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Spin depolarizing effect in collisions with neutral hydrogen

II. Application to simple/complex ions in spherically symmetric states

M. Derouich[1,⋆] and P. S. Barklem[2]

[1] Instituto de Astrofísica de Canarias, 38205 La Laguna, Tenerife, Spain
e-mail: moncef@iac.es
[2] Department of Astronomy and Space Physics, Uppsala University, Box 515, 751 20 Uppsala, Sweden

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ABSTRACT

Aims. We develop an accurate and general semi-classical formalism that deals with the definition and the calculation of the collisional depolarizing constants of the levels of simple and complex singly-ionized atoms in arbitrary *s*-states perturbed by collisions with hydrogen atoms. The case of ions with hyperfine structure is investigated fully.

Methods. We obtain potential energy curves based on the MSMA exchange perturbation theory by employing the Unsöld approximation. These potentials enter the Schrödinger equation to determine the collisional T-matrix elements in a semi-classical description. We use the T-matrix elements for the calculation of the collisional depolarization rates of simple atoms. Then, we use these rates to calculate the collisional coefficients in cases of ions with hyperfine structure.

Results. We evaluate the collisional depolarization and polarization transfer rates of the ground levels of the ionized alkaline earth metals Be II, Mg II, Ca II, Sr II, and Ba II. We study the variation of the collisional rates with effective principal quantum number n^* characterizing an arbitrary *s*-state of a perturbed simple ion. We find that the collisional rates for simple ions obey simple power laws as a function of n^*. We present direct and indirect formulations of the problem of the calculation of the depolarization and polarization transfer rates of levels of complex atoms and hyperfine levels from those for simple atoms. In particular, the indirect method allows a quick and simple calculation with its simple power-law relations. For the state 4s $^2S_{1/2}$ of Ca II, our computed rate of the destruction of orientation differs from existing quantum chemistry calculations by only 4% at $T = 5000$ K.

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

1. Introduction

The interaction of an atomic system with anisotropic unpolarized radiation can create atomic linear polarization, i.e. population imbalances and quantum coherences among the Zeeman sub-levels. As a result one obtains a linearly polarized spectrum when observing close to the solar limb (the so-called "second solar spectrum"). Under the physical conditions of the solar photosphere and the low chromosphere, the isotropic collisions between the atomic system and a bath of hydrogen atoms can partially or completely destroy the linear polarization of the levels. Thus, the role of these collisions should be considered when analyzing the linear polarization of the spectral lines.

We consider the problem of theoretical modelling of a binary collision between an ion in an arbitrary (i.e. not necessarily a ground state) *s*-state and the hydrogen atom in its ground *s*-state. Since the impact approximation is well satisfied for isotropic collisions between neutral hydrogen atoms and emitting/absorbing atoms in the solar photosphere, the collisional depolarization rates are simply obtained by multiplying the rates for a binary collision by the hydrogen density.

The atomic polarization of the J-level of an emitting or absorbing atom is affected during the collision by an interaction potential depending on its projection M_J; i.e., the interaction potential is *anisotropic* or, in other words, it depends on the orientation of the total angular momentum of the perturbed ion[1]. For an atom or an ion in an *s*-state interacting with the hydrogen atom in its ground *s*-state, the anisotropic part of the interaction potential comes from the effect of the spin.

Evaluation of the depolarization rates of the ground states of the ionized alkaline earth metals Be II, Mg II, Ca II, Sr II, and Ba II has been carried out. We have compared our results for the Ca II case with the results of Kerkeni et al. (2003) where quantum chemistry potentials and a fully quantal description of the dynamics have been employed. Very satisfactory agreement is obtained. In fact, at $T = 5000$ K the difference is 4%.

We went on to define the collisional depolarization rates for the case where the hyperfine structure of the odd isotopes is taken into account. In the framework of the frozen nuclear spin approximation, we obtain these rates using both a direct and an indirect method for the case of Ba II. For any value of the nuclear spin of any ion, the hyperfine collisional depolarization rates can be obtained via simple power law relations and algebraic coefficients which are specified.

We obtain the depolarization rates of the *s*-states 4f5d6s and 4f^{4}6s of the complex ions Ce II and Nd II, respectively, which are of particular astrophysical interest. Manso Sainz et al. (2006) studied the second solar spectrum of the Ce II, and found that the collisional depolarization rates are needed in order to better

⋆ Also associated researcher at CNRS UMR 8112 – LERMA, Observatoire de Paris, Section de Meudon, 92195 Meudon, France.

[1] In fact, this property is general, i.e. regardless of whether the perturbed particle is an ion, atom, or molecule, only the anisotropic part of the interaction potential affects the atomic polarization.

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understand the role of the atomic polarization of the lower levels on the observed scattering polarization.

2. Potentials

In a recent paper (Derouich et al. 2005b, hereafter Paper I), a method for computing potentials using MSMA (Murrell & Shaw 1967; Musher & Amos 1967) exchange perturbation theory, employing the Unsöld approximation, was described for the case of the interaction of a hydrogen atom with an atom in a spherically symmetric s-state. For the present problem, we need to extend the theory to the interaction of a hydrogen atom with a singly ionized atom. The theory for the case of ions was addressed by Barklem et al. (1998), but neglecting exchange i.e. employing the Rayleigh-Schrödinger perturbation theory where spin is not considered, and then applied to collisional depolarization and polarization transfer involving p and d states in Derouich et al. (2004). Using these two works as starting points, it is not difficult to extend the method to s-states of ions.

The general theory is essentially the same as the one outlined in Paper I, with three changes. First, we note that the interaction term V in the Hamiltonian must account for the increased charge of the core of the perturbed ion, and is now

$$V = \frac{2}{R} + \frac{1}{r_{12}} - \frac{2}{p_1} - \frac{1}{r_2}. \tag{1}$$

Second, we note that in Paper I some terms in the second-order energy expression, which were within the same order of magnitude as the first order energy were neglected. In this work for ions, due to the increased magnitude of the interaction and thus the larger first-order energy, we found it to be important to retain these terms as they partially cancel the first-order term. Finally the introduction of the Unsöld approximation, including separation of dispersive and inductive interactions (see Barklem et al. 1998), is made. We define the inductive part of the interaction as

$$V_{\rm ind} = \frac{1}{R} - \frac{1}{p_1}. \tag{2}$$

Following the notation of Paper I, the expressions for the first and second order energies are found to be

$$E^{(1)} = \frac{\langle a_0 b_0|V|a_0 b_0\rangle \pm \langle a_0 b_0|V|b_0 a_0\rangle}{1 \pm S_{00}}, \tag{3}$$

and

$$\begin{aligned} E^{(2)} \approx & -\frac{(E^{(1)})^2}{E_{\rm p}({\rm dir})} - E^{(1)} + \langle a_0 b_0|V|a_0 b_0\rangle \\ & + \frac{1}{1 \pm S_{00}} \left\{ \frac{1}{E_{\rm p}({\rm dir})} \left[\langle a_0 b_0|V^2|a_0 b_0\rangle - \langle a_0 b_0|V^2_{\rm ind}|a_0 b_0\rangle \right] \right. \\ & + \frac{1}{E_{\rm p}({\rm ind})} \langle a_0 b_0|V^2_{\rm ind}|a_0 b_0\rangle \\ & \left. \pm \frac{1}{E_{\rm p}({\rm exch})} \langle a_0 b_0|V^2|b_0 a_0\rangle \right\}, \end{aligned} \tag{4}$$

where $S_{00} = \langle a_0 b_0|b_0 a_0\rangle = \langle a_0|b_0\rangle^2$ is the wavefunction overlap. The singlet and triplet potentials, $V^{1\Sigma}$ and $V^{3\Sigma}$ respectively, to the second order are given by $E^{(1)} + E^{(2)}$ where the upper signs (+) correspond to the singlet case and lower signs (−) to the triplet case.

The appropriate choice for $E_{\rm p}({\rm ind})$ is $-4/9$ atomic units, as this term represents the interaction of the hydrogen atom with the excess charge of the ion (see Barklem et al. 1998). Appropriate values of $E_{\rm p}({\rm dir})$ and $E_{\rm p}({\rm exch})$ must be chosen. Barklem et al. (1998) described how the appropriate choice of $E_{\rm p}({\rm dir})$ may be inferred from the long-range van der Waals interaction constant C_6, and from how C_6 may be calculated. In that paper and in Barklem & O'Mara (2000), $E_{\rm p}({\rm dir})$ has been calculated for the interactions of ions of the alkaline earth metals Be II, Mg II, Ca II, Sr II, and Ba II, in their ground states and some excited states. It is the ground s-states of these species that are of interest here, and these values for $E_{\rm p}({\rm dir})$ may be adopted. The choice of $E_{\rm p}({\rm exch})$ is more difficult, and as in Paper I we obtain guidance from quantum chemistry type potentials. We investigated the cases of the ground states of BeH^+, MgH^+, and CaH^+. For BeH^+ we used the $X^1\Sigma^+$ and $a^3\Sigma^+$ potentials from Machado & Ornellas (1991), for MgH^+ the $1^1\Sigma^+$ and $1^3\Sigma^+$ potentials from García-Madroñal et al. (1992), and for CaH^+ the $X^1\Sigma^+$ and $a^3\Sigma^+$ potentials from Kerkeni et al. (2003). We then performed calculations varying $E_{\rm p}({\rm exch})$ to obtain the best fit to the exchange splitting $V^{3\Sigma} - V^{1\Sigma}$ in the region of potential around $R \sim 6$–8, 9, $12a_0$, the upper limits of the fitting region corresponding to the Be II, Mg II, and Ca II cases, respectively. From these fits we obtain $E_{\rm p}({\rm exch}) = -26.9$, -18.1 and -6.3 atomic units for the three cases respectively. Note that these values are significantly lower than those found for ground states of neutral alkali atoms, which is expected. As mentioned in Paper I and as noted by Musher & Amos (1967), the major contribution to the exchange integral sum comes from continuum states, which is a natural consequence of the fact that when a wavefunction centred on one atom is expanded about the other atom, the most important contributions will come from continuum states. As the electronic wavefunctions of ions are much more compact than for neutrals, we expect that the contributing continuum states have higher energy, leading to a higher value of $|E_{\rm p}({\rm exch})|$.

As found in Paper I for ground states of neutral alkali atoms, $E_{\rm p}({\rm exch})$ correlates well with effective principal quantum number $n^* = [2E_\infty]^{-1/2}$, E_∞ being the binding energy of the state in atomic units. Following that work we may make a fit to these values,

$$E_{\rm p}({\rm exch}) = -0.4444 - \exp(-3.710n^* + 9.7742). \tag{5}$$

Using this fit we may extrapolate to the cases of the ground states of Sr II and Ba II ($n^* = 2.221$ and 2.332, respectively), so potentials for SrH^+ and BaH^+ were calculated in this manner. We may also attempt to infer something about the general behaviour of the depolarization rates with n^*. A grid of potentials was computed for a range of n^*, adopting $E_{\rm p}({\rm dir}) = -4/9$ and $E_{\rm p}({\rm exch})$ as given by Eq. (5) for this purpose.

3. Definitions of the depolarization and polarization transfer probabilities

3.1. Fine structure levels

Let us consider collisions between a singly ionized atom in an s-state with angular momentum $\boldsymbol{J}$ ($J = 1/2$) and a bath of neutral hydrogen atoms in their ground state with angular momenta J_2 ($J_2 = 1/2$).

In the framework of the impact approximation, the contribution of the collisions is simply added to the contribution of the radiative rates in the statistical equilibrium equations (SEE). We define the collisional depolarization and transfer of polarization rates in a way similar to that often adopted for the radiative rates, based on the formalism of the irreducible spherical tensors. In fact, the density matrix formalism expressed in the basis

of the irreducible tensorial operators ${}^{J,J'}T^{k_J}_{q_J}$ has been shown to be the most suitable for formulating the problem of the formation of polarized spectral lines (e.g. Sahal-Bréchot 1977; Landi Degl'Innocenti & Landolfi 2004). On this basis, the internal state of the ion is described by the density matrix elements ${}^{J}\rho^{k_J}_{q_J}$.

In the absence of hyperfine structure (i.e. the nuclear spin $I = 0$ or the hyperfine structure has a negligible effect), the contribution of the isotropic collisions is:

$$\left(\frac{\mathrm{d}\,{}^{J}\rho^{k_J}_{q_J}}{\mathrm{d}t}\right)_{\mathrm{coll}} = -D^{k_J}(J,T)\,{}^{J}\rho^{k_J}_{q_J} - {}^{J}\rho^{k_J}_{q_J}\sum_{J'\neq J}\sqrt{\frac{2J'+1}{2J+1}}D^0(J\to J',T) + \sum_{J'\neq J}D^{k_J}(J\leftarrow J',T)\,{}^{J'}\rho^{k_J}_{q_J} \tag{6}$$

where $D^{k_J}(J,T)$, $D^0(J\to J',T)$, and $D^{k_J}(J\leftarrow J',T)$ are the depolarization, the population transfer, and the polarization transfer rates, respectively.

The polarization transfer from J to J' levels of a perturbed atom or ion due to isotropic collisions with neutral hydrogen atoms is given in the basis of ${}^{J,J'}T^{k_J}_{q_J}$ by

$$\langle P^{k_J}(J\to J',b,v)\rangle_{\mathrm{av}} = \sum_{\mu_1,\mu_1',\nu_1,\nu_1'}\sum_{\gamma_2,\gamma_2'}\frac{1}{2J_2+1}\langle J\mu_1|\langle J_2\gamma_2|T(\boldsymbol{b},\boldsymbol{v})|J_2\gamma_2'\rangle|J'\mu_1'\rangle \times\langle J\nu_1|\langle J_2\gamma_2|T(\boldsymbol{b},\boldsymbol{v})|J_2\gamma_2'\rangle|J'\nu_1'\rangle^* \times\sum_{\alpha_1}(-1)^{J-J'+\mu_1-\mu_1'}\begin{pmatrix}J' & J' & k_J\\ \nu_1' & -\mu_1' & \alpha_1\end{pmatrix}\begin{pmatrix}J & J & k_J\\ \nu_1 & -\mu_1 & \alpha_1\end{pmatrix} \tag{7}$$

and the depolarization probability of a J-level is

$$\langle P^{k_J}(J,b,v)\rangle_{\mathrm{av}} = \langle P^0(J\to J,b,v)\rangle_{\mathrm{av}} - \langle P^{k_J}(J\to J,b,v)\rangle_{\mathrm{av}}. \tag{8}$$

Each collision is characterized by an impact-parameter vector $\boldsymbol{b}$ and a relative velocity vector $\boldsymbol{v}$. The symbol $\langle\ \rangle_{\mathrm{av}}$ denotes an average of the probabilities over all the orientations of the collision plane $(\boldsymbol{b},\boldsymbol{v})$.

Because of the semi-classical character of our approach, the collisional cross sections are obtained after an integration of the collisional depolarization and polarization transfer probabilities over the impact parameter b. Then the corresponding depolarization rates $D^k(J,T)$ and polarization transfer rates $D^k(J\to J',T)$ are calculated for a local temperature T by an integration over a Maxwell distribution of the relative velocities (see Eq. (12) of Paper I).

3.2. Hyperfine structure levels

Many enigmatic features of the second solar spectrum require a careful study taking the nuclear spin effects into account, i.e. the hyperfine structure contribution. For example, for the studies of the still not understood complications of the D_1-D_2 type systems of sodium, barium, lithium, potassium, etc. (see e.g. Casini & Manso Sainz 2005), one needs an accurate formulation including hyperfine collisional depolarization rates. In the remainder of this section we consider a particular isotope having nuclear spin I, and, total angular momentum $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$.

In the spherical tensorial representation ${}^{F,F'}T^{k_F}_{q_F}$, the contribution of the isotropic collisions in the case of a multilevel atom with hyperfine structure is

$$\left(\frac{\mathrm{d}\,{}^{JI}\rho^{k_F}_{q_F}}{\mathrm{d}t}(F,F')\right)_{\mathrm{coll}} = -\sum_{F''F'''}D^{k_F}((JI)FF';(JI)F''F''',T)\,{}^{JI}\rho^{k_F}_{q_F}(F'',F''') - \sum_{F''F''',J'\neq J}\zeta((JI)FF'\to(J'I)F''F''',T)\,{}^{JI}\rho^{k_F}_{q_F}(F'',F''') + \sum_{F''F''',J'\neq J}D^{k_F}((JI)FF'\leftarrow(J'I)F''F''',T)\,{}^{J'I}\rho^{k_F}_{q_F}(F''F''') \tag{9}$$

where $D^{k_F}((JI)FF';(JI)F''F''',T)$ is the destruction rate of the order k that is given by

$$D^k((JI)FF';(JI)F''F''',T) = \zeta^0((JI)FF'\to(JI)F''F''',T) - \zeta^k((JI)FF'\to(JI)F''F''',T) \tag{10}$$

where

$$\zeta^{k_F}((JI)FF'\to(J'I)F''F''',T)\ (J=J' \text{ and } J\neq J') = n_{\mathrm{H}}\int_0^\infty vf(v)\mathrm{d}v\left(\pi b_0^2 + 2\pi\int_{b_0}^\infty\langle P^{k_F}((JI)FF'\to(J'I)F''F''',b,v)\rangle_{\mathrm{av}}\,b\,\mathrm{d}b\right) \tag{11}$$

and

$$\langle P^{k_F}((JI)FF'\to(J'I)F''F''',b,v)\rangle_{\mathrm{av}} = \sum_{\substack{\mu_1,\mu_1'\\ \nu_1,\nu_1'}}\sum_{\gamma_2,\gamma_2'}\frac{1}{2J_2+1}\langle(JI)F\mu_1|\langle J_2\gamma_2|T(\boldsymbol{b},\boldsymbol{v})|J_2\gamma_2'\rangle|(J'I)F''\mu_1'\rangle \times\langle(JI)F'\nu_1|\langle J_2\gamma_2|T(\boldsymbol{b},\boldsymbol{v})|J_2\gamma_2'\rangle|(J'I)F'''\nu_1'\rangle^* \times\sum_{\alpha_1}(-1)^{F+F''+k+\mu_1-\mu_1'}\begin{pmatrix}F' & F & k_F\\ \nu_1 & -\mu_1 & -\alpha_1\end{pmatrix}\begin{pmatrix}F''' & F'' & k_F\\ -\nu_1' & \mu_1' & \alpha_1\end{pmatrix}. \tag{12}$$

We choose $b_0 = 3\,a_0$ as the cutoff impact-parameter, and $f(v)$ is the Maxwellian distribution function for relative velocity v.

The hyperfine polarization transfer rates by isotropic collisions are

$$D^{k_F}((JI)FF'\to(J'I)F''F''',T) = \zeta^{k_F}((JI)FF'\to(J'I)F''F''',T), \tag{13}$$

and in particular if $k_F = 0$,

$$D^0((JI)FF'\to(J'I)F''F''',T) = \zeta^0((JI)FF'\to(J'I)F''F''',T) = \delta(F,F')\,\delta(F'',F''')\sqrt{\frac{2F+1}{2F''+1}} \times\zeta((JI)FF'\to(J'I)F''F''',T), \tag{14}$$

where $\zeta((JI)FF'\to(J'I)F''F''',T)$ are the collisional rates of the transitions between the levels $|(JI)FF'\rangle$ and $|(J'I)F''F'''\rangle$ averaged over all possible orientations of the collision plane $(\boldsymbol{b},\boldsymbol{v})$.

Our semi-classical theory developed in the previous papers should allow the calculation of the hyperfine rates involving states with electronic angular momentum $l > 0$. The definitions given in this section are the same independently of l. In the next sections, we examine the case of a singly ionized atom having electronic angular momentum $l = 0$ (s-state).

4. Depolarization rates of the fine structure levels with $I = 0$

The quantum defect and thus the effective quantum number n^* is used to characterize the state of the ion, and the interaction potentials $V^{1\Sigma}$ and $V^{3\Sigma}$ calculated for n^* in the interval [1.5, 3] were used to compute depolarization rates. The potentials $V^{1\Sigma}$ and $V^{3\Sigma}$ enter the semi-classical coupled differential equations, derived from the time-dependent Schrödinger equation (Eq. (7) of Paper I, Roueff 1974). The computed T-matrices are then employed to compute the tensorial components $\zeta^0(J = 1/2,\ T)$ and $\zeta^1(J = 1/2,\ T)$, and the destruction rate of orientation:

$$D^1(1/2,\ T) = \zeta^0(J = 1/2) - \zeta^1(J = 1/2) \tag{15}$$

for each n^*. We found that these rates obey a power law of the form $D^1(1/2,\ T = 5000\ \mathrm{K})(\frac{T}{5000})^{(1-\lambda^1)/2}$. The velocity exponent $\lambda^1(1/2)$ exhibits only a weak variation with n^* and is approximately equal to 0.42.

Interestingly, $D^1(1/2,\ T = 5000\ \mathrm{K})$, $\zeta^0(J = 1/2,\ T)$, and $\zeta^1(J = 1/2,\ T)$ have striking power law behaviours with n^*, which are, with correlation coefficients $R > 0.9$, fit by:

$$\begin{aligned} D^1(1/2,\ T = 5000\ \mathrm{K}) &\simeq 1.35 \times 10^{-9}\ n_{\mathrm{H}} \times n^{*^{1.22}} \\ \zeta^0(1/2,\ T = 5000\ \mathrm{K}) &\simeq 7.01 \times 10^{-9}\ n_{\mathrm{H}} \times n^{*^{1.22}} \\ \zeta^1(1/2,\ T = 5000\ \mathrm{K}) &\simeq 5.65 \times 10^{-9}\ n_{\mathrm{H}} \times n^{*^{1.22}}. \end{aligned} \tag{16}$$

The tensorial components $\zeta^0(J)$ and $\zeta^1(J)$ describe the elastic scattering of order zero and one, respectively. They are sensitive to the *diagonal* elements of the $T(\boldsymbol{b}, \boldsymbol{v})$-matrix. This leads to $\zeta^0(J)$ and $\zeta^1(J)$ being clearly larger than $D^1(J)$ because the latter depends only on the *off-diagonal* elements. Note that all the *diagonal* elements of the $T(\boldsymbol{b}, \boldsymbol{v})$-matrix are non-zero and usually larger than the *off-diagonal* elements.

The relationships of Eq. (16) will be used in the next sections to calculate the depolarization rates of hyperfine structure levels and levels of complex ions. The present method is not specific for a given perturbed atom and thus allows the calculation of the depolarization rates of any s-state.

The effective principal quantum numbers of the Be II, Mg II, Ca II, Sr II, and Ba II ground states are $n^* \simeq 1.7288$, 1.9025, 2.1411, 2.2213, and 2.3325, respectively. The destruction rates of orientation for the ground states of alkaline earth ions can be either determined directly from the numerical code associated to our theory or inferred from Eq. (16). We used our code to directly compute the rates for $100 \leq T \leq 10\,000$ K, and we find the following analytical expressions in units of s^{-1}:

– Be II ($2\mathrm{s}\ ^2\mathrm{S}_{1/2}$)- H I ($1\mathrm{s}\ ^2\mathrm{S}_{1/2}$):

$$D^1(2\ 1\ 1/2,\ T) = 2.67 \times 10^{-9} \times n_{\mathrm{H}} \left(\frac{T}{5000}\right)^{0.414}$$

– Mg II ($3\mathrm{s}\ ^2\mathrm{S}_{1/2}$)-H I ($1\mathrm{s}\ ^2\mathrm{S}_{1/2}$):

$$D^1(3\ 1\ 1/2,\ T) = 2.88 \times 10^{-9} \times n_{\mathrm{H}} \left(\frac{T}{5000}\right)^{0.407}$$

– Ca II ($4\mathrm{s}\ ^2\mathrm{S}_{1/2}$)-H I ($1\mathrm{s}\ ^2\mathrm{S}_{1/2}$):

$$D^1(4\ 1\ 1/2,\ T) = 3.43 \times 10^{-9} \times n_{\mathrm{H}} \left(\frac{T}{5000}\right)^{0.422}$$

– Sr II ($5\mathrm{s}\ ^2\mathrm{S}_{1/2}$)-H I ($1\mathrm{s}\ ^2\mathrm{S}_{1/2}$):

$$D^1(5\ 1\ 1/2,\ T) = 3.60 \times 10^{-9} \times n_{\mathrm{H}} \left(\frac{T}{5000}\right)^{0.415}$$

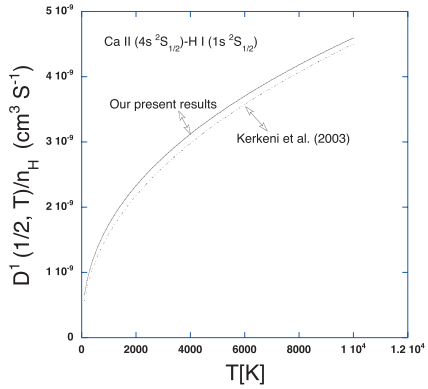

Fig. 1. Destruction rates of the orientation in $\mathrm{cm}^3\ \mathrm{s}^{-1}$ for the the Ca II ($4\mathrm{s}\ ^2\mathrm{S}_{1/2}$) level from the present calculations (solid line) and from Kerkeni et al. (2003) (dotted line).

– Ba II ($6\mathrm{s}\ ^2\mathrm{S}_{1/2}$)-H I ($1\mathrm{s}\ ^2\mathrm{S}_{1/2}$):

$$D^1(6\ 1\ 1/2,\ T) = 3.78 \times 10^{-9} \times n_{\mathrm{H}} \left(\frac{T}{5000}\right)^{0.422}.$$

The only existing result available for comparison is the quantal destruction rate of the orientation obtained in the case of the Ca II ($4\mathrm{s}\ ^2\mathrm{S}_{1/2}$), which equals $3.29 \times 10^{-9} \times n_{\mathrm{H}}$ at $T = 5000$ K as given by Eq. (11) of Kerkeni et al. (2003). As seen in Fig. 1, a very small difference of 4% at $T = 5000$ K is found.

5. Depolarization and polarization transfer rates of the hyperfine structure levels

Levels with total angular momentum $J = 1/2$ cannot be aligned, but if for example a level with $J = 1/2$ is split into hyperfine levels due to coupling with a nuclear spin $I = 3/2$, both hyperfine levels $F = 1$ and $F = 2$ can be aligned.

As can be seen in Eq. (12), an exact calculation of the hyperfine depolarization and polarization transfer rates first requires the calculation of the required atomic wavefunctions and interaction potentials fully taking the effect of the nuclear spin into account. Second, the time-dependent Schrödinger equations have to be solved on the basis of the set of eigenfunctions $|(JI)FM_F J_2 M_{J_2}\rangle$. This is a very complicated problem. As discussed in the next section, we resort to an approximate treatment by assuming that the nuclear spin is conserved during the collision.

In the typical solar conditions where the temperature is about 5700 K, the relative kinetic velocity of the collision is ~9.7 $\mathrm{km\,s}^{-1}$ (i.e. relative kinetic energy of ~0.5 eV). With a typical interatomic distance $R \sim 10$ Å, the inverse of the typical time duration of a collision between a hydrogen atom and the perturbed ion is $1/\tau \sim 10^{13}\ \mathrm{s}^{-1}$ (i.e. $1/\tau \sim 334\ \mathrm{cm}^{-1}$). In these conditions, the hyperfine splitting is usually much smaller than $1/\tau$, so that one can assume that the nuclear spin is conserved during the collision[2]. This validates the frozen nuclear spin approximation.

[2] It is important, however, not to confuse this condition with the fact that the SEE (Eq. (9)) must be solved for the hyperfine levels when the inverse of the lifetime of the level is smaller than the hyperfine splitting; i.e. the hyperfine levels are separated. In the second solar spectrum, the inverse of the lifetime is often small compared to the hyperfine splitting (if it exists).

5.1. A direct formulation with hyperfine scattering matrix in the dyadic basis

We adopt the frozen nuclear spin approximation, so the T-matrix is diagonal in I and its elements do not depend on M_I. The hyperfine structure T-matrix elements $\langle (JI)FM_F|T|(J'I)F'M'_F\rangle$ can be written as a linear combination of the $\langle JM_J|T|J'M'_J\rangle$, dropping the symbol $|J_2M'_{J_2}\rangle$ for brevity:

$$\langle (JI)FM_F|T|(J'I)F'M'_F\rangle \simeq \sum_{M_J,M'_J,M_I} (-1)^{2I-2J+M_F+M'_F}\sqrt{(2F+1)(2F'+1)} \times \begin{pmatrix} I & J & F \\ M_I & M_J & -M_F \end{pmatrix}\begin{pmatrix} I & J' & F' \\ M_I & M'_J & -M'_F \end{pmatrix}\langle JM_J|T|J'M'_J\rangle. \quad (17)$$

This reasoning, which gives Eq. (17), is equivalent to expressing the interaction potential elements $\langle FM_FJ_2M_{J_2}|V|F'M'_FJ_2M_{J'_2}\rangle$ as a linear combination of the singlet and triplet potentials $V^{1\Sigma}$ and $V^{3\Sigma}$.

To calculate the depolarization rates one has to

1. determine all the matrix elements given by Eq. (17);
2. calculate the depolarization and polarization transfer probabilities in the tensorial matrix basis ${}^{F,F'}T^{k_F}_{q_F}$;
3. integrate these probabilities over impact parameters and velocities (see Eq. (11)).

As an example, we compute the destruction rate of the alignment of the level $F = 1$. According to Eq. (17), the nine ($F = 1$) transition matrix elements $\langle FM_F|T|F'M_{F'}\rangle$ are given as a function of the five ($J = 1/2$) elements $\langle JM_J|T|J'M'_J\rangle$ by

$$\begin{aligned}
\langle 1-1|T|1-1\rangle &= \frac{3}{4}\times\left\langle \frac{1}{2}\ \frac{1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle + \frac{1}{4}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{-1}{2}\right\rangle \\
\langle 1-1|T|10\rangle &= -\frac{1}{\sqrt{8}}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle \\
\langle 1-1|T|11\rangle &= 0 \qquad (18)\\
\langle 10|T|1-1\rangle &= -\frac{1}{\sqrt{8}}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle \\
\langle 10|T|10\rangle &= \frac{1}{2}\times\left\langle \frac{1}{2}\ \frac{1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle + \frac{1}{2}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{-1}{2}\right\rangle \\
\langle 10|T|11\rangle &= -\frac{1}{\sqrt{8}}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle \\
\langle 11|T|1-1\rangle &= 0 \\
\langle 11|T|10\rangle &= -\frac{1}{\sqrt{8}}\times\left\langle \frac{1}{2}\ \frac{1}{2}|T|\frac{1}{2}\ \frac{-1}{2}\right\rangle \\
\langle 11|T|11\rangle &= \frac{1}{4}\times\left\langle \frac{1}{2}\ \frac{1}{2}|T|\frac{1}{2}\ \frac{1}{2}\right\rangle + \frac{3}{4}\times\left\langle \frac{1}{2}\ \frac{-1}{2}|T|\frac{1}{2}\ \frac{-1}{2}\right\rangle.
\end{aligned}$$

Following steps 2 and 3 above we obtain:

$$D^2((JI)11;(JI)11,T) = 0.68\times 10^{-9}\times n_{\rm H}\left(\frac{T}{5000}\right)^{0.439}\ {\rm s}^{-1}. \quad (19)$$

This is a "direct" but computationally consuming method. We propose an "indirect" and more practical way that allows the calculation of the hyperfine depolarization and polarization transfer rates via the values of $D^1(1/2,\ T)$, $\zeta^0(J = 1/2,\ T)$, and $\zeta^1(J = 1/2,\ T)$ given by Eq. (16).

5.2. An indirect formulation in the irreducible tensorial operator basis

One considers an uncoupled basis ${}^JT^{k_J}_{q_J}\otimes{}^IT^{k_I}_{q_I}$ in which the total orbital angular momentum and the nuclear spin are considered independently. Due to the frozen nuclear spin approximation, the depolarization matrix is spin-independent – the order k_I of the nuclear spin is not affected by the isotropic collisions. The values of the collisional rates $D^1(1/2,\ T)$, $\zeta^0(J = 1/2,\ T)$, and $\zeta^1(J = 1/2,\ T)$ associated with the J-levels over the irreducible tensorial operator basis ${}^JT^{k_J}_{q_J}$ are known.

As pointed out by Nienhuis (1976) and Omont (1977),

$$\zeta^{k_F}((JI)FF'\to(J'I)F''F''',T) = \sqrt{(2F+1)(2F'+1)(2F''+1)(2F'''+1)} \times\sum_{k_J}(2k_J+1)\zeta^{k_J}(J\to J',T) \times\sum_{k_I}(2k_I+1)\begin{Bmatrix} J & I & F \\ J & I & F' \\ k_J & k_I & k_F\end{Bmatrix}\begin{Bmatrix} J' & I & F'' \\ J' & I & F''' \\ k_J & k_I & k_F\end{Bmatrix}, \quad (20)$$

in particular

$$D^2((JI)11;(JI)11,T) = \zeta^0((JI)11\to(JI)11,T) - \zeta^2((JI)11\to(JI)11,T) \quad (21)$$

and, according to Eq. (20),

$$\zeta^0((JI)11\to(JI)11,T) = \frac{6}{16}\times\zeta^0(1/2,T) + \frac{10}{16}\times\zeta^1(1/2,T) \quad (22)$$

$$\zeta^2((JI)11\to(JI)11,T) = \frac{3}{16}\times\zeta^0(1/2,T) + \frac{13}{16}\times\zeta^1(1/2,T)$$

then

$$D^2((JI)11;(JI)11,T) = \frac{3}{16}\times D^1(J,T) = 0.709\times 10^{-9}\times n_{\rm H}\left(\frac{T}{5000}\right)^{0.422}. \quad (23)$$

The difference between the value of $D^2((JI)11;(JI)11,T)$ obtained by this indirect method and that of Eq. (19) is only 4%.

Taking into account the symmetry property

$$D^k((JI)FF'\to(J'I)F''F''',T) = D^k((JI)F''F'''\to(J'I)FF',T), \quad (24)$$

all the hyperfine depolarization rates associated to the $J = 1/2$ and $I = 3/2$ where $k = 2$ are

$$\begin{aligned}
D^2((JI)11;(JI)11,T) &= \frac{3}{16}\times(\zeta^0(J,T)-\zeta^1(J,T)) \qquad (25)\\
&= \frac{3}{16}\times D^1(J,T)\\
D^2((JI)11;(JI)22,T) &= \frac{\sqrt{60}-\sqrt{21}}{16}\times D^1(J,T)\\
D^2((JI)12;(JI)12,T) &= -\frac{3}{16}\times\zeta^0(J,T) - \frac{3}{16}\times\zeta^1(J,T)\\
D^2((JI)12;(JI)21,T) &= \frac{3}{16}\times D^1(J,T)
\end{aligned}$$

$$D^2((JI)12;(JI)11,T) = -\frac{3}{16}\times D^1(J,T)$$
$$D^2((JI)21;(JI)11,T) = \frac{3}{16}\times D^1(J,T)$$
$$D^2((JI)12;(JI)22,T) = -\frac{\sqrt{21}}{16}\times D^1(J,T)$$
$$D^2((JI)21;(JI)22,T) = \frac{\sqrt{21}}{16}\times D^1(J,T)$$
$$D^2((JI)22;(JI)22,T) = \frac{3}{16}\times D^1(J,T).$$

Of course we recall that by definition $D^{k=0}((JI)FF' \rightarrow (JI)F''F''',T) \equiv 0$ (see Eq. (10)). Using the indirect method, one can easily calculate the higher-order terms of $D^k((JI)FF' \rightarrow (J'I)F''F''',T)$ with $k > 2$ when they play a non-negligible role in the SEE. Note that the observed linear polarization spectrum is the footprint of only the even orders k of the atom, and thus only depolarization and polarization transfer rates with even k are needed to study such a spectrum.

6. Depolarization and polarization transfer rates of the levels of complex atoms with $l = 0$

The ionized alkaline earth metals Be II, Mg II, Ca II, Sr II, and Ba II in their ground states are simple ions because they have only one valence electron above a filled subshell. In contrast, the electronic configuration of a complex ion has one valence electron above an incomplete (open) subshell within the core. We denote by $\boldsymbol{L}_c$ the total orbital angular momentum of the core and by $\boldsymbol{S}_c$ its total spin.

6.1. Direct formulation

To infer the depolarization and polarization transfer rates of complex ions, we adopt the same strategy as for complex neutral atoms (Paper I). The orbital angular momentum of the valence electron is $\boldsymbol{l} = \boldsymbol{0}$ and the total angular momentum of the simple atom is $\boldsymbol{J} = \boldsymbol{s}$. The total orbital momentum of the atom is $\boldsymbol{L} = \boldsymbol{L}_c + \boldsymbol{l} = \boldsymbol{L}_c$. The total spin is $\boldsymbol{S} = \boldsymbol{S}_c + \boldsymbol{s}$ and $\boldsymbol{\mathcal{J}} = \boldsymbol{L} + \boldsymbol{S} = \boldsymbol{L}_c + \boldsymbol{S}$ is the total angular momentum of the complex ion. This coupling scheme is similar to the coupling scheme presented in Derouich et al. (2005a) for $l > 0$. Thus, the expression for the transition matrix elements of complex ions is easily obtained from the formulae given by Eq. (7) in Derouich et al. (2005a) if we make formal substitutions:

$$\langle \mathcal{J}M_{\mathcal{J}}|T(\text{complex})|\mathcal{J}'M_{\mathcal{J}'}\rangle = \tag{26}$$
$$(-1)^{\mathcal{J}+\mathcal{J}'+M_{\mathcal{J}}+M_{\mathcal{J}'}}\sqrt{(2\mathcal{J}+1)(2\mathcal{J}'+1)}$$
$$\times\sqrt{(2L_c+1)(2L_c+1)}\sum_{\mathcal{J}''}(2\mathcal{J}''+1)\begin{Bmatrix} S_c & S & J \\ L_c & S & \mathcal{J}' \\ J & \mathcal{J} & \mathcal{J}'' \end{Bmatrix}$$
$$\times\sum_{M_J,M'_J,M_{\mathcal{J}''}}\langle JM_J|T(\text{simple})|JM'_J\rangle\begin{pmatrix} J & \mathcal{J}' & \mathcal{J}'' \\ M'_J & M_{\mathcal{J}'} & M_{\mathcal{J}''}\end{pmatrix}$$
$$\times\begin{pmatrix} J & \mathcal{J} & \mathcal{J}'' \\ M_J & M_{\mathcal{J}} & M_{\mathcal{J}''}\end{pmatrix}.$$

Our collisional numerical code is adapted to the calculations of the depolarization rate of the level 4f 5d (^{3}F) 6s ($^4F_{3/2}$) of the Ce II complex ion[3]. For the Ce II state 4f 5d (^{3}F) 6s ^{4}F, we have $n^* = 2.274$, $L_c = 3$, $J = 1/2$, $L = 3$, $S = 3/2$, $S_c = 1$, and $\mathcal{J}$ takes the values 3/2, 5/2, 7/2, and 9/2. We calculate the collisional transition matrix $\langle JM_J|T(\text{simple})|JM'_J\rangle$ by solving the Schrödinger equation for the appropriate n^*, followed by the transition matrix $\langle \mathcal{J}M_{\mathcal{J}}|T(\text{complex})|\mathcal{J}'M_{\mathcal{J}'}\rangle$ according to Eq. (26) above, and thus we obtain the depolarization rates $D^2(\mathcal{J} = 3/2,\ T)$:

$$D^2(\mathcal{J} = 3/2,\ T) = 0.485\times 10^{-9}\, n_{\rm H}\left(\frac{T}{5000}\right)^{0.412}\ \text{s}^{-1}. \tag{27}$$

Any calculations of the depolarization and the transfer of the polarization rates involving complex ions must proceed level by level if one uses the above direct method. In the next section, we present and demonstrate an indirect method of quickly calculating all the rates of complex ions.

6.2. Indirect formulation

As we have shown in Paper I for neutral complex atoms, the collisional spherical tensor components associated to the $\mathcal{J}$-levels of a complex ion are:

$$\begin{aligned}\zeta^k(L\mathcal{J}\rightarrow L\mathcal{J}',T) &= \sum_{k_J=0}^{1}\zeta^{k_J}(J,T)\mathcal{A}^k(L\mathcal{J}\rightarrow L\mathcal{J}';k_J)\\ &= \zeta^0(J,T)\mathcal{A}^k(L\mathcal{J}\rightarrow L\mathcal{J}';0)\\ &\quad+\zeta^1(J,T)\mathcal{A}^k(L\mathcal{J}\rightarrow L\mathcal{J}';1),\end{aligned} \tag{28}$$

where the depolarization and polarization transfer rates are respectively:

$$\begin{aligned}D^k(\mathcal{J},T) &= \zeta^0(L\mathcal{J}\rightarrow L\mathcal{J},T)-\zeta^k(L\mathcal{J}\rightarrow L\mathcal{J},T)\\ D^k(\mathcal{J}\rightarrow\mathcal{J}',T) &= \zeta^k(L\mathcal{J}\rightarrow L\mathcal{J}',T)(\mathcal{J}\neq\mathcal{J}').\end{aligned} \tag{29}$$

Then, $\mathcal{A}^k(L\mathcal{J}\rightarrow L\mathcal{J}';k_J)$ is the depolarization coefficient of the state $|L\mathcal{J}\rangle$ of the complex atom, the expression for which is given in Eq. (28) of Paper I. Also, $\zeta^{k_J}(J,T)(k_J = 0,1)$ is given by Eq. (16) as a function of the effective quantum number n^*. Since

$$\begin{aligned}\zeta^0(L\,\mathcal{J}=3/2,T) &= 0.4\times\zeta^0(1/2,T)+0.6\times\zeta^1(1/2,T)\\ \zeta^2(L\,\mathcal{J}=3/2,T) &= 0.28\times\zeta^0(1/2,T)+0.72\times\zeta^1(1/2,T),\end{aligned} \tag{30}$$

then

$$D^2(\mathcal{J} = 3/2,\ T) = \zeta^0(L\,\mathcal{J}=3/2,T)-\zeta^2(L\,\mathcal{J}=3/2,T) =$$
$$0.12\times D^1(J,T) = 0.441\times 10^{-9}\, n_{\rm H}\left(\frac{T}{5000}\right)^{0.420}. \tag{31}$$

As expected, the values of $D^2(\mathcal{J} = 3/2,\ T)$ for Ce II calculated by the direct method (Eq. (27)) and those obtained via the indirect method (Eq. (31)) are in close agreement. In fact, the difference is 8%, slightly higher than the value of 4% obtained in the case of the hyperfine rates. We notice, however, that the difference can be attributed to the fact that individual detailed calculations are not perfectly reproduced by the simple power-law relations. In addition, the population and the alignment transfer

[3] As can be seen in Eq. (26), a given level of a complex atom/ion is mainly characterized by an effective principal quantum number n^*, by quantum numbers of the optical electron, and by the electrons in the core.

rates from $\mathcal{J} = 3/2$ to $\mathcal{J} = 5/2$ can be expressed respectively by:

$$D^0(\mathcal{J} = 3/2 \rightarrow \mathcal{J}' = 5/2,\ T) = 0.801 \times 10^{-9}\, n_{\rm H} \left(\frac{T}{5000}\right)^{0.420} \tag{32}$$

$$D^2(\mathcal{J} = 3/2 \rightarrow \mathcal{J}' = 5/2,\ T) = 0.588 \times 10^{-9}\, n_{\rm H} \left(\frac{T}{5000}\right)^{0.420}.$$

For the Nd II state $4f^4$ (^{5}I) 6s ^{6}I, $n^* = 2.253$, $L_c = 6$, $L = 6$, $S = 5/2$, $S_c = 2$, and $\mathcal{J}$ takes the values 7/2, 9/2, 11/2, 13/2, 15/2, and 17/2. The collisional depolarization rate of the level $\mathcal{J} = 7/2$ and the polarization transfer rates between $\mathcal{J} = 7/2$ and $\mathcal{J} = 9/2$ are given by:

$$D^2(\mathcal{J} = 7/2,\ T) = 0.135 \times 10^{-9}\, n_{\rm H} \left(\frac{T}{5000}\right)^{0.420} \tag{33}$$

$$D^0(\mathcal{J} = 7/2 \rightarrow \mathcal{J}' = 9/2,\ T) = 0.510 \times 10^{-9}\, n_{\rm H} \left(\frac{T}{5000}\right)^{0.420}$$

$$D^2(\mathcal{J} = 7/2 \rightarrow \mathcal{J}' = 9/2,\ T) = 0.468 \times 10^{-9}\, n_{\rm H} \left(\frac{T}{5000}\right)^{0.420}.$$

Similarly, all the other rates for the states of Ce II and Nd II can be estimated by simple calculations of the depolarization coefficients $\mathcal{A}^k(L\mathcal{J} \rightarrow L\mathcal{J}'; k_J)$ and the simple relations of Eq. (16).

To obtain the depolarization rates of hyperfine levels of a complex ion (if the complex ion has a nuclear spin), the procedure is exactly the same as the one illustrated in the Sect. 5 for simple ions.

7. Conclusion

We have presented a general, semi-classical method that may be used to determine a large number of the depolarization and the polarization transfer rates for the collisions of simple and complex ions in an arbitrary s-state with neutral hydrogen. The collisional depolarization of the lines of the hyperfine structured ions is fully treated. Simple power-law relations are given that constitute a powerful tool for obtaining accurate data quickly.

We have demonstrated how to calculate of the destruction rate of the alignment by two equivalent methods: a) the direct method of reference where the scattering matrix is calculated by solving the Schrödinger equation and integrations over the impact parameters and the relative velocities are performed; b) the useful indirect method based on the simple power-law relations for $D^1(J,T)$, $\zeta^0(J,T)$, and $\zeta^1(J,T)$ as a function of the effective quantum number n^*.

The comparison of our semi-classical destruction rate of orientation to the quantal rate obtained in the case of Ca II by Kerkeni et al. (2003) gives a very good agreement, the difference being only 4% at $T = 5000$ K.

The depolarization and polarization transfer rates obtained with our general approach are important ingredients for studies concerned with determining weak unresolved magnetic fields by their Hanle effect on the scattering polarization.

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