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On the collisional depolarization and transfer rates of spectral lines by atomic hydrogen

III. Application to f-states of neutral atoms

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Abstract. The theory of collisional depolarization of spectral lines by atomic hydrogen (Derouich et al. 2003a; Derouich et al. 2003b) is extended to f-atomic levels ($l = 3$). Depolarization rates, polarization and population transfer rates are calculated and results are given. Each cross section as a function of the effective quantum number for a relative velocity of 10 km s^{-1} is given together with an exponent λ, if it exists, with the assumption that the cross section varies with velocity as $v^{-\lambda}$. The general trends of depolarization rates, polarization transfer rates and population transfer rates are discussed.

Key words. Sun: atmosphere – atomic processes – line: formation – polarization

1. Introduction

The observation of the so-called "second solar spectrum" (a term first suggested by V. V. Ivanov; see Stenflo & Keller 1997; Stenflo et al. 2000; Stenflo 2001; Gandorfer 2000; Gandorfer 2002), which is the spectrum of the linear polarization observed near the limb, is due to the scattering of the underlying anisotropic radiation. The atomic polarization may be modified by several factors, in particular the magnetic field (Hanle effect), and also the isotropic collisions with the neighboring particles of hydrogen. Therefore the depolarization rates, polarization and population transfer rates by collisions with hydrogen are needed in order to quantitatively interpret the observed polarization in terms of magnetic fields in solar quiet regions.

In Derouich et al. (2003a) and Derouich et al. (2003b) (hereafter Papers I and II, respectively), a semi-classical theory for the calculation of depolarization rates, polarization and population transfer rates has been developed and applied to p ($l = 1$) and d ($l = 2$) atomic states. In the present paper we extend this theory to f-atomic levels ($l = 3$). This paper presents the first calculations of the depolarization and the collisional transfer rates for f-atomic states.

Our semi-classical theory is not specific for a given atom and its application is possible even to heavy atoms (Ti, Fe, ...), for which there are no data available for depolarization rates, transfer of polarization and population rates. The extension of this method permits calculation of depolarization and collisional transfer rates of p ($l = 1$), d ($l = 2$) and f ($l = 3$) atomic levels. It should now be possible to rapidly obtain the large amount of data needed for the interpretation of the second solar spectrum. Using our method, the general trends of all rates for p ($l = 1$), d ($l = 2$) and f ($l = 3$) atomic levels with orbital angular momentum quantum number l can be discussed for the first time.

2. Method

The method used to determine depolarization rates, transfer of polarization and population rates is the same as the one previously introduced in Papers I and II. We denote as $D^k(nlJ, T)$ the collisional depolarization rate for the statistical tensor of rank k. Each level of total angular momentum J relaxes with $2J+1$ independent depolarization rates. In particular $D^0(nlJ, T)$ is the destruction rate of population, which is zero since elastic collisions do not alter the population of an atomic level (nlJ). $D^1(nlJ, T)$ is the destruction rate of orientation (circular polarization) and $D^2(nlJ, T)$ is the destruction rate of alignment (linear polarization) which is of interest in the understanding of the second solar spectrum. If quenching must be taken into account, $D^k(nlJ \rightarrow nlJ', T)$ corresponds to collisional transfer of population ($k = 0$), orientation ($k = 1$) and alignment ($k = 2$) (Paper II). Since potentials are computed in the rotating frame, which is obtained from the fixed laboratory frame by means of the geometrical rotation $R\ (\beta, \frac{\pi}{2}, \frac{\pi}{2})$, the interaction potential

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matrix is diagonal (see, for example, Paper I). The extension of our calculations to f-atomic levels ($l = 3$) requires the determination of seven RSU potentials $V_{\mathrm{eff,m}}$ ($-3 \leq m \leq 3$). For more details we refer the reader to Paper I and Paper II and to the ABO papers (Anstee 1992; Anstee & O'Mara 1991, 1995; Anstee et al. 1997; Barklem 1998; Barklem & O'Mara 1997; Barklem et al. 1998). The total wave function $|\psi\rangle$ of the system is developed over the basis formed by the eigenvectors $|M_l\rangle$:

$$\big|\psi(t)\rangle = \sum_{M_l} a_{M_l}(t) \mathrm{e}^{-\mathrm{i}E^0_{M_l}t} \big|M_l\rangle \tag{1}$$

where the $E^0_{M_l}$ are the energy eigenvalues of the isolated atoms. For f-states, seven semi-classical coupled linear differential equations describing the evolution of the manifold of states are obtained by using the time-dependent Schrödinger equation (see Barklem et al. 1998). After integration of these coupled equations over an entire collision, we obtain the $a_{M_l}(t)$ coefficients and then the transition T-matrix elements (Paper I, Paper II). All rates are obtained after integration over impact parameters and velocities, of transition probabilities given by Eq. (39) in Paper I and Eq. (11) in Paper II.

3. Results

As for the p and d atomic state calculations, in most cases the behaviour of the cross sections with the relative velocity v obeys a power law of the form:

$$\sigma^k(n3J \to n3J', v)(J = J' \text{ and } J \neq J') = \sigma^k(n3J \to n3J', v_0)\left(\frac{v}{v_0}\right)^{-\lambda^k(n3J\to n3J')}, \tag{2}$$

where v_0 (=10 km s^{-1}) is a typical velocity where the cross section is calculated. Tables 1 and 2 give respectively variation of cross sections with the effective principal quantum number n^* and the corresponding velocity exponents. n^* is related to E_{nl} by $n^* = [2(E_\infty - E_{nl})]^{-1/2}$, E_∞ and E_{nl} being the binding energy of the ground state and the energy of the state of the valence electron respectively. Cross sections for other velocities can be obtained from Tables 1 and 2 using Eq. (2). Tables 1 and 2 can be interpolated for an appropriate n^* corresponding to a given observed line in order to obtain the needed rates (Paper I, Paper II). For cross sections obeying Eq. (2), the collisional depolarization and transfer rates can be expressed by Eq. (13) of Paper II. Sometimes, especially for the alignment transfer calculations, such behaviour was not obeyed (the cross sections showed oscillations with relative velocities) and so $\lambda^k(n3J \to n3J')$ is not reported (Table 2). We have to calculate directly the cross sections for each velocity. The collisional depolarization and transfer rates $D^k(nlJ \to nlJ', T)$ ($J = J'$ and $J \neq J'$) follow from numerical integration over the velocities.

Figure 1 shows the alignment depolarization rates ($k = 2$) as a function of the local temperature T and n^* for $l = 3$. The population transfer rates ($k = 0$) and the linear polarization transfer rates ($k = 2$) as a function of T and n^* are displayed in Figs. 2 and 3. All these rates increase with temperature. For a temperature $T \leq 10\,000$ K, the destruction rate of alignment $D^2(n\ 3\ 5/2)/n_{\mathrm{H}} \leq 7 \times 10^{-14}$ rad m^3 s^{-1}, $D^2(n\ 3\ 3)/n_{\mathrm{H}} \leq 12 \times 10^{-14}$ rad m^3 s^{-1} and $D^2(n\ 3\ 7/2)/n_{\mathrm{H}} \leq 7 \times 10^{-14}$ rad m^3 s^{-1}. The population transfer rate $D^0(n\ 3\ 5/2 \to n\ 3\ 7/2)/n_{\mathrm{H}} \leq 7 \times 10^{-14}$ rad m^3 s^{-1} and the linear polarization transfer rate $D^2(n\ 3\ 5/2 \to n\ 3\ 7/2)/n_{\mathrm{H}} \leq 5 \times 10^{-15}$ rad m^3 s^{-1}. These numerical values are given for $n^* \leq 5$ which includes most of the lines of interest.

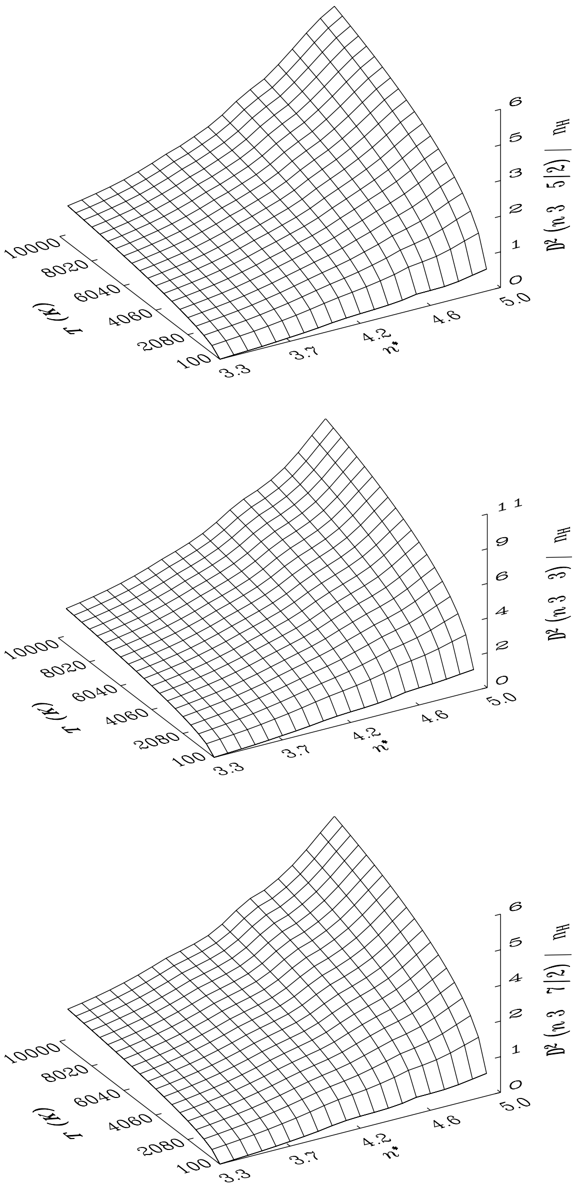

Fig. 1. Depolarization rates per unit H-atom density as a function of temperature T and n^*. For $l = 3$, each figure: $S = \frac{1}{2}$ and $J = \frac{5}{2}$; $S = 0$ and $J = 3$; $S = \frac{1}{2}$ and $J = \frac{7}{2}$. Depolarization rates are given in 10^{-14} rad m^3 s^{-1}.

4. General trends

For a given effective quantum number n^*, and for the cases $l = 1$, $l = 2$, and $l = 3$, destruction rates of alignment are such that $D^2(n\ 3\ 3, T) < D^2(n\ 2\ 2, T) < D^2(n\ 1\ 1, T)$. A similar result has been obtained for the broadening of spectral lines. In fact, Barklem et al. (1998) have previously shown that, also for

Table 1. Variation of the cross sections, for the relative velocity of 10 km s^{-1}, with the effective principal number. Cross sections are in atomic units.

n^*	$\sigma^2(n3\frac{5}{2})$	$\sigma^2(n33)$	$\sigma^2(n3\frac{7}{2})$	$\sigma^0(n3\frac{5}{2} \to n3\frac{7}{2})$	$\sigma^2(n3\frac{5}{2} \to n3\frac{7}{2})$
3.3	426	782	491	478	40
3.4	451	831	521	518	44
3.5	489	892	561	565	51
3.6	535	962	603	616	58
3.7	584	1055	654	684	67
3.8	637	1151	708	768	81
3.9	695	1249	765	865	96
4	759	1365	824	962	101
4.1	835	1467	875	1031	110
4.2	890	1572	899	1119	108
4.3	1024	1777	1051	1188	114
4.4	1077	1908	1097	1297	121
4.5	1236	2166	1247	1418	121
4.6	1249	2279	1306	1508	116
4.7	1420	2411	1432	1503	125
4.8	1485	2515	1485	1529	118
4.9	1521	2587	1504	1630	132
5	1928	3135	1845	1786	130

Table 2. Velocity exponents $\lambda^k(nlJ \to nlJ')$ ($J = J'$ and $J \neq J'$) corresponding to the cross sections of Table 1.

n^*	$\lambda^2(n3\frac{5}{2})$	$\lambda^2(n33)$	$\lambda^2(n3\frac{7}{2})$	$\lambda^0(n3\frac{5}{2} \to n3\frac{7}{2})$	$\lambda^2(n3\frac{5}{2} \to n3\frac{7}{2})$
3.3	0.228	0.277	0.301	0.280	–
3.4	0.249	0.295	0.315	0.283	–
3.5	0.252	0.303	0.325	0.288	–
3.6	0.260	0.311	0.331	0.289	–
3.7	0.275	0.329	0.346	0.289	–
3.8	0.275	0.334	0.354	0.296	–
3.9	0.282	0.342	0.367	0.301	0.103
4	0.306	0.363	0.402	0.320	0.117
4.1	0.298	0.362	0.412	0.344	0.176
4.2	0.278	0.336	0.384	0.351	0.267
4.3	0.240	0.306	0.333	0.370	0.328
4.4	0.235	0.304	0.319	0.394	0.384
4.5	0.262	0.333	0.349	0.415	0.396
4.6	0.215	0.317	0.311	0.440	0.411
4.7	0.181	0.289	0.284	0.435	0.497
4.8	0.192	0.268	0.269	0.409	0.600
4.9	0.218	0.248	0.268	0.363	0.587
5	0.222	0.224	0.242	0.331	0.500

a given n^*, lines with upper p-states ($l = 1$) are more broadened than lines with upper d-states ($l = 2$), and similarly lines with upper d-states are more broadened than lines with upper f-states ($l = 3$). This effect is similar to that first seen observationally in the solar spectrum by Carter (1949). In general, when the orbital angular momentum quantum number l increases, the depolarization rates and transfer of polarization and population rates decrease for a given value of the energy of the state of the valence electron E_{nl}.

For f-states, when $J = 7/2$ and $J' = 5/2$ we have: $D^0(n\ 3\ 7/2 \to n\ 3\ 5/2, T) > D^1(n\ 3\ 7/2 \to n\ 3\ 5/2, T) > D^2(n\ 3\ 7/2 \to n\ 3\ 5/2, T) > D^4(n\ 3\ 7/2 \to n\ 3\ 5/2, T) > D^3(n\ 3\ 7/2 \to n\ 3\ 5/2, T) > D^5(n\ 3\ 7/2 \to n\ 3\ 5/2, T)$. We recall that $D^k(n\ l\ J \to n\ l\ J', T)$ is a linear combination

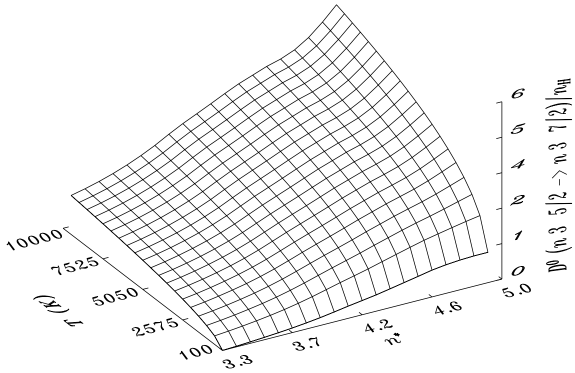

Fig. 2. Population transfer rate per unit H-atom density ($k = 0$) as a function of temperature T and n^*. $l = 3$, $S = \frac{1}{2}$, $J = \frac{5}{2}$ and $J' = \frac{7}{2}$. Population transfer rate is given in 10^{-14} rad m^3 s^{-1}.

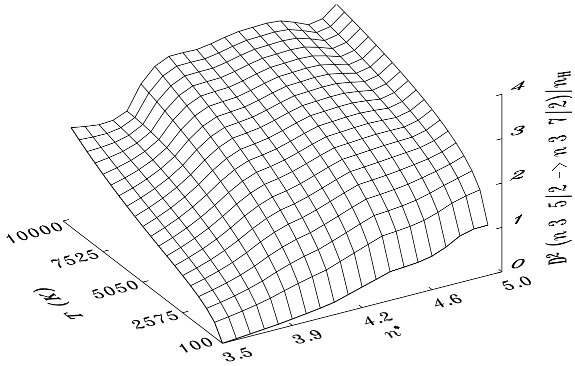

Fig. 3. Linear polarization transfer rate per unit H-atom density ($k = 2$) as a function of temperature T and n^*. $l = 3$, $S = \frac{1}{2}$, $J = \frac{5}{2}$ and $J' = \frac{7}{2}$. Linear polarization transfer rate is given in 10^{-15} rad m^3 s^{-1}.

of $\zeta(nlJM_J \rightarrow nlJ'M'_J, T)$ (Eq. (3) in Paper II). The population transfer rate is the greater transfer rate because for $k = 0$ the coefficients of this linear combination are positive. These coefficients are constant and equal to $1/\sqrt{(2J+1)(2J'+1)}$ which leads to a $D^0(nlJ \rightarrow nlJ', T)$ which is proportional to $\zeta(nlJ \rightarrow nlJ', T)$ (Eq. (5) in Paper II). However, the sign of the coefficients of the linear combination for transfer rates of rank $k \geq 1$ is sometimes positive and sometimes negative. For example, these coefficients have the sign of $M_J \times M'_J$ for orientation transfer rates ($k = 1$) and the sign of $(3M_J^2 - J(J+1)) \times (3M_J'^2 - J'(J'+1))$ for alignment transfer rates. The other coefficients of the linear combination for $k > 2$ may be obtained on request from the authors. We conclude that, for $k \neq 0$, the collisional transfer rates may be positive or negative as a function of transition probabilities between the Zeeman sublevels which depend on n^*. The depolarization rates are usually positive.

All rates were found to increase with temperature T. The functional form $D(T) = AT^{(1-\lambda)/2}$ may be accurately fitted to the depolarization rates and the population transfer rates (Paper I, Paper II). However, sometimes the collisional transfer rates with $k \neq 0$, cannot be fitted by the power-law $AT^{(1-\lambda)/2}$ and so λ is not reported (Table 2 in the present paper and Table 2 in Paper II). This is due to the fact that these collisional transfer rates are the sum of incoherent contributions from the states $|nlJM_J\rangle$ and $|nlJ'M'_J\rangle$. We notice that the above remarks are valid also for p and d-atomic states.

5. Discussion

Unfortunately, there are neither experimental nor quantum chemistry depolarization and collisional transfer rates for f-states for comparison. We expect that the main differences between the RSU potentials and those from quantum chemistry, which are considered as more realistic, occur for the short-range interactions. We have verified that these close collisions do not influence the computed depolarization and collisional transfer rates for f-states. The decisive contribution to the depolarization and collisional transfer rates occurs at intermediate-range interactions. In Paper I, which is concerned with p-states, comparison with quantum chemistry results in Kerkeni (2002) gives depolarization rates in agreement to better than 20%. Extrapolating our results obtained for p and d states (Paper I, Paper II), we expect a rather good agreement (relative difference less than 20% at solar temperatures) between our rates obtained for f-states and a full quantum mechanical treatment.

6. Conclusion

This paper is a continuation of a series concerned with theoretical calculations of the depolarization and collisional transfer rates. Thanks to the extension to f-atomic states ($l = 3$), we can draw the first general conclusions about the trends of all rates as a function of orbital angular momentum quantum number l. An extrapolation for $l > 3$ would be useful for a more complete interpretation of the "second solar spectrum". This work is in progress. An extension of our theory to the case of ions will be the subject of further papers.

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