d}b\, 2\pi\, b \left\langle \sum_{j \neq i} \left|T_{ij}\right|^2 + \sum_{j' \neq f} \left|T_{fj'}\right|^2 - \left|T_{ii} - T_{ff}^*\right|^2 \right\rangle_{angle.avg.} \qquad (9)$$

The cross-sections appearing in Eq. (9) are inelastic, while T_{ii} and T_{ff}^* are elastic scattering terms. Thus, the broadening effects of the inelastic scattering add incoherently, while those of the elastic scattering subtract coherently (Baranger 1962, p.517). This leads to an interference term after development of this formula.

5.1. Development of the Baranger's formula for the width using the T-matrix

After some angular algebra calculations, the full width at half maximum intensity $2w$ reads:

$$
\begin{aligned}
2w = N_P \int_0^\infty \mathrm{d}v\, v\, f(v) \Bigg[& \sum_{\alpha J \neq \alpha_i J_i} \sigma(\alpha_i J_i \to \alpha J, v) + \sum_{\alpha' J' \neq \alpha_f J_f} \sigma(\alpha_f J_f \to \alpha' J', v) \\
& + \sigma(\alpha_i J_i \leftrightarrow \alpha_i J_i, v) + \sigma(\alpha_f J_f \leftrightarrow \alpha_f J_f, v) \\
& - 2 \int_0^\infty \mathrm{d}b\, 2\pi\, b \\
& \times \sum_{M_i\, M_i'\, M_f\, M_f'\, m} (-1)^{2J_f + M_f + M_f'} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & m & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M_i' & m & M_f' \end{pmatrix} \\
& \times \mathrm{Re} \left\{ \langle \alpha_i J_i M_i | T(v,b) | \alpha_i J_i M_i' \rangle \langle \alpha_f J_f M_f | T^*(v,b) | \alpha_f J_f M_f' \rangle \right\} \Bigg] .
\end{aligned}
\tag{10}
$$

The collisional decay of the two levels appears in the first line of Eq. (10), as well as the elastic cross-sections $\sigma(\alpha_i J_i \leftrightarrow \alpha J, v)$ of the two levels (averaged over N_H and v) in the second line.

The subsequent lines represent the so-called "interference term" (Griem 1974, p.92) between the initial level i and final level f of the transition. This upper-lower (i-f) interference term mixes the two levels. The presence of the elastic cross sections of the initial and final level of the transition and of the interference term shows that there is a major difference between collisional line broadening studies and collisional depolarization studies.

5.2. Numerical example: the case of the D lines of Na I colliding with neutral hydrogen under solar conditions

As known for a very long time (Roueff & van Regemorter 1969), the atom-hydrogen interaction potential differs significantly from the Van der Waals model, because the typical impact parameters playing a role in solar conditions are much smaller. So a more realistic potential must be derived. In addition, the S-matrix elements have to be determined. Quantum chemistry methods are the most accurate. However, the hydrogen perturber can be treated as a classical particle moving along a classical path (a straight line), because the solar atmosphere temperature is high enough. Consequently the S-matrix elements can be obtained through the solution of the semi-classical, first-order, close-coupling differential equations, provided that the interaction potential is known.

The numerical results in Table 1 are taken from Roueff (1974). They are the first results using a realistic Na-H interaction potential and semi-classical close-coupling methods for the calculation of the S-matrix.

This table shows that the contribution of the interference term is very important (and negative in this case). Both contributions of elastic collisions and the ground state are also very important. The collisional FWHM, W, which is equal to $2\,\gamma_{21}$ of formula (60) of Omont et al. (1972), is made of all these terms. This table also shows that, even if there are similarities between the theories of collisional broadening and collisional depolarization (same basic theory, same S-matrix to calculate), there also are

Table 1. Results for $T = 4500$K, in rad s^{-1} (angular frequency units), for a hydrogen density equal to $N_H = 1\,\mathrm{cm}^{-3}$. W is the full width at half maximum (FWHM), $W = 2w$, cf. Eq. (10).

	D1 line	D2 line
Natural width A_{21}	6.14×10^{7}	6.16×10^{7}
Shift d	-0.64×10^{-9}	-0.55×10^{-9}
Full width W	16.46×10^{-9}	15.94×10^{-9}
– Excited state contribution to W	12.64×10^{-9}	12.60×10^{-9}
– Ground state contribution to W	14.3×10^{-9}	14.3×10^{-9}
– Interference term contribution to W	-10.48×10^{-9}	-10.96×10^{-9}
Fine structure collision rate $\gamma_2^{(c)}$	5.12×10^{-9}	2.56×10^{-9}

important differences. The linear combinations of the S-matrix elements are different. Depolarization (and polarization transfer) rates affect levels, and there are no T-matrix elastic terms $\alpha JM \leftrightarrow \alpha JM$ where M is conserved. Broadening instead affects the radiative transition between two levels, with a quantum interference term between the levels, and a contribution from the T-matrix elastic elements $\alpha JM \leftrightarrow \alpha JM$.

6. Collisional broadening and depolarization by collisions with hydrogen

Collisional depolarization was an important subject of research in the seventies and eighties. It enjoyed a revival over the last twenty years thanks to the development of studies of the second solar spectrum. In the present paper, we do not report all the necessary coefficients. We only recall that collisional depolarization affects the levels, and that the same S-matrix as the one for the broadening is required. However, the linear combinations are different, and there are no T-matrix elastic elements $\alpha JM \leftrightarrow \alpha JM$.

7. The interaction potential

Regarding the interaction potential, we recall that the Van der Waals model is inadequate and should be deprecated. This is due to the fact that the typical impact parameters b are small (about 10–20 atomic units), and thus an expansion in terms of $1/b$ is invalid. Modern quantum chemistry methods are able to obtain accurate interaction potentials (e.g., Kerkeni 2002), but the calculations are very long, and it is practically impossible to derive the numerous results that are needed for astrophysical applications. A good approximation is the ABO interaction potential (Brueckner 1971; Omara 1976). We refer to Barklem et al. (1998) and references therein for the case of broadening. Derouich et al. (2003b,a, 2004a,b, 2005) extended the use of the ABO interaction potential to collisional depolarization calculations, which has permitted to obtain many useful results. During the second decade of the present century, this so-called DSB method coupled to genetic programming methods was used to obtain a great number of

analytical results (Derouich et al. 2015; Derouich 2017; Derouich et al. 2017; Derouich 2018).

8. Conclusion

First, the width and shift of a spectral line due to collisions interests both levels of the corresponding radiative transition. In particular, the interference term between the two levels that was described in this paper can be important. The expressions of the line width and shift also contain elastic terms of the form $\alpha JM \leftrightarrow \alpha JM$. Polarization transfer and depolarization rates interest instead the individual levels. There are no elastic terms $\alpha JM \leftrightarrow \alpha JM$, but only those of the form $\alpha JM \rightarrow \alpha JM'$, with $M \neq M'$. So, it is impossible to find any analytical relationship between the line width and the depolarization rates. Interestingly, numerical relations were recently obtained, using numerical fitting methods based on genetic programming and artificial intelligence techniques (Derouich et al. 2015). Second, numerical calculations have to be performed both for broadening and depolarization. The semi-classical approximation is sufficient, but the perturbation expansion of the S-matrix is not valid. Close-coupling calculations are necessary, and a long range expansion of the interaction potential is invalid, because the typical impact parameters are too small (about 10-20 atomic units). Adapted interaction potentials are essential.

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