Collisional line broadening

versus

Collisional depolarization: Similarities and differences

S. Sahal-Bréchot[1] and V. Bommier[2]

1 *Observatoire de Paris, LERMA CNRS UMR 8112, France*
2 *Observatoire de Paris, LESIA CNRS UMR 8109, France*

Atomic polarization -1
What is atomic polarization?
And what is collisional depolarization?

What is "atomic polarization" ?

The Zeeman sublevels of the radiating atom are not in LTE:

Different populations (diagonal elements of the atomic density matrix) : $N(\alpha JM) \neq N(\alpha JM')$

Coherent superposition of states (off-diagonal elements of the density matrix)

Then the emitted line can be polarized

Needs: Anisotropy (or dissymmetry) of excitation of the levels:

e.g.Directive incident radiation

e.g.Directive collisional excitation

Modification of the atomic polarization:

Magnetic field vector (Hanle effect)

Anisotropic velocity fields

Isotropic collisions restore LTE (collisional depolarization)

Multiple scattering (not optically thin lines): depolarizing effect

Short remind -1-
Polarization matrix of radiation and Stokes parameters

E electric vector of the radiation

E_x

E

E_y

x

z

y

Radiation field propagating along z
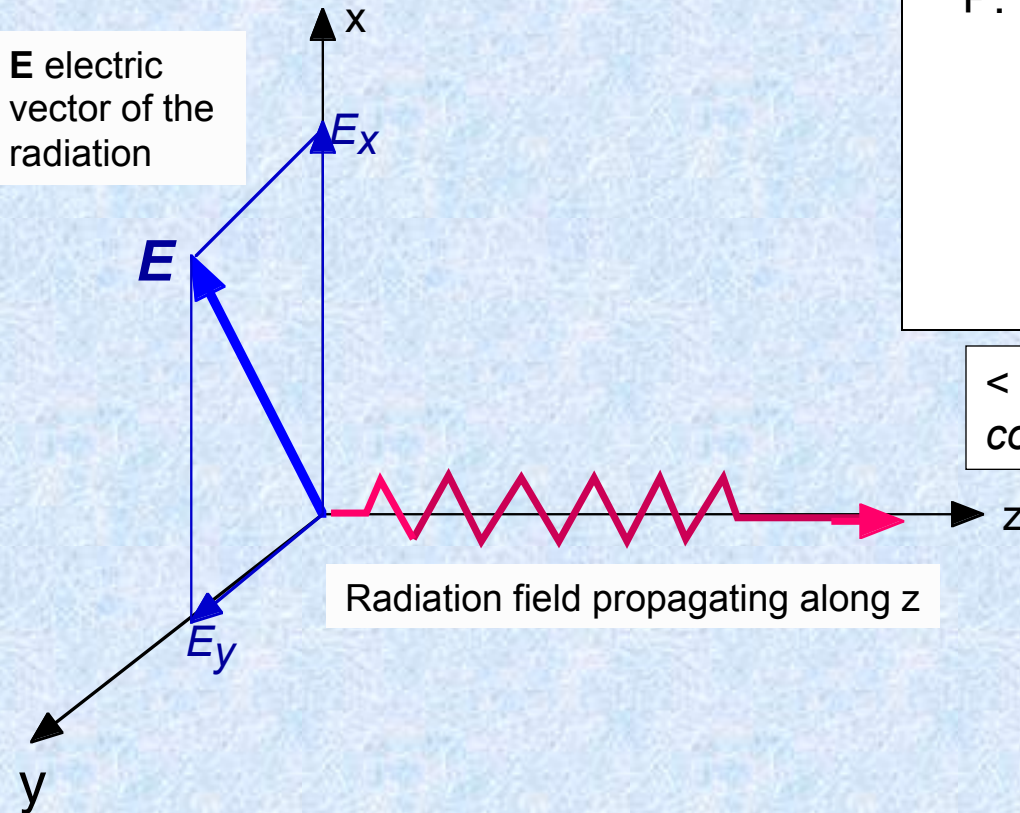
P: Polarization matrix

$$\Pi = \begin{pmatrix} \left\langle E_x(t)E^*_x(t) \right\rangle & \left\langle E_x(t)E^*_y(t) \right\rangle \\ \left\langle E_y(t)E^*_x(t) \right\rangle & \left\langle E_y(t)E^*_y(t) \right\rangle \end{pmatrix}$$

< …> = *average over a time interval large compared to the wave period*

Stokes Parameters:
$$\begin{cases} I = \Pi_{xx} + \Pi_{yy} \\ Q = \Pi_{xx} - \Pi_{yy} \\ U = \Pi_{xy} + \Pi_{yx} \\ V = i(\Pi_{xy} - \Pi_{yx}) \end{cases}$$

Short remind -2-
Physical meaning of the Stokes parameters

Intensity of the radiation: *I*

Measured Intensity: analyser axis *OX*, angle α with *Ox*:

$$I_X(\alpha) = \frac{1}{2}\left(Q\cos 2\alpha + U\sin 2\alpha + I \right)$$
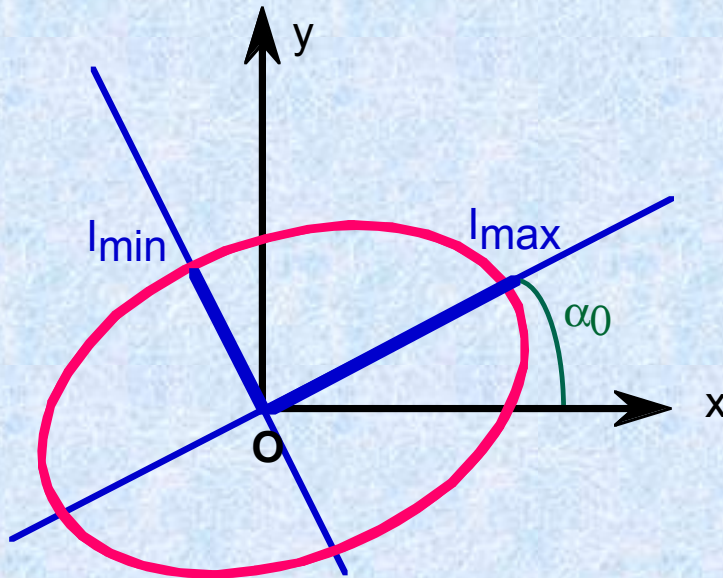
$$I_{\max} = \frac{1}{2}\left(I + \sqrt{Q^2 + U^2} \right)$$

$$I_{\min} = \frac{1}{2}\left(I - \sqrt{Q^2 + U^2} \right)$$

Circular polarization degree

I_- = right circular component = $\langle E_+(t)\, E^*_+(t) \rangle$

I_+ = left circular component = $\langle E_-(t)\, E^*_-(t) \rangle$

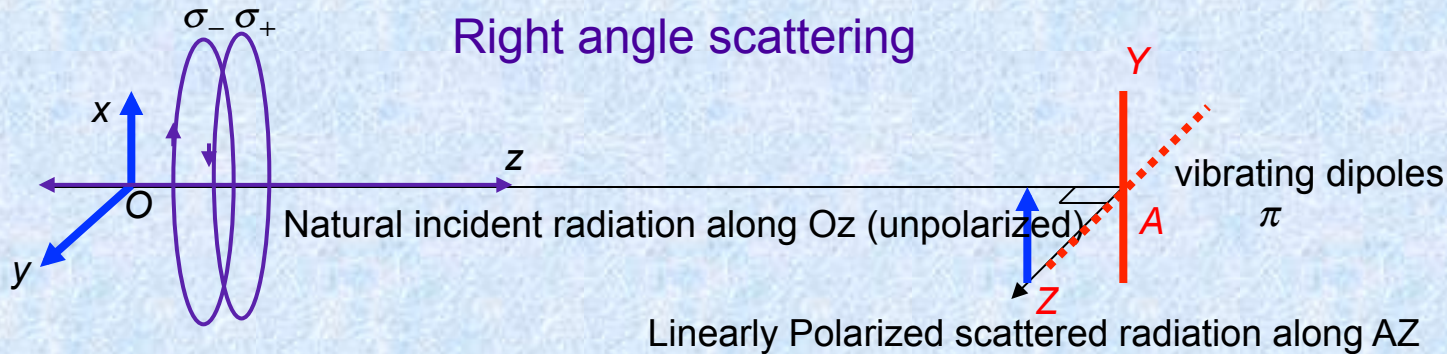$$p_c = \frac{I_- - I_+}{I_+ + I_-} = -\frac{V}{I}$$

- Linear polarization degree p_l
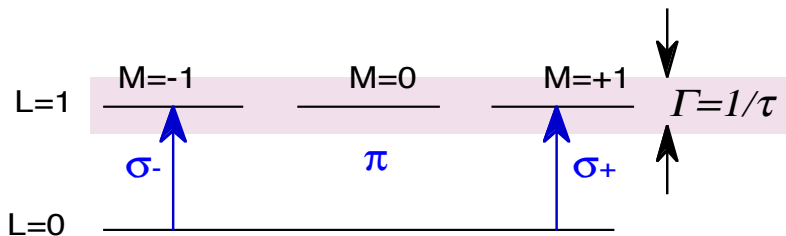**- polarization direction α_0 (within π)**

$$p_l = \frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}} = \frac{\sqrt{Q^2 + U^2}}{I}$$

$$\cos 2\alpha_0 = \frac{Q}{\sqrt{Q^2 + U^2}} \quad \text{et} \quad \sin 2\alpha_0 = \frac{U}{\sqrt{Q^2 + U^2}}$$

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Linear polarization due to radiative scattering: basic quantum interpretation

Right angle scattering

$\sigma_- \; \sigma_+$

x

O

z

y

Natural incident radiation along Oz (unpolarized)

Y

A

Z

vibrating dipoles

π

Linearly Polarized scattered radiation along AZ

Resonance scattering: quantum aspect (normal Zeeman triplet)

L=1   M=-1   M=0   M=+1 $\Gamma = 1/\tau$

σ- π σ+

L=0

•Quantization axis :Symmetry axis (direction of incident radiation) $\mapsto$ Zeeman LM states

•Photons σ_+ and σ_- excite the sublevels
    M=1 and M=-1 are equally populated.
    M=0 is not populated

*The Zeeman sublevels are **aligned***

•Polarization matrix of the scattered radiation mirrors that of the atomic excited level

•Projection on the direction of observation (AZ) $\mapsto$ Stokes Parameters of the observed radiation (linearly polarized along AY)

Polarization degree $\tau = \dfrac{3\eta \sin^2 \theta}{1 - \left(3\cos^2 \theta - 1\right)\eta}$

with $\eta = $ $(I_\pm - I_0)/(I_0 + 2I_\pm)$

$\eta = \dfrac{N(1\pm 1) - N(10)}{N(10) + 2N(1\pm 1)}$ *N(LM)* populations of the sublevels

Vocabulary:

Alignment : populations of M and -M are equal
➔ **linear polarization**

Orientation: Imbalance of populations of Zeeman sublevels M and -M
➔ **circular polarization**

Maximum polarization degree

J_{upper}	J_{lower}	p_{max}
1	0	1
0	1	0
1/2	3/2	0
3/2	1/2	3/7

Line broadening and Atomic polarization: brief survey of the theory

The density matrix ρ of the whole system is solution of the **Schrödinger equation**

$$H = H_A + H_{\mathrm{magn}} + H_B + H_{AB},$$

$$H_B + H_{AB} = H_R + H_{AR} + H_P + H_{AP},$$

$$i\hbar \frac{d\rho}{dt} = [H, \rho(t)];$$

$$\rho_A(t) = \mathrm{Tr}_B[\rho(t)],$$

$$\rho_B(t) = \mathrm{Tr}_A[\rho(t)].$$

A is the atomic subsystem

B is the bath of perturbers (P) and photons (R) and are assumed independent

H_A *gives the atomic wave functions (unperturbed) and the atomic energies*

The reduced density matrices $\rho_A(t)$ and $\rho_B(t)$ are not described by an hamiltonian and thus are not solution of a Schrödinger equation

They are solution of a **master equation**

Collisional line broadening: short survey of the theory

Intensity (Baranger 1958abc)

$$I = \frac{4\omega^4}{3c^3}\left|\langle f|\mathbf{d}|i\rangle\right|^2$$

$$I = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\omega s}\Phi(s)\,\mathrm{d}s,$$

$$\Phi(s) = \mathrm{Tr}\left[\mathbf{d}\, T^*(s)\mathbf{d}\, T(s)\rho\right].$$

ρ is the density matrix of the system: atom (A)+ bath B (R photons, P perturbers)

$\mathbf{d}$ is the atomic dipole moment

$T(s)$ the evolution operator of the system

Two keys approximations:

- **No back reaction**: $\rho = \rho_A \otimes \rho_B$
- **Impact approximation**

    Mean duration of an interaction <<mean interval between two interactions

$\rho_R(t)$ and $\rho_P(t)$ are decoupled and their interactions with the atom are decoupled
⇒The atom-perturber **interaction** is **complete** (no emission of photon during the time of interest). The collisional S-matrix will appear

The calculation of the line profile becomes an application of the theory of **collisions**

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Collisional broadening: short survey of the theory Isolated lines

No overlap of close levels
(with $\Delta l=1$ for electron impacts) due to collisional level-widths

$\Rightarrow$**The profile is lorentzian**

$$I(\omega) = \rho_A\left(\alpha_i J_i\right)\frac{4\omega^4}{3c^3}F(\omega)$$

$$F(\omega) = \frac{1}{\pi}\int_0^\infty e^{i\omega s}\Phi(s)ds$$

$$\Phi(s) = e^{-(w+id)s}$$

ρ_A is the atomic density matrix

Without polarization: only diagonal elements:
- LTE: Boltzman factor,

- Out of LTE, its elements are solutions of the statistical equilibrium equations (collisional radiative model

Emissivity = Profile x Population of the upper level
This is **complete redistribution**

Baranger's formula for an isolated line $i(\alpha_i J_i) - f(\alpha_f J_f)$

Tr$_P$: trace over the perturbers, i.e. average over all perturbers =

$$N_P \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho \, d\rho \oint \frac{d\Omega}{4\pi}$$

$$w + i d = N_P \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho \, d\rho \left\langle 1 - S_{ii} S_{ff}^* \right\rangle_{angular\,average}$$

$$= N_P \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho \, d\rho \times$$

$$\left[1 - \sum_{\substack{M_i M'_i \\ M_f M'_f \\ \mu}} (-1)^{2J_f + M_f + M'_f} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & \mu & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M'_i & \mu & M'_f \end{pmatrix} \times \right.$$

$$\left. \left\langle \alpha_f J_f M_f \left| S* \right| \alpha_f J_f M'_f \right\rangle \left\langle \alpha_i J_i M_i \left| S \right| \alpha_i J_i M'_i \right\rangle \right]$$

The scattering *S* matrix is symmetric and unitary

expression of the Baranger's formula for the width

With the *T* matrix: *T*=1-*S,* and using *T*T*= 2 Re *(T)*

$$W = 2w = N_P \int v f(v) \mathrm{d}v \left[\left(\sum_{\alpha J} \sigma\left(\alpha_i J_i \to \alpha J\right) + \sum_{\alpha' J'} \sigma\left(\alpha_f J_f \to \alpha' J'\right) \right) - 2\,\mathrm{Re} \int_0^\infty 2\pi \rho\, \mathrm{d}\rho \times \left[1 - \sum_{\substack{M_i M'_i \\ M_f M'_f \\ \mu}} (-1)^{2J_f + M_f + M'_f} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & \mu & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M'_i & \mu & M'_f \end{pmatrix} \times \left\langle \alpha_f J_f M_f \left| T * \right| \alpha_f J_f M'_f \right\rangle \left\langle \alpha_i J_i M_i \left| T \right| \alpha_i J_i M'_i \right\rangle \right] \right]$$
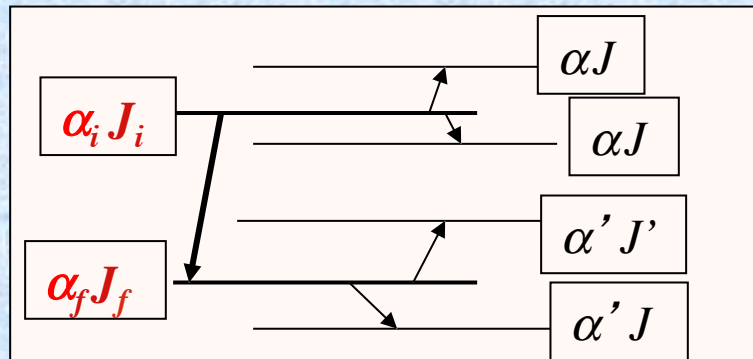
Atomic polarization:
brief survey of the theory
calculation of the atomic density matrix

1- H_A gives the atomic wave functions (unperturbed)

      and the atomic energies

*2-**Same key approximations as for collisional line broadening***:

• First key approximation: **no back reaction**

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

• Second key approximation: the **impact approximation**

    Mean duration of an interaction <<mean interval between two interactions

    $\Rightarrow \rho_R(t)$ and $\rho_P(t)$ are decoupled and their interactions with the atom are decoupled

−4- The atom-perturber **interaction** is **complete** during the time of interest (S-matrix appears)

−5 **Markov approximation**: evolution of $\rho_A(t)$ only depends $\rho_A(t_0)$ on and not on his past history

−6 **Secular approximation**

Atomic polarization:
brief survey of the theory:
calculation of the atomic density matrix

7-The radiation is weak:

Perturbation theory sufficient for atom radiation interaction

8-Consequence of Second order perturbation theory + Markov:

Transitions can only be done with exact resonance in energy,

so:

Profile cannot be taken into account: δ-profile

Atomic polarization is a global information

Atomic polarization:
brief survey of the theory:
processes to take into account in the calculation of the atomic density matrix

Atomic polarisation (master equation):

•Excitation by anisotropic process responsible for the polarization (**only alignment in astrophysics and thus only linear polarization**) : radiation or beam of particles (energetic electrons, protons)
  Quantization axis in the direction of the preferrred excitation

•Excitation by radiative or isotropic collisional processes (decrease alignment)

•Breakdown of the cylindrical symmetry: apparition of coherences in the master equation and thus modification of the degree and direction of polarization

  •e.g. interaction with a magnetic field B: Hanle effect. *Quantization axis in the direction of **B***

•**Depolarization and transfer of alignment by isotropic collisions**

•Followed by deexcitation (radiative and collisional)

•*If the (hyper)fine levels are separated (no overlap by the lifetime), the atomic polarization is different for the different (hyper)fine lines*

Atomic polarization: brief survey of the theory:
expression of the atomic density matrix and of the radiation polarization matrix

•At the stationary state $\rho_A(t) = \rho_A$
ρ_A**is solution of the "statistical equilibrium equations"** leading to populations (diagonal elements of ρ_A) and coherences (off-diagonal elements pf ρ_A) in the standard *JM* representation

•and at the stationary state
$\rho_R(t) = \rho_R$
$\Rightarrow$**The matricial transfer equation** of the Stokes operators *(I Q U V)*

Case of a two-level atom without polarization of the lower level in the irreducible tensorial T^K_Q representation
Master equation for the atomic density matrix:

$$\frac{d}{dt}\left(\sqrt{2J'+1}\,^{bb}\rho_Q^K\right) =$$
$$-i\omega_L g_{J'}Q\sqrt{2J'+1}\,^{bb}\rho_Q^K$$
$$+B_{ab}\sqrt{2J+1}\,^{aa}\rho_0^0$$
$$\times \int d\nu_1\,(-1)^Q\,\Phi_Q^{K,K'}(J,J';\nu_1)\,J_{-Q}^{K'}(\nu_1)\,,$$
$$-\sqrt{2J'+1}\,^{bb}\rho_Q^K\left(A_{ba}+C_{ba}+D_b^{(K)}\right)$$
$$+\sqrt{2J+1}\,^{aa}\rho_0^0 C_{ab}\delta_{K,0}\delta_{Q,0}$$

Population: K=0
Orientation: K=1
Alignment: K=2
Coherences: Q≠0

Examples of expressions

Rates beween the Zeeman sublevels
(standard atomic basis αJM)

Angular average : Gordeyev et al. (1969, 1971), Masnou-Seeuws & Roueff (1972), Omont (1977), Sahal-Bréchot (1974), Sahal-Bréchot et al. (A&A 2007)

$$\langle P(\alpha JM \rightarrow \alpha' J' M') \rangle_{\text{Ang Av}} = |\langle \alpha JM |T| \alpha' J' M' \rangle|^2_{\text{Ang Av}} =$$

$$\sum_{mm'nn'} \sum_{K=|J-J'|}^{J+J'} (2K+1) \sum_x \begin{pmatrix} J & J' & K \\ M & M' & x \end{pmatrix} \sum_k \begin{pmatrix} J & J' & K \\ m & n' & k \end{pmatrix} \begin{pmatrix} J & J' & K \\ n & m' & k \end{pmatrix} \langle \alpha Jm| T | \alpha' J' m' \rangle \langle \alpha Jn| T | \alpha' J' n' \rangle^* .$$

The summations over x and k are reduced to only a single term, owing to the selection rules over the "3-j" symbols:

$x = -(M + M')$, and $m + n' = n + m' = -k$.

Examples of expressions
(cf. for instance Sahal-Bréchot et al. (A&A 2007)

T^k_q basis (irreducible tensorial operators)

- **Master equation: off-diagonal elements**

$$P^k(\alpha J \to \alpha' J') = \sum_{\mu\mu'\nu\nu'} \langle \alpha J\mu |T| \alpha' J'\mu' \rangle \langle \alpha J\nu |T| \alpha' J'\nu' \rangle^* (-1)^{J-J'} \sum_x (-1)^{\nu-\nu'} \begin{pmatrix} J & J & k \\ \nu & -\mu & x \end{pmatrix} \begin{pmatrix} J' & J' & k \\ \nu' & -\mu' & x \end{pmatrix}, \qquad (14)$$

where the T-matrix can now be calculated in any frame. We note that $\nu - \mu = \mu' - \nu'$, owing to the selection rules on the "3-j" coefficients.

- **Master equation:diagonal elements:**
  Sum of contributions of
  - elastic collisions (*k*-pole depolarization rates)
  - inelastic collisions (relaxation rates,independent of *k*): loss terms

$$P^k(\alpha J) + \sum_{\alpha' J' \neq \alpha J} P(\alpha J \to \alpha' J') =$$

$$- \sum_{\substack{M \\ M' \neq M}} (2k+1)(-1)^{M-M'} \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix} \begin{pmatrix} J & k & J \\ -M' & 0 & M' \end{pmatrix} \langle P(\alpha JM \to \alpha JM') \rangle_{\text{Ang Av}}$$

$$+ \sum_{\substack{M \\ \alpha' J' M' \\ \text{and } M \neq M' \text{ if } \alpha J = \alpha' J'}} (2k+1) \begin{pmatrix} J & k & J \\ -M & 0 & M \end{pmatrix}^2 \langle P(\alpha JM \to \alpha' J'M') \rangle_{\text{Ang Av}} . \qquad (23)$$

The contribution of elastic collisions ($\alpha J = \alpha' J'$) in Eq. (23) is equal to $P^k(\alpha J)$, the depolarization probability due to elastic collisions. The contribution of inelastic collisions leads to the relaxation probability $\sum_{\alpha' J' \neq \alpha J} P(\alpha J \to \alpha' J')$.

Collisions with neutral Hydrogen broadening and depolarization
- Calculation of the S-matrix
- the interaction potential

1. Semiclassical approximation is sufficient :
        classical path for the perturber

1. Perturbation expansion of the S-matrix is not valid:
        Close-coupling necessary:
        First order semiclassical differential equations to solve

3. Long range expansion (Van der Waals) not valid
        Typical impact parameters 10–20 a_0

4. Integration over the impact parameter:
        A lower cutoff has to be introduced

From hydrogen collisional broadening to depolarization: the ABO method

Nineties: Line broadening by collisions with neutral hydrogen: a new and powerful approximate method: the so-called ABO method

O'Mara and Anstee, Barklem:(Anstee & O'Mara 1991, 1995, 1997; Barklem & O'Mara 1997, Barklem et al. 1998ab, 2000)

- **Semiclassical close-coupling theory**
- **Approximate interaction potential** : time-independent second-order perturbation theory without exchange, Unsöld approximation, allowing the Lindholm-Foley average over *m* states to be removed
  (Brueckner 1971; O'Mara 1976)

2000-2007: Extension of this method to line depolarization
Derouich, Sahal-Bréchot & Barklem, A&A 2003, 2004ab, 2005ab, 2007
Derouich, thesis 2004, Derouich 2006, Derouich & Barklem 2007
Good results when compared to quantum chemistry calculations (20%)

Broadening and Depolarization by isotropic collisions

The fine structure (and a fortiori hyperfine structure) can be most often neglected during the collision in astrophysical conditions (high temperatures): The spin has no time to rotate during the collision time

⇒ if LS coupling is valid, the fine structure components have the same width and shift, that of the multiplet.

For collisional depolarization rates the linear combinations of the *T*-matrix elements are different from those of the width
And expressions between J levels are required

Diagonal elements of the S-matrix appear in the broadening formula and do not play a role in depolarization

Numerical calculations have to be performed both for broadening and for depolarization.

No analytical relation (even approximate) between the collisional width and the disalignment, disorientation, alignment transfer, and orientation transfer collisional rates.

Beyond the impact and Markov approximation for atom-radiation interaction

Coupling of the atomic density matrix to the line profile and redistribution of radiation:

First work by Bommier A&A 1997: two level atom with unpolarized lower level

Higher orders of the perturbation development of the atom-radiation interaction taken into account:
⇒two photons can interact with the atom at the same time (resonant scattering)

Beyond the Markov approximation:
⇒the past memory is taken into account
⇒the lifetimes are no longer ignored

⇒ Introduction of the line profile in the master equation and thus in the Stokes parameters of the observed line

Thank you for your attention

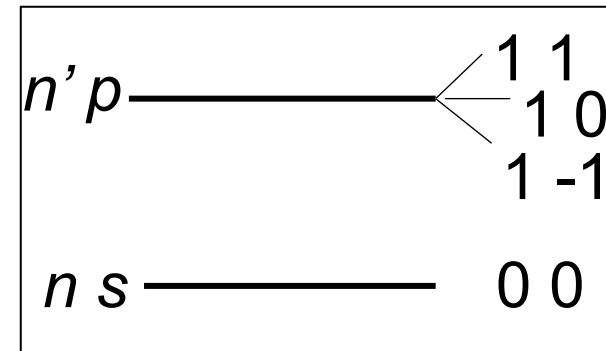# Broadening and Depolarization by isotropic collisions example of collisions with neutrals (Hydrogen)

N.B. remind : T-matrix is symmetric, $<JM|T|J'M'>=<J'M'|T|JM>$
and $|<JM|T|J'M'>|^2_{Ang.Av}= |<J-M|T|J'-M'>|^2_{Ang.Av}$

For collisions with neutrals The **quenching is negligible**.
Processes to take into account: **elastic** and **fine structure inelastic** collisions

Example : normal Zeeman triplet: p-s transition without spin: $n\ p\ ^1P^o_1 - n'\ s\ ^1S_0$

$J_i=1$, $M_i=0\pm1$ (upper level)   Notation: $<1M|T|1M'>= T_{MM'}$
$J_f=0$, $M_f=0$ (lower level) $<00|T|00>=t_{00}$

Disorientation $D^{(1)} \propto |T_{01}|^2_{Ang.Av}+2|T_{-1+1}|^2_{Ang.Av}$
Disalignment $D^{(2)} \propto 3|T_{01}|^2_{Ang.Av}$

$$
\begin{array}{ll}
n'\,p & \underset{}{\overbrace{}} \begin{array}{l} 1\ 1 \\ 1\ 0 \\ 1\ -1 \end{array} \\
\\
n\,s & \underline{} \qquad 0\ 0
\end{array}
$$

Particular case: one state case*: $t_{00}=0$ (does not work wit collisions with H)
width= elastic collision rate of the upper level:

$$
2w \propto \frac{1}{3}\sum_{MM'}|T_{MM'}|^2 = \frac{1}{3}\left[2|T_{01}|^2+2|T_{-11}|^2+2|T_{0-1}|^2\right]+\frac{1}{3}\left[|T_{00}|^2+|T_{11}|^2+|T_{-1-1}|^2\right]=\left|\langle1|T|1\rangle\right|^2
$$

$$
2w \propto (1/3)\,[\,4\,|T_{01}|^2_{Ang.Av}+2\,|T_{-1+1}|^2_{Ang.Av}\,] + (1/3)\,[T_{-1-1}|^2_{Ang.Av}+[T_{11}|^2_{Ang.Av}+[T_{00}|^2_{Ang.Av}\,]
$$

Broadening and Depolarization by isotropic collisions example of collisions with neutrals (Hydrogen) (following)
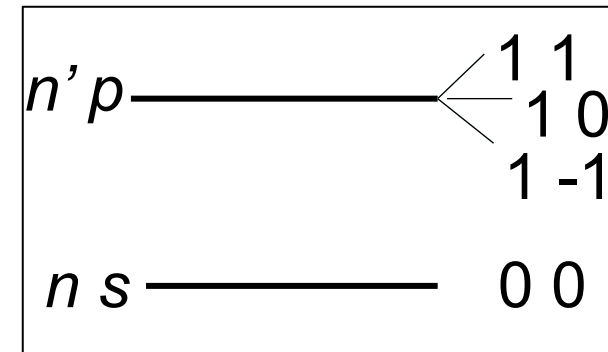
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and │<JM│T│J'M'>│$^2_{Ang.Av}$= │<J-M│T│J'-M'>│$^2_{Ang.Av}$

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J_i=1, M_i= 0±1 (upper level) Notation: <1M│T│1M'>= $T_{MM'}$
J_f=0, M_f=0 (lower level) <00│T│00>=t_{00}

Disorientation $D^{(1)} \propto |T_{01}|^2_{Ang.Av} + 2|T_{-1+1}|^2_{Ang.Av}$
Disalignment $D^{(2)} \propto 3|T_{01}|^2_{Ang.Av}$

$$
\begin{array}{ll}
n'p\ \rule{3cm}{0.4pt} & \begin{array}{l} 1\ 1 \\ 1\ 0 \\ 1\ \text{-}1 \end{array} \\
\\
n\ s\ \rule{3cm}{0.4pt} & 0\ 0
\end{array}
$$

General case: two state case: t_{00}≠0 *(case of collisions with H)*
width= elastic collision rate of the upper level+elastic collision rate of the lowerr level+
interference term

$$2w \propto \left|\langle 1|T|1\rangle\right|^2 + \left|\langle 0|T|0\rangle\right|^2 - 2\mathrm{Re}\left[1 - \frac{1}{3}t_{00}\left(T_{11} + T_{-1-1} + T_{00}\right)\right]$$