XTAT, a new multilevel-multiline polarized radiative transfer code with PRD

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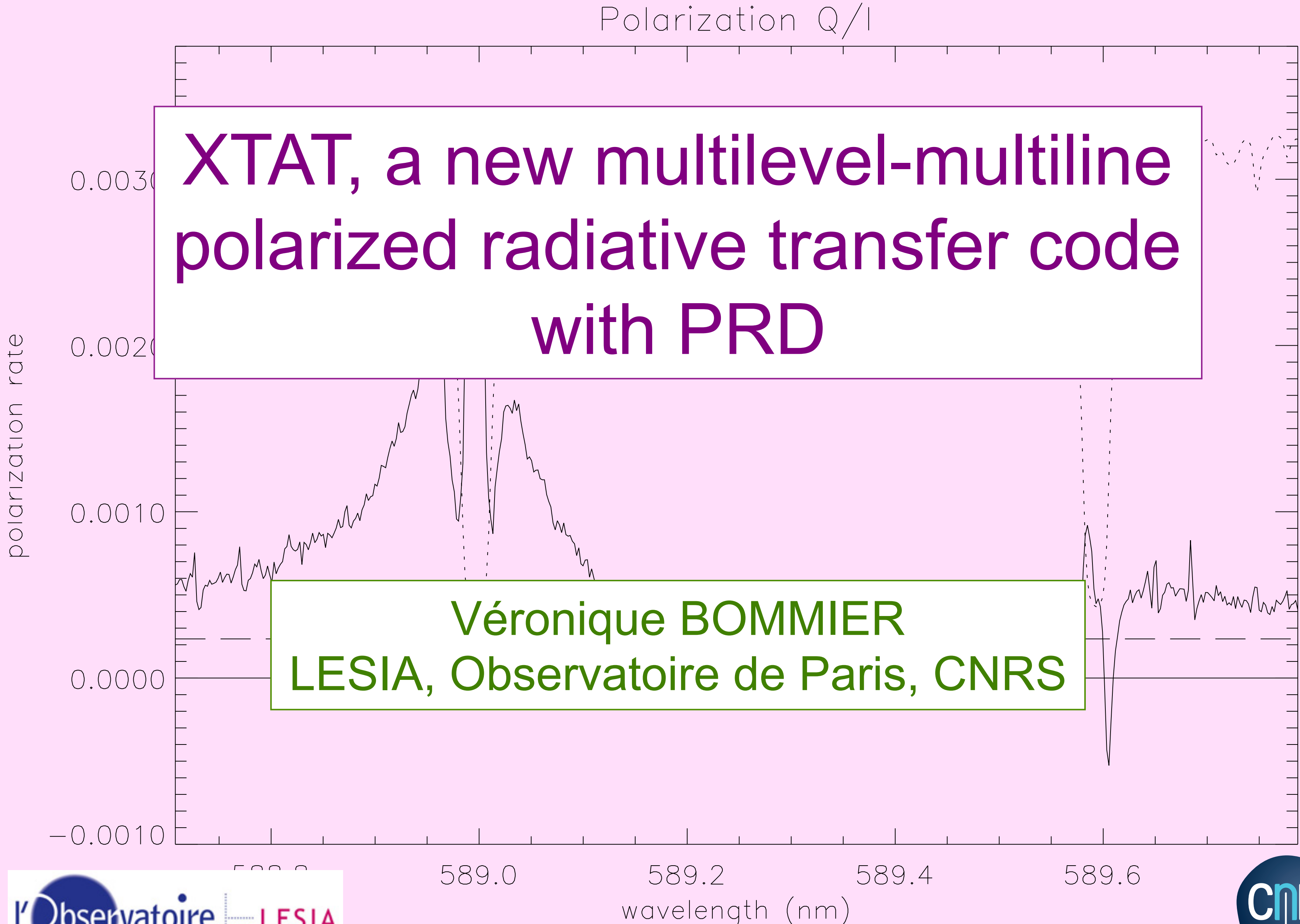


COST Action MP1104, Prague, 5-9 May 2014

Objective

– Modeling the line profile formation **including polarization**

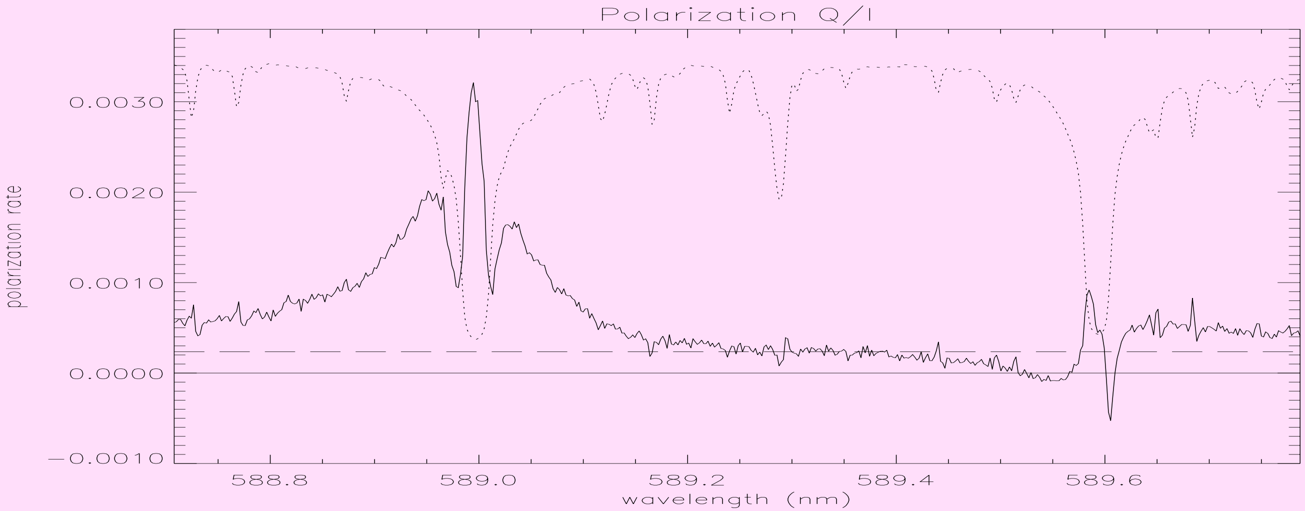
Magnetic field, multilevel-multiline, polarization profile, far wings

Solving the coupled statistical equilibrium and radiative transfer equations, for the polarized atom

– Interpreting the **Second Solar Spectrum** (Stenflo, 1996)

Linear polarization formed by scattering and observed inside the solar limb

Na I D lines



from Bommier & Molodij, 2002, A&A 381, 241, THEMIS observation

– 30% of the lines display a M-type polarization profile with far wings

Belluzzi & Landi Degl'Innocenti, 2009, A&A 495, 577, & Belluzzi's PhD

Going out of the 2-level approximation

is solving the system of statistical equilibrium equations (SEE)

But how taking into account the partial redistribution (PRD) ?

The SEE accounts for
- absorption
- emission

But how taking into account
- absorption *followed* by emission ?
- how the system may have "memory" ?

Answer:
- by going out of the "short memory" approximation
- i.e., by overcoming the Markov approximation

  (Bommier, 1997, A&A 328, 706 & 726)

This will also help for line profiles in SEE

The Markov approximation

Hamiltonian atom+radiation: $H = H_0 + V$

Schrödinger equation in interaction representation: $i\hbar \frac{d}{dt}\tilde{\rho}(t) = \left[\tilde{V}(t), \tilde{\rho}(t)\right]$

which can be integrated in: $\tilde{\rho}(t) = \tilde{\rho}(0) + \frac{1}{i\hbar}\int_0^t \left[\tilde{V}(t-\tau), \tilde{\rho}(t-\tau)\right] d\tau$

Markov approximation: $\tilde{\rho}(t) = \tilde{\rho}(0) + \frac{1}{i\hbar}\int_0^t \left[\tilde{V}(t-\tau), \tilde{\rho}(t)\right] d\tau$

– Physical meaning: ρ does not keep memory of his past history

Validity: the characteristic ρ evolution time Γ^{-1} >> the interaction correlation time τ_c
Cohen-Tannoudji (1975): the validity condition is fulfilled for weak radiation field

Consequence: the ρ finite life-time Γ^{-1} is not taken into account in the process
the line width, or profile, is discarded from the formalism
at its place, one has

$$\int_0^{+\infty} e^{-(\omega-\omega_0)\tau} d\tau = \frac{1}{2}\delta(\omega-\omega_0) + i P(\omega-\omega_0)$$

P : Cauchy Principal Value

Overcoming the Markov approximation

The Markov approximation intervenes in a perturbation development

Reporting the integral equation in the differential one

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}(t)=\frac{1}{\mathrm{i}\hbar}\left[\tilde{V}(t),\tilde{\rho}(0)\right]-\frac{1}{\hbar^2}\int_0^t\left[\tilde{V}(t)\left[\tilde{V}(t-\tau),\tilde{\rho}(t-\tau)\right]\right]\mathrm{d}\tau$$

Markov approximation closes the development:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}(t)=\frac{1}{\mathrm{i}\hbar}\left[\tilde{V}(t),\tilde{\rho}(0)\right]-\frac{1}{\hbar^2}\int_0^t\left[\tilde{V}(t)\left[\tilde{V}(t-\tau),\tilde{\rho}(t)\right]\right]\mathrm{d}\tau$$

Getting out of the Markov approximation is reporting several times the integral equation
This is pursuing the perturbation development

at order-4:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}(t)=\frac{1}{\hbar^4}\int_0^t\mathrm{d}\tau\int_0^{t-\tau_1}\mathrm{d}\tau\int_0^{t-\tau_1-\tau_2}\mathrm{d}\tau\left[\tilde{V}(t),\left[\tilde{V}(t-\tau_1),\left[\tilde{V}(t-\tau_1-\tau_2),\left[\tilde{V}(t-\tau_1-\tau_2-\tau_3),\tilde{\rho}(t-\tau_1-\tau_2-\tau_3)\right]\right]\right]\right]$$

Markov approximation closes again the development

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}(t)=\frac{1}{\hbar^4}\int_0^t\mathrm{d}\tau\int_0^{t-\tau_1}\mathrm{d}\tau\int_0^{t-\tau_1-\tau_2}\mathrm{d}\tau\left[\tilde{V}(t),\left[\tilde{V}(t-\tau_1),\left[\tilde{V}(t-\tau_1-\tau_2),\left[\tilde{V}(t-\tau_1-\tau_2-\tau_3),\tilde{\rho}(t)\right]\right]\right]\right]$$

and so on.

Resummation

The statistical equilibrium equation remains the same as usual, except that
in place of the δ function, at the profile place, appears a quantity of the generic form

Perturbation development manually written

$$\varphi\left\{1-\frac{A_{ba}}{2}\varphi+\frac{A_{ba}^2}{2^2}\varphi^2-\frac{A_{ba}^3}{2^3}\varphi^3+\dots\right\}$$

One sees that it behaves as

$$\varphi\left\{\sum_{n=0}^{\infty}\left[-\frac{A_{ba}}{2}\varphi\right]^n\right\}$$

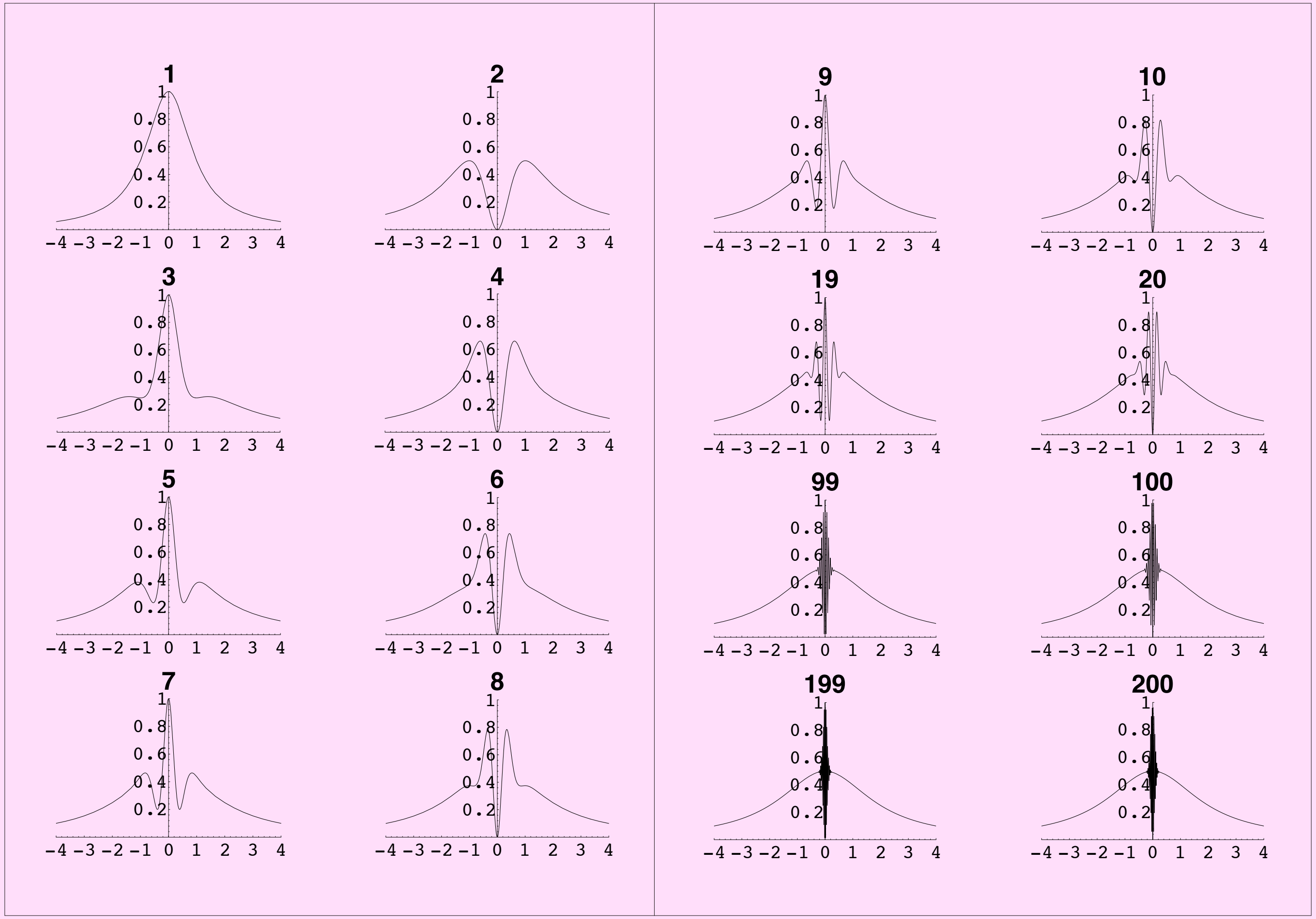
which can be resummed in

$$\frac{\varphi}{1+\frac{A_{ba}}{2}\varphi}$$

which introduces A_{ba} as a half-half-width in the profile

The resummed theory is non-perturbative

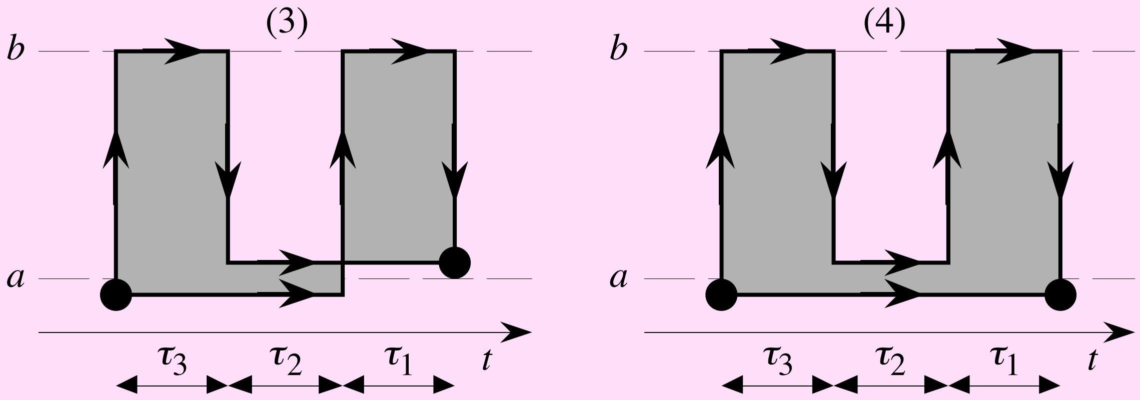
Resummation effect on the line width



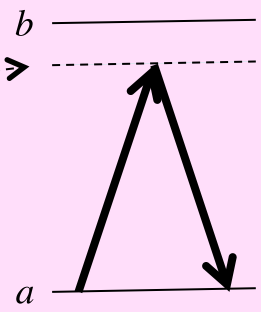
the resummation broadens the line

2^{nd} effect: new term at order-4 in the emissivity

New processes appear at order-4, that can be represented as:



The two transition amplitude do not stay at the same time in the upper level b



The b level is « never populated », or « virtual »
There is no absorption, nor emission
There is only scattering, with frequency conservation
This is Rayleigh scattering (can be generalized to Raman scattering)
This intervenes in the far wings

There is frequency coherence between the « absorbed » and the « emitted » photons,
Such a coherence which was rendered impossible by the Markov approximation

Bibliography

– this theory, for a 2-level atom, with polarization and magnetic field
Bommier, V., 1997, A&A, 328, 706 & 726
+ Bommier, V., 1999, ASSL 243 (SPW2), 43
for Raman scattering and Doppler redistribution
(the statistical equilibrium has to be solved for each velocity class of the atoms)

– full agreement about the redistribution functions
and the physical description of the Rayleigh scattering
with Omont, Smith, Cooper, 1972, ApJ, 175, 185

– previous papers make use of the emissivity developed in two terms,
but from empirical derivation
Hubeny, Oxenius, Simonneau, 1983, JQSRT, 29, 495
Hubeny, I., 1985, Bull. Astron. Inst. Czechosl., 36, 1
Hubeny & Lites, 1995, ApJ, 455, 376
Uitenbroek, H., 1989, A&A, 213, 360

SEE: Statistical Equilibrium Equations

Atomic Density Matrix

Evolution of a coherence between the levels (J_1M_1) and $(J_1'M_1')$, α_1 representing the other quantum numbers, of a mean atom at position $\vec{r}$ with velocity $\vec{v}$

$$\frac{d}{dt}\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}(\vec{r},\vec{v}) =$$

$$-\frac{i}{\hbar}\left[E(\alpha_1 J_1 M_1) - E(\alpha_1 J_1' M_1')\right]\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}(\vec{r},\vec{v}) \qquad \text{Hanle effect term}$$

$$+\sum_{\alpha_2 J_2 J_2' M_2 M_2'} \Gamma_{\alpha_1 J_1 J_1' M_1 M_1' \leftarrow \alpha_2 J_2 J_2' M_2 M_2'}\,{}^{\alpha_2 J_2 J_2'}\rho_{M_2 M_2'}(\vec{r},\vec{v}) \qquad \text{"populating" contributions}$$

$$-\frac{1}{2}\sum_{J_1'' M_1''}\left\{\sum_{\alpha_2 J_2 M_2} \Gamma_{\alpha_2 J_2 J_2 M_2 M_2 \leftarrow \alpha_1 J_1'' J_1 M_1'' M_1}\,{}^{\alpha_1 J_1'' J_1'}\rho_{M_1'' M_1'}(\vec{r},\vec{v}) \right. \qquad \text{"depopulating" contributions}$$

$$\left. + \sum_{\alpha_2 J_2 M_2} \Gamma_{\alpha_2 J_2 J_2 M_2 M_2 \leftarrow \alpha_1 J_1' J_1'' M_1' M_1''}\,{}^{\alpha_1 J_1 J_1''}\rho_{M_1 M_1''}(\vec{r},\vec{v}) \right\}$$

What about the atomic velocity ?
The Doppler redistribution

The atomic velocity is an external freedom degree

In solar conditions, velocity-changing collisions are rare.
The time between two such collisions >> the level radiative lifetime

It can be shown (Sahal-Bréchot, Bommier, Feautrier, 1998, A&A 340, 579
that the SEE have to be solved for each velocity class,
i.e. for each density matrix $\rho(\vec{v})$

The line profile in SEE is the one in the atomic frame,
in which the atomic velocity is taken into account by the Doppler effect

$$\tilde{\nu} = \nu\left(1 - \frac{\vec{\Omega}\cdot\vec{v}}{c}\right)$$

Radiation Field Tensors

Landi Degl'Innocenti, 1983, Solar Phys. 85, 3

$$J_{qq'}(\nu) = \oint \frac{d\vec{\Omega}}{4\pi} \sum_{i=0}^{3} \mathscr{T}_{qq'}(i, \vec{\Omega})\, S_i(\nu, \vec{\Omega})$$

$q, q' = -1, 0, +1$

i : reference index for Stokes parameters $i = 0, \ldots, 3$

ν : radiation frequency

$\vec{\Omega}$: radiation propagation direction

$S_i(\nu, \vec{\Omega})$: Stokes parameter i at frequency ν propagating along $\vec{\Omega}$

$\mathscr{T}_{qq'}(i, \vec{\Omega})$: spherical tensor for polarimetry defined by Landi Degl'Innocenti (1983, Table II)

Fine-structure algebra

$$X\left(\alpha_2 J_2 J_2' \to \alpha_1 J_1 J_1'\right) =$$

$$(-1)^{J_1' - J_1 + J_2' - J_2} \sqrt{(2J_1+1)(2J_2+1)(2J_1'+1)(2J_2'+1)}$$

$$\times (2L_2+1) \begin{Bmatrix} J_1 & 1 & J_2 \\ L_2 & S & L_1 \end{Bmatrix} \begin{Bmatrix} J_1' & 1 & J_2' \\ L_2 & S & L_1 \end{Bmatrix}$$

(analogous expression for hyperfine structure)

Line profiles

Lorentz

$$\tfrac{1}{2}\Phi_{ba}\left(\nu_0-\nu\right)=\frac{1}{\gamma_{ba}+i\left(\omega_0-\omega+\Delta_{ba}\right)}$$

with $\int \Phi_{ba}\left(\nu_0-\nu\right)\ d\nu=1$

$\omega=2\pi\nu$ is the pulsation

Δ_{ba} is a shift term due to the interaction

$b,a:$ line upper and lower level

$\gamma_{ba}=\tfrac{1}{2}\left(\Gamma_R+\Gamma_I+\Gamma_E\right):$ radiative and collisional line broadening

$\nu_0\ (\omega_0):$ line central frequency (pulsation)

Level profiles
Lorentz

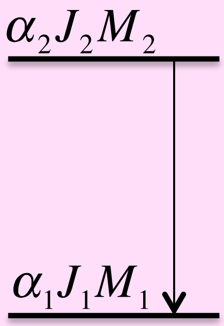
$$\tfrac{1}{2}\Phi_a(\nu_1-\nu_2)=\frac{1}{\gamma_a+i(\omega_1-\omega_2)}$$

with $\int \Phi_a(\nu_1-\nu_2)\ d\nu_1=1$

$\omega=2\pi\nu$ is the pulsation

$a:$ one level

$\gamma_a=(\Gamma_R+\Gamma_I):$ radiative and collisional level broadening



Radiative Transition Probabilities

spontaneous emission

$$\Gamma^{\mathrm{sp}}_{\alpha_1 J_1 J_1' M_1 M_1' \leftarrow \alpha_2 J_2 J_2' M_2 M_2'} =$$

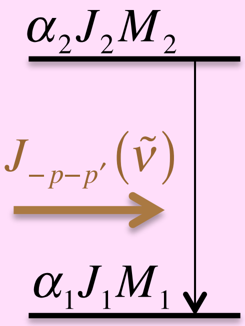
$$X\left(\alpha_2 J_2 J_2' \to \alpha_1 J_1 J_1'\right) A\left(\alpha_2 L_2 S \to \alpha_1 L_1 S\right)$$

$$\times \begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & -p & M_2 \end{pmatrix} \begin{pmatrix} J_1' & 1 & J_2' \\ -M_1' & -p & M_2' \end{pmatrix}$$

(isotropic)
+ analogous for collisional transitions

Radiative Transition Probabilities

induced emission



$$\Gamma^{\text{ind}}_{\alpha_1 J_1 J_1' M_1 M_1' \leftarrow \alpha_2 J_2 J_2' M_2 M_2'} =$$

$$X\left(\alpha_2 J_2 J_2' \to \alpha_1 J_1 J_1'\right) 3B\left(\alpha_2 L_2 S \to \alpha_1 L_1 S\right)$$

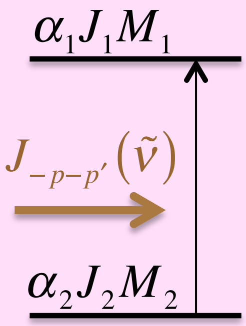
$$\times \int d\nu \oint \frac{d\vec{\Omega}}{4\pi} (-1)^{M_1 - M_1'} J_{-p-p'}(\tilde{\nu})$$

$$\times \begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & -p' & M_2 \end{pmatrix} \begin{pmatrix} J_1' & 1 & J_2' \\ -M_1' & -p & M_2' \end{pmatrix}$$

$$\times \left[\tfrac{1}{2} \Phi^*_{ba}\left(\nu_{\alpha_2 J_2' M_2', \alpha_1 J_1' M_1'} - \tilde{\nu}\right) + \tfrac{1}{2} \Phi_{ba}\left(\nu_{\alpha_2 J_2 M_2, \alpha_1 J_1 M_1} - \tilde{\nu}\right) \right]$$

$$\text{where } \nu_{\alpha_2 J_2 M_2, \alpha_1 J_1 M_1} = \frac{1}{h}\left[E\left(\alpha_2 J_2 M_2\right) - E\left(\alpha_1 J_1 M_1\right)\right]$$

+ analogous for collisional transitions
(but isotropic)



Radiative Transition Probabilities

absorption

$$\Gamma^{\text{abs}}_{\alpha_1 J_1 J_1' M_1 M_1' \leftarrow \alpha_2 J_2 J_2' M_2 M_2'} =$$

$$X\left(\alpha_2 J_2 J_2' \to \alpha_1 J_1 J_1'\right) 3B\left(\alpha_2 L_2 S \to \alpha_1 L_1 S\right)$$

$$\times \int d\nu \oint \frac{d\vec{\Omega}}{4\pi} (-1)^{M_1 - M_1' + p + p'} J_{-p-p'}(\tilde{\nu})$$

$$\times \begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & p & M_2 \end{pmatrix} \begin{pmatrix} J_1' & 1 & J_2' \\ -M_1' & p' & M_2' \end{pmatrix}$$

$$\times \left[\tfrac{1}{2} \Phi_{ba}\left(\nu_{\alpha_1 J_1' M_1', \alpha_2 J_2' M_2'} - \tilde{\nu}\right) + \tfrac{1}{2} \Phi^*_{ba}\left(\nu_{\alpha_1 J_1 M_1, \alpha_2 J_2 M_2} - \tilde{\nu}\right) \right]$$

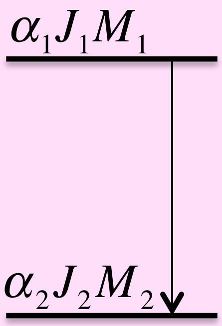
where $\nu_{\alpha_2 J_2 M_2, \alpha_1 J_1 M_1} = \dfrac{1}{h}\left[E\left(\alpha_2 J_2 M_2\right) - E\left(\alpha_1 J_1 M_1\right) \right]$

+ analogous for collisional transitions
(but isotropic)

RTE: Radiative Transfer Equation

$$\frac{d}{ds}\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = \underbrace{\begin{pmatrix} \varepsilon_I \\ \varepsilon_Q \\ \varepsilon_U \\ \varepsilon_V \end{pmatrix}}_{\text{spontaneous emission}} + \underbrace{\begin{pmatrix} \eta_I^s & \eta_Q^s & \eta_U^s & \eta_V^s \\ \eta_Q^s & \eta_I^s & \rho_V^s & -\rho_U^s \\ \eta_U^s & -\rho_V^s & \eta_I^s & \rho_Q^s \\ \eta_V^s & \rho_U^s & -\rho_Q^s & \eta_I^s \end{pmatrix}}_{\text{induced emission}} \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$

$$- \underbrace{\begin{pmatrix} \eta_I & \eta_Q & \eta_U & \eta_V \\ \eta_Q & \eta_I & \rho_V & -\rho_U \\ \eta_U & -\rho_V & \eta_I & \rho_Q \\ \eta_V & \rho_U & -\rho_Q & \eta_I \end{pmatrix}}_{\text{absorption}} \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$



Radiative Transfer Equation Coefficients

emissivity

$$
\begin{aligned}
&\varepsilon_i^{(2)}\left(\vec{r},\nu,\vec{\Omega}\right)= \\
&\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1 J_1 J_1' M_1 M_1' \alpha_2 J_2 M_2}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p-p'}\left(i,\vec{\Omega}\right) \\
&\times X\left(\alpha_1 J_1 J_1' \rightarrow \alpha_2 J_2 J_2\right) 3A\left(\alpha_1 L_1 S \rightarrow \alpha_2 L_2 S\right) \\
&\times\begin{pmatrix} J_2 & 1 & J_1 \\ -M_2 & -p' & M_1 \end{pmatrix}\begin{pmatrix} J_2 & 1 & J_1' \\ -M_2 & -p & M_1' \end{pmatrix} \\
&\times\left[\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_1 J_1' M_1',\alpha_2 J_2 M_2}-\tilde{\nu}\right)+\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_1 J_1 M_1,\alpha_2 J_2 M_2}-\tilde{\nu}\right)\right]
\end{aligned}
$$

Radiative Transfer Equation Coefficients
emissivity, new second coefficient

$$\varepsilon_i^{(4)}\left(\vec{r},\nu,\vec{\Omega}\right)=$$

$$\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1J_1J_1'M_1M_1'\alpha_2J_2J_2'M_2M_2'\alpha_3J_3M_3}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1J_1J_1'}\rho_{M_1M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p''-p'''}\left(i,\vec{\Omega}\right)$$

$$\times\int d\nu_1\left(-1\right)^{M_1-M_1'}J_{-p-p'}\left(\tilde{\nu}_1\right)$$

$$\times X\left(\alpha_1J_1J_1'\rightarrow\alpha_2J_2J_2\right)3B\left(\alpha_1L_1S\rightarrow\alpha_2L_2S\right)$$

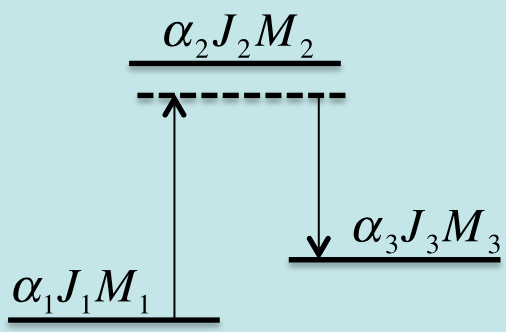
$$\times X\left(\alpha_2J_2J_2'\rightarrow\alpha_3J_3J_3\right)3A\left(\alpha_2L_2S\rightarrow\alpha_3L_3S\right)$$

$$\times\begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & -p & M_2 \end{pmatrix}\begin{pmatrix} J_1' & 1 & J_2' \\ -M_1' & -p' & M_2' \end{pmatrix}$$

$$\times\begin{pmatrix} J_3 & 1 & J_2 \\ -M_3 & -p''' & M_2 \end{pmatrix}\begin{pmatrix} J_3 & 1 & J_2' \\ -M_3 & -p'' & M_2' \end{pmatrix}$$

$$\times\left\{\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_2J_2'M_2',\alpha_1J_1'M_1'}-\tilde{\nu}_1\right)\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_2J_2M_2,\alpha_1J_1M_1}+\nu_{\alpha_1J_1'M_1',\alpha_3J_3M_3}-\tilde{\nu}\right)\tfrac{1}{2}\Phi_{ca}\left(\tilde{\nu}-\tilde{\nu}_1-\nu_{\alpha_1J_1'M_1',\alpha_3J_3M_3}\right)\right.$$

$$\left.+\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_2J_2M_2,\alpha_1J_1M_1}-\tilde{\nu}_1\right)\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_2J_2'M_2',\alpha_1J_1'M_1'}+\nu_{\alpha_1J_1M_1,\alpha_3J_3M_3}-\tilde{\nu}\right)\tfrac{1}{2}\Phi_{ca}^{*}\left(\tilde{\nu}-\tilde{\nu}_1-\nu_{\alpha_1J_1M_1,\alpha_3J_3M_3}\right)\right\}$$

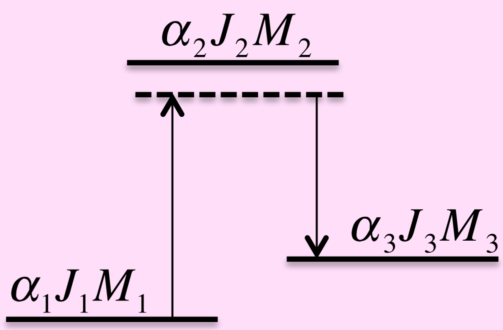


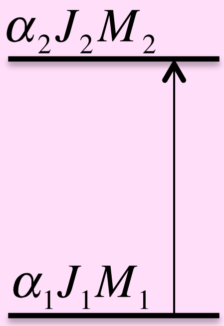
Radiative Transfer Equation Coefficients

emissivity, new second coefficient

The order-4 term in the emissivity:

– its integral over one or the other of the frequencies is zero
– it redistributes the frequencies inside the emission profile
– the result is a decoupling between atom and radiation

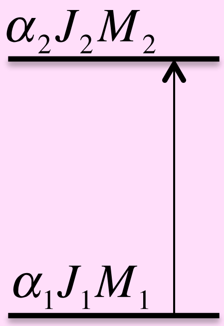




Radiative Transfer Equation Coefficients

absorption coefficient

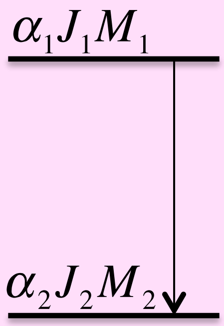
$$
\begin{aligned}
&\eta_i\left(\vec{r},\nu,\vec{\Omega}\right)= \\
&\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1 J_1 J_1' M_1 M_1' \alpha_2 J_2 M_2}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p-p'}\left(i,\vec{\Omega}\right)\left(-1\right)^{M_1-M_1'} \\
&\times X\left(\alpha_1 J_1 J_1' \rightarrow \alpha_2 J_2 J_2\right) 3B\left(\alpha_1 L_1 S \rightarrow \alpha_2 L_2 S\right) \\
&\times\begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & -p & M_2 \end{pmatrix}\begin{pmatrix} J_1' & 1 & J_2 \\ -M_1' & -p' & M_2 \end{pmatrix} \\
&\times\left[\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_2 J_2 M_2,\alpha_1 J_1 M_1}-\tilde{\nu}\right)+\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_2 J_2 M_2,\alpha_1 J_1' M_1'}-\tilde{\nu}\right)\right]
\end{aligned}
$$



Radiative Transfer Equation Coefficients

absorption coefficient, magneto-optical effects

$$
\begin{aligned}
&\rho_i\left(\vec{r},\nu,\vec{\Omega}\right)= \\
&\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1 J_1 J_1' M_1 M_1' \alpha_2 J_2 M_2}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p-p'}\left(i,\vec{\Omega}\right)(-1)^{M_1-M_1'} \\
&\times X\left(\alpha_1 J_1 J_1' \rightarrow \alpha_2 J_2 J_2\right) 3B\left(\alpha_1 L_1 S \rightarrow \alpha_2 L_2 S\right) \\
&\times\begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & -p & M_2 \end{pmatrix}\begin{pmatrix} J_1' & 1 & J_2 \\ -M_1' & -p' & M_2 \end{pmatrix} \\
&\times(-i)\left[\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_2 J_2 M_2,\alpha_1 J_1 M_1}-\tilde{\nu}\right)-\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_2 J_2 M_2,\alpha_1 J_1' M_1'}-\tilde{\nu}\right)\right]
\end{aligned}
$$



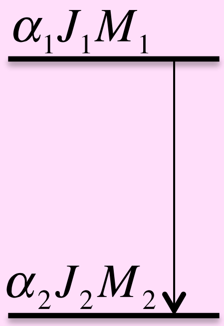
Radiative Transfer Equation Coefficients

induced emission coefficient

$$
\begin{aligned}
&\eta_i^{s}\left(\vec{r},\nu,\vec{\Omega}\right)= \\
&\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1 J_1 J_1' M_1 M_1' \alpha_2 J_2 M_2}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p-p'}\left(i,\vec{\Omega}\right) \\
&\times X\left(\alpha_1 J_1 J_1' \to \alpha_2 J_2 J_2\right) 3B\left(\alpha_1 L_1 S \to \alpha_2 L_2 S\right) \\
&\times\begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & p' & M_2 \end{pmatrix}\begin{pmatrix} J_1' & 1 & J_2 \\ -M_1' & p & M_2 \end{pmatrix} \\
&\times\left[\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_1 J_1' M_1', \alpha_2 J_2 M_2}-\tilde{\nu}\right)+\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_1 J_1 M_1, \alpha_2 J_2 M_2}-\tilde{\nu}\right)\right]
\end{aligned}
$$

Radiative Transfer Equation Coefficients

induced emission coefficient: magneto-optical effects



$$
\begin{aligned}
&\rho_i^{s}\left(\vec{r},\nu,\vec{\Omega}\right)= \\
&\frac{h\nu}{4\pi}\mathscr{N}\sum_{\alpha_1 J_1 J_1' M_1 M_1' \alpha_2 J_2 M_2}\int d^3\vec{v}\, f\left(\vec{v}\right)\,{}^{\alpha_1 J_1 J_1'}\rho_{M_1 M_1'}\left(\vec{r},\vec{v}\right)\mathscr{T}_{-p-p'}\left(i,\vec{\Omega}\right) \\
&\times X\left(\alpha_1 J_1 J_1' \rightarrow \alpha_2 J_2 J_2\right) 3B\left(\alpha_1 L_1 S \rightarrow \alpha_2 L_2 S\right) \\
&\times\begin{pmatrix} J_1 & 1 & J_2 \\ -M_1 & p' & M_2 \end{pmatrix}\begin{pmatrix} J_1' & 1 & J_2 \\ -M_1' & p & M_2 \end{pmatrix} \\
&\times(-i)\left[\tfrac{1}{2}\Phi_{ba}\left(\nu_{\alpha_1 J_1' M_1',\alpha_2 J_2 M_2}-\tilde{\nu}\right)-\tfrac{1}{2}\Phi_{ba}^{*}\left(\nu_{\alpha_1 J_1 M_1,\alpha_2 J_2 M_2}-\tilde{\nu}\right)\right]
\end{aligned}
$$

Irreducible Tensors basis ρ_Q^K

on the example of a $J = 1$ level, 9 density matric elements

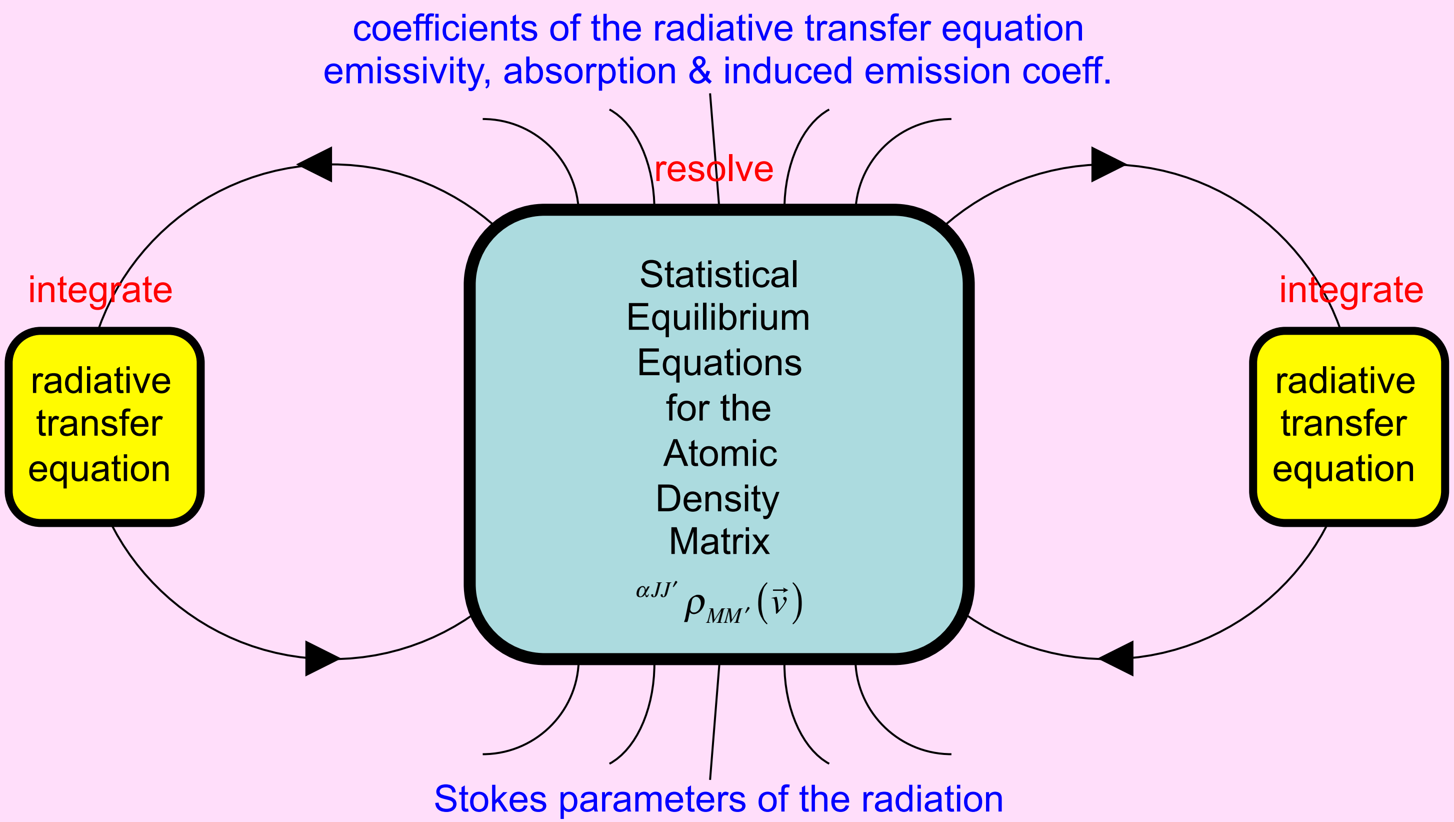
- atom in cylindrical symmetry, without structure & without magnetic field
  2 non-zero density matrix elements: $\underbrace{\rho_0^0}_{\text{population}}$ & $\underbrace{\rho_0^2}_{\text{alignment}}$
- atom in cylindrical symmetry, without structure but with magnetic field
  6 non-zero density matrix elements: $\underbrace{\rho_0^0}_{\text{population}}, \underbrace{\rho_{-2}^2, \rho_{-1}^2, \rho_0^2, \rho_1^2, \rho_2^2}_{\text{alignment}}$
- atom in cylindrical symmetry, with structure & magnetic field
  9 non-zero density matrix elements: $\underbrace{\rho_0^0}_{\text{population}}, \underbrace{\rho_{-1}^1, \rho_0^1, \rho_1^1}_{\text{orientation}}, \underbrace{\rho_{-2}^2, \rho_{-1}^2, \rho_0^2, \rho_1^2, \rho_2^2}_{\text{alignment}}$
  (alignment to orientation effect)

Conclusion: in the general case, there is no symmmetry
and therefore no gain (reduction of element number)
in applying the irreducible tensors algebra

the dyadic basis will be used $\rho_{MM'}$

XTAT, a code based on this theory for modeling the polarized line formation

Centered on statistical equilibrium resolution for the multilevel atom
(iterative method)



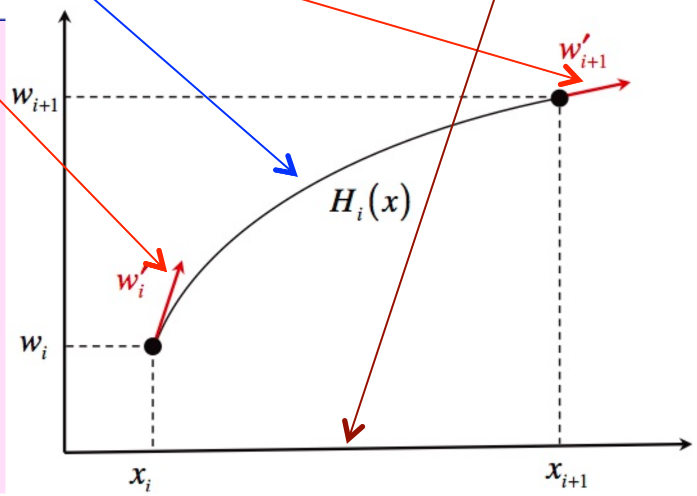
hybrid MPI-OpenMP PARALLELIZED

Integration of the RTE

Short characteristics method by Ibgui et al., 2013, A&A 549, A126, inspired by Auer (2003):

Piecewise cubic locally monotonic interpolation between grid-points (nodes):

- Interpolant: Cubic Hermite Polynomial
- Derivatives at nodes from Brodlie (1980), Fritsch & Butland (1984)
- Taylor expansion up to the 3rd order for $\Delta\tau < 0.05$



Numerics

- Discretizations:
  - 1024 depths
  - 7 line frequencies (about each line center frequency)
  - 6 atomic velocities (Maxwell distribution for the global atom)
  - 4 inclination angles (radiation & velocities)
  - 8 azimut angles (radiation & velocities)

- Integrations: Gauss methods
  - finite integral limits (angles): Gauss-Legendre
  - inifinite integral limits (frequencies, velocities): Gauss-Hermite

Parallelization

- Massive: 32768 threads running simultaneously

- Hybrid:

  ➔ loop MPI parallelized
    - 1024 depths

  ➔ grouped in one single loop OpenMP parallelized (shared memory saves memory)
    - 4 inclination angles (radiation & velocities)
    - 8 azimut angles (radiation & velocities)

- Machine: IBM Blue Gene/Q (IDRIS, Orsay, France)

Line profiles

- in the SEE, for each atomic velocity class:
  natural width << incident line width
  ➔ incident radiation assumed constant along the natural width

- for the RTE coefficients:
  there are not enough velocity nodes
  ➔ the emission/absorption profile is replaced,
  for each velocity node,
  by a Voigt profile.

Acceleration

The method is Λ-iteration.
It is well-known to require acceleration for convergence

- Ng acceleration:
  - requires to keep in memory 3 or 4 previous iteration results

  ➔we do not have enough memory

- Preconditioning (Rybicki & Hummer 1991, 1992, 1994)
  - method: replacing the level population contribution to the incident radtion, by the new unknown value
  - very efficient for isolated levels/lines
  - the more levels are involved, the less efficient is the method

    "The preconditioning of some [several] terms may have little effect on the convergence rate" (Rybicki & Hummer, 1992, "Overlapping transitions"

  ➔we have lots of sublevels and atomic coherences

Initialisation & run conditions

– initialisation: LTE density matrix populations

– Na I D1 & D2 observed near the solar limb, inside "Second Solar Spectrum"

– Solar atmosphere model: FAL-C

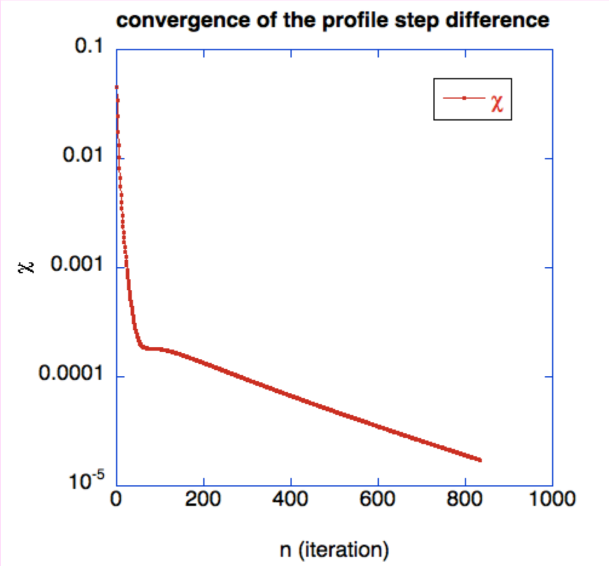
– Ionization: Saha equilibrium is assumed

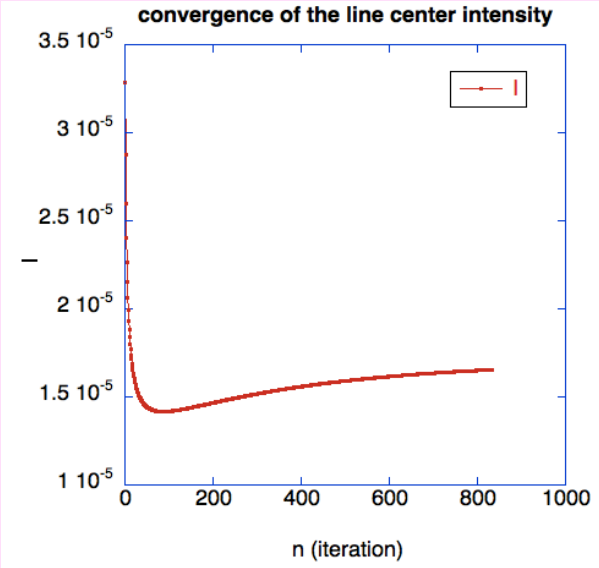
– Collisions rates:
  - elastic (or quasi-elastic) $\mathrm{Na} + \mathrm{H}$
    Kerkeni & Bommier (2002)
  - inelastic $\mathrm{Na} + e^{-}$
    semi-classical perturbation method of Sahal-Brechot (1969) improved by taking into account the energy and moment transfer during the collision by Bommier (2006, SPW4)

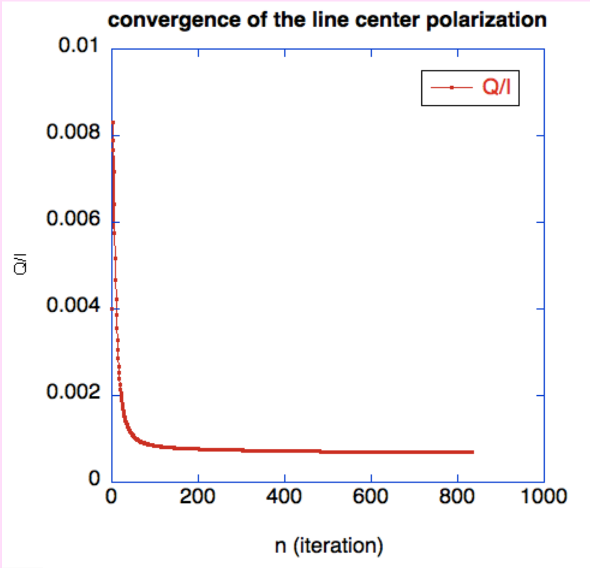
– no hyperfine structure
– no PRD, only CRD

Convergence

$\varepsilon \approx 10^{-3}$

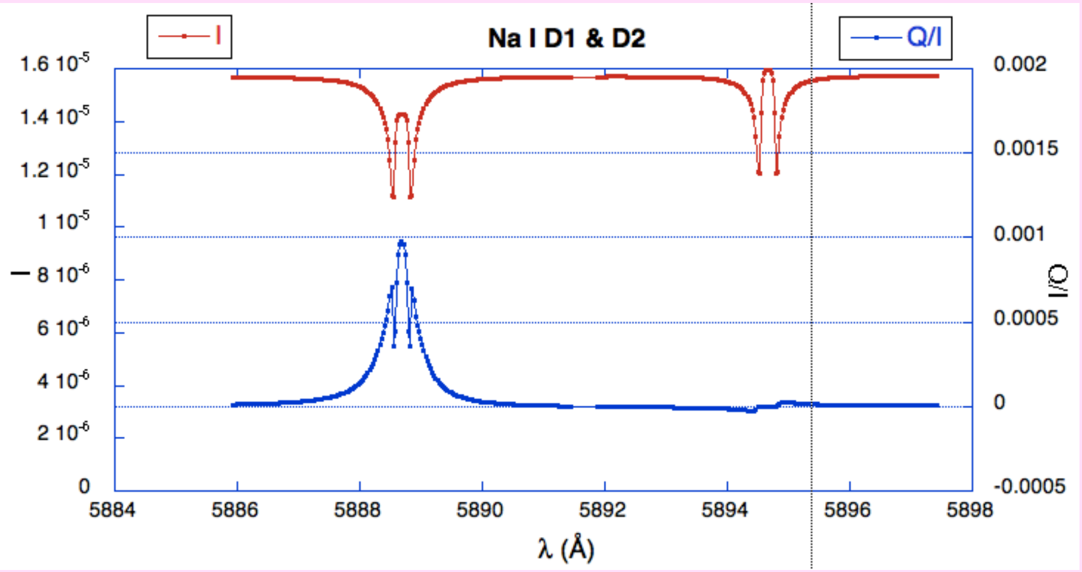


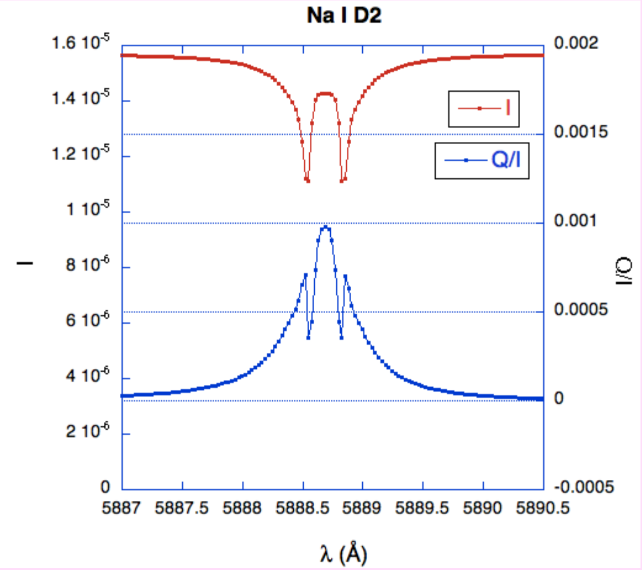


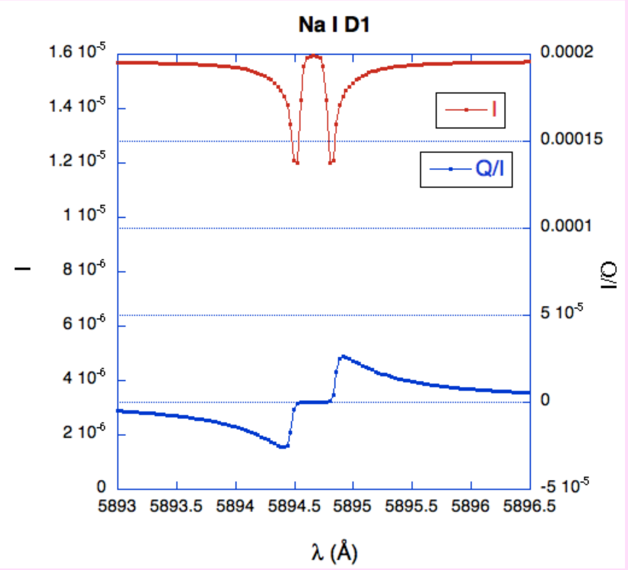


– no hyperfine structure
– no PRD, only CRD

Results

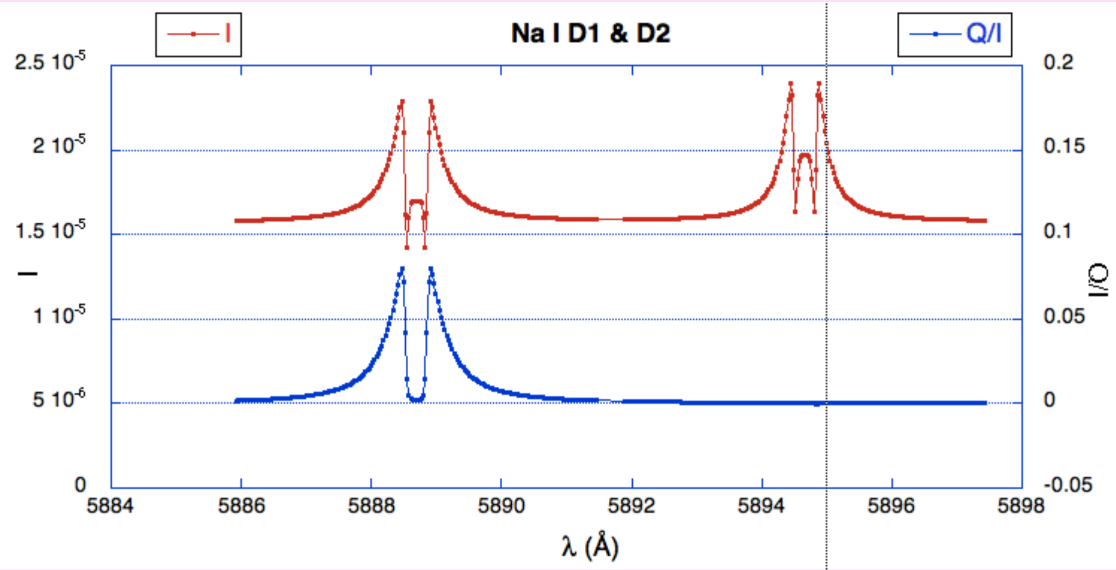


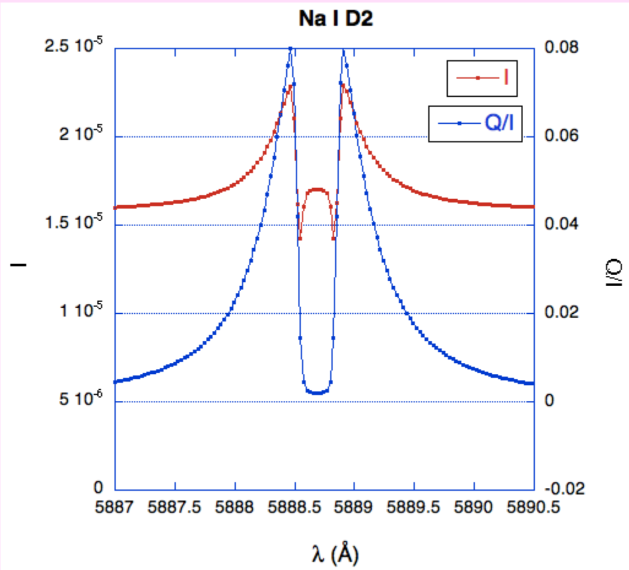


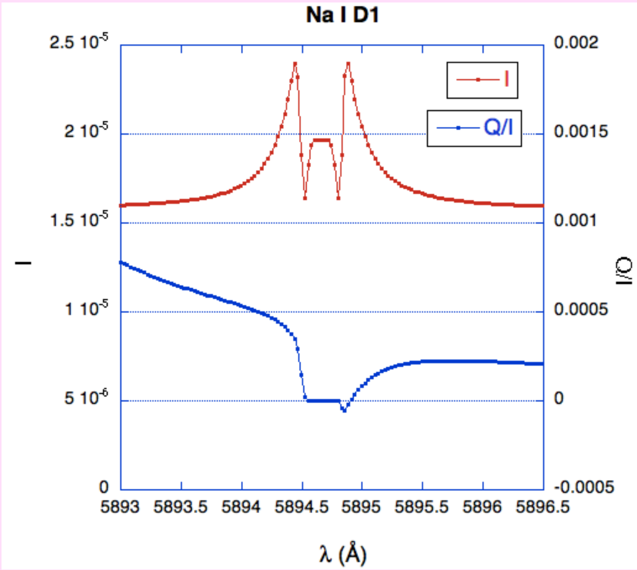


– no hyperfine structure
– with PRD

Results

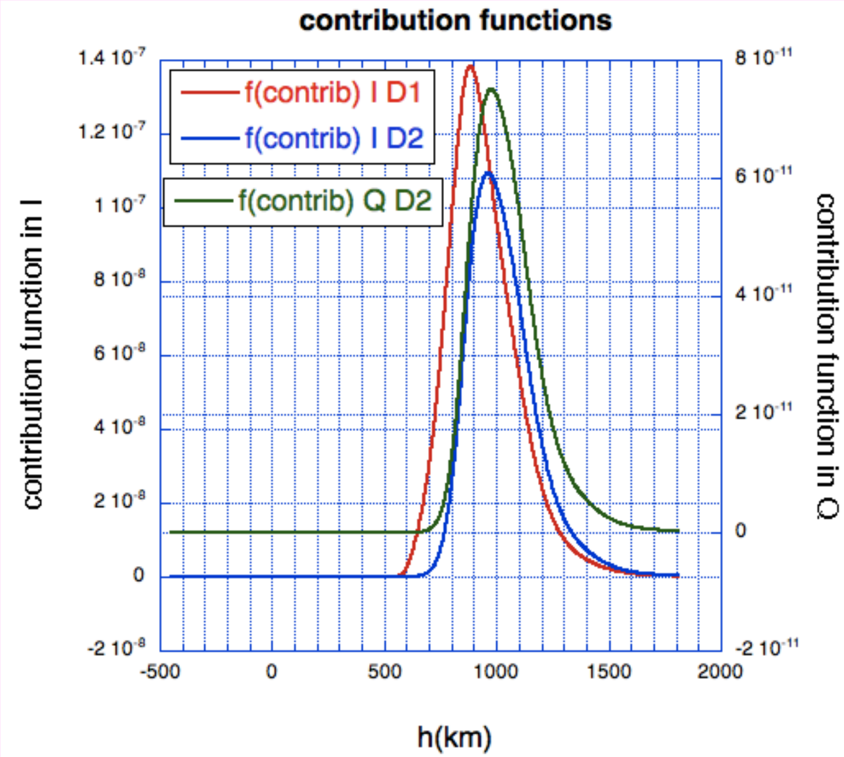




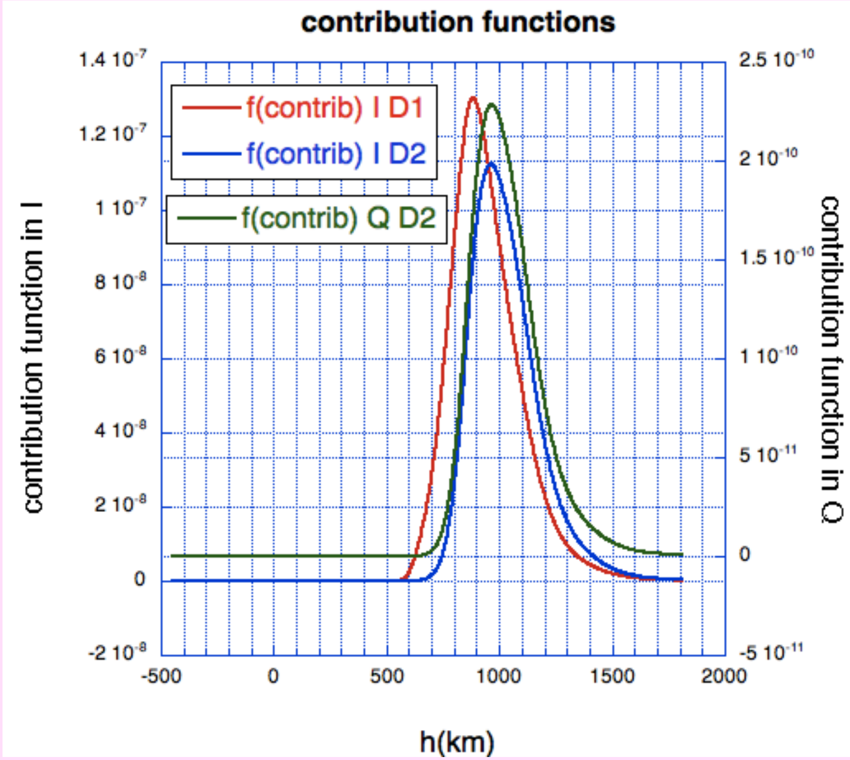


Contribution Functions

at line center
for a line-of-sight inclined at 85° (= 5" inside the limb)

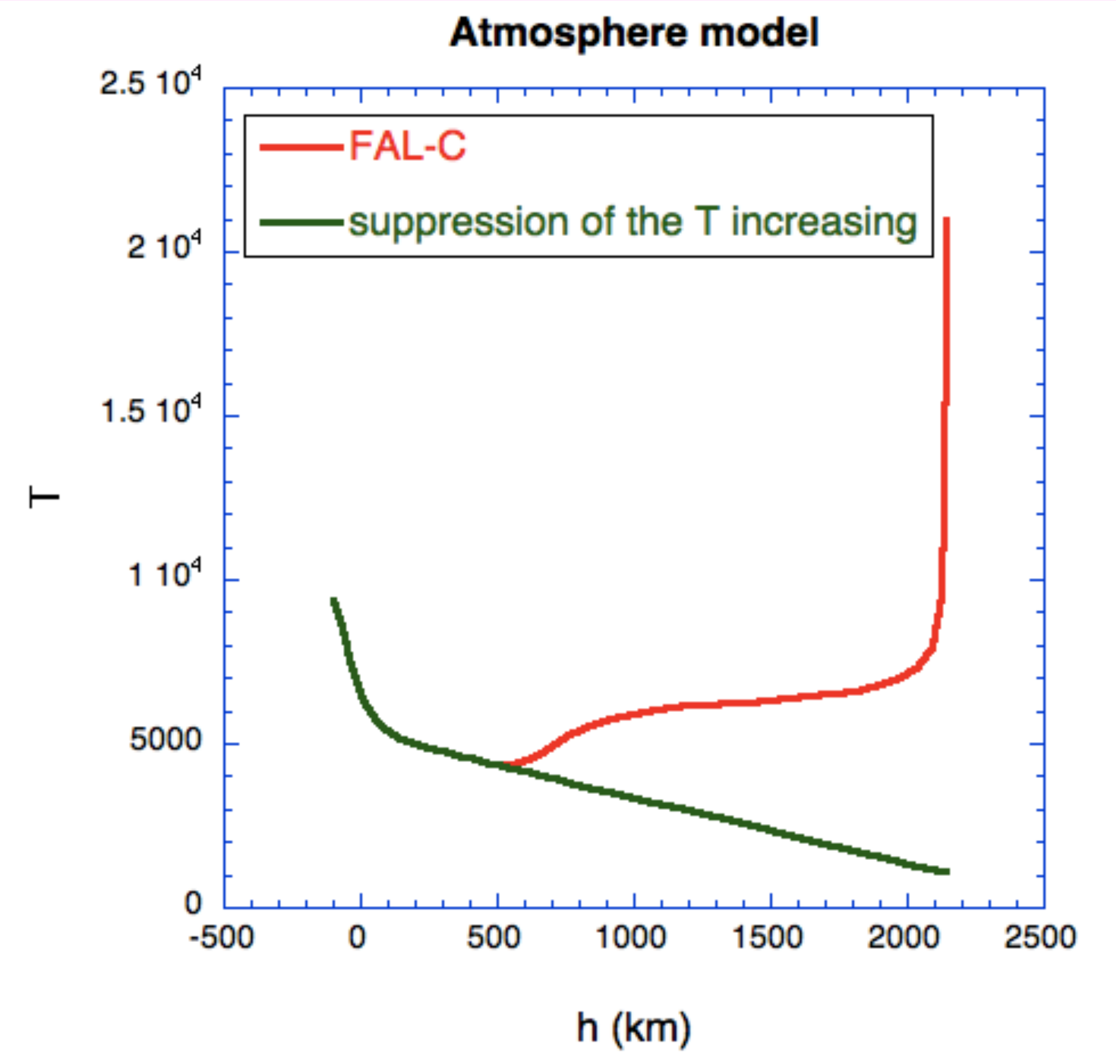


– no hyperfine structure
– with PRD



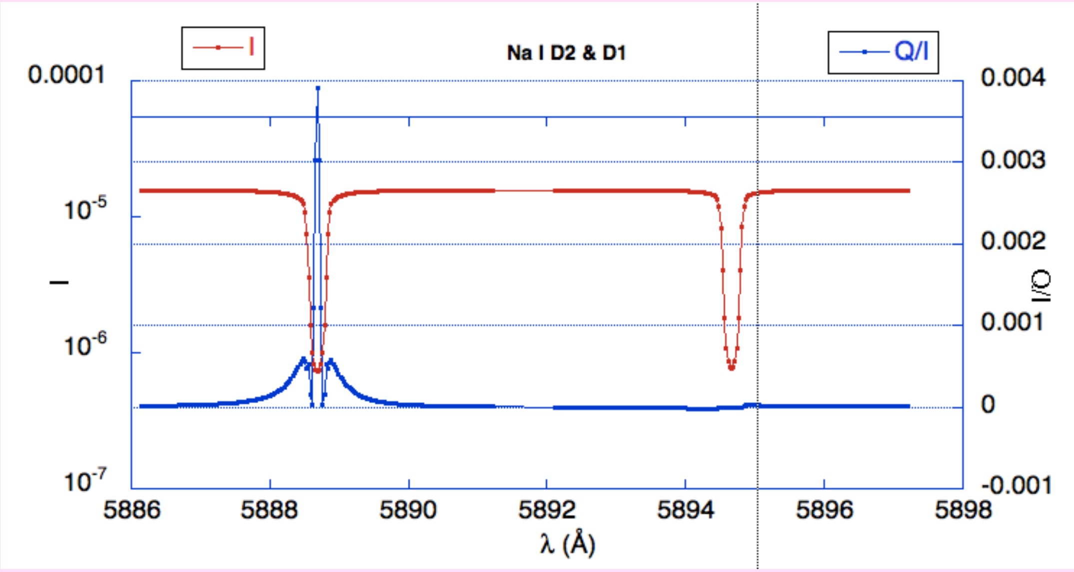
– no hyperfine structure
– with PRD

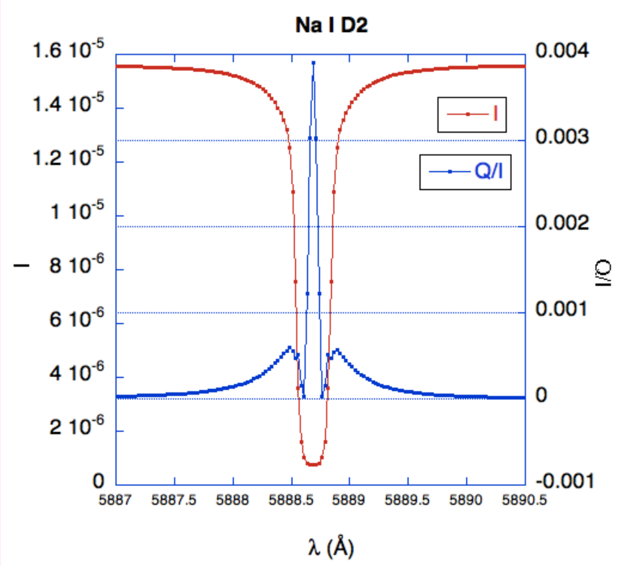
Atmosphere model

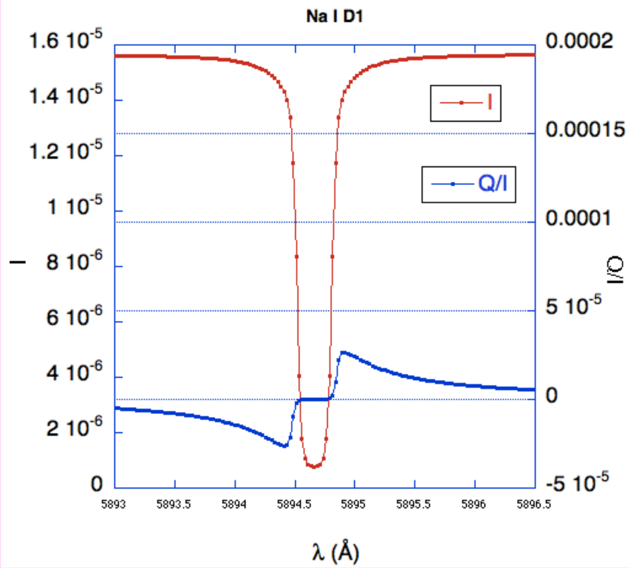


- no hyperfine structure
- no PRD, only CRD

Results

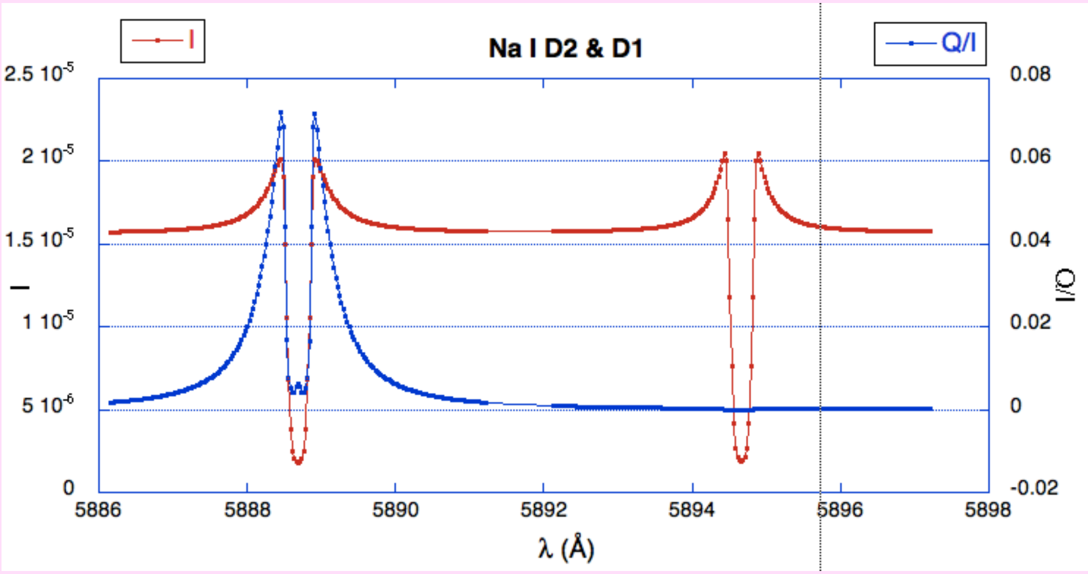


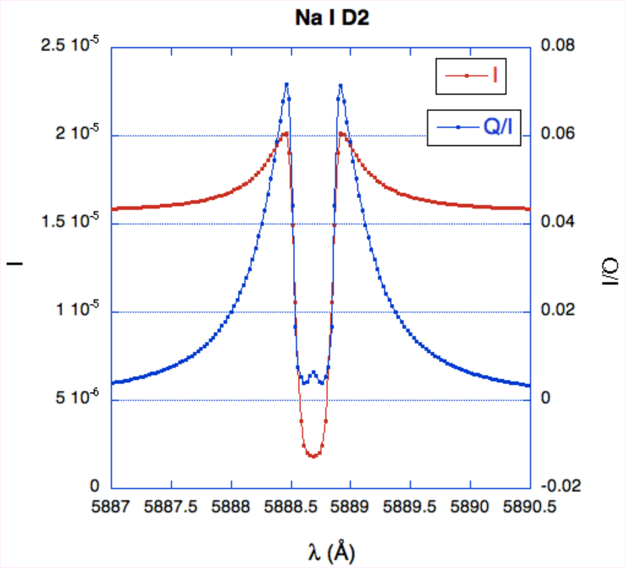


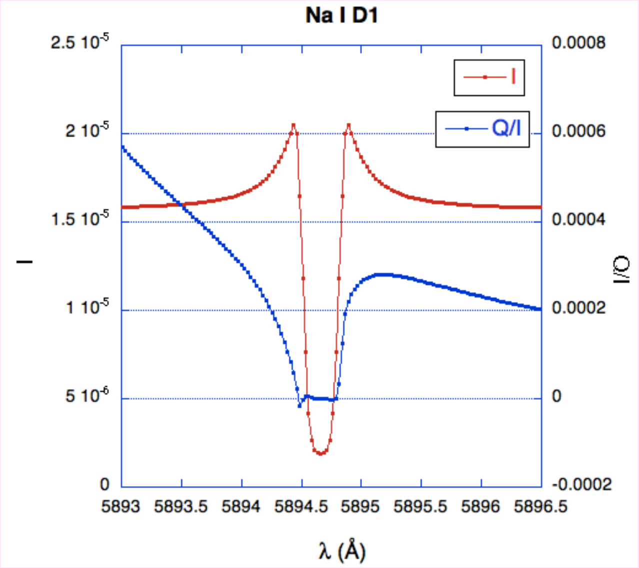


– no hyperfine structure
– with PRD

Results







2nd effect: new term at order-4 in the emissivity

$$\varepsilon =$$

order-2
$$\frac{h\nu}{4\pi}\frac{\nu^3}{\nu_0^3}N\rho_{bb}A_{ba}\phi_{ba}\left(\nu_0-\nu\right)$$

order-4
$$+\frac{h\nu}{4\pi}\frac{\nu^3}{\nu_0^3}N\rho_{aa}B_{ab}\int \mathrm{d}\nu_1 J\left(\nu_1\right)$$
$$\left[\frac{1}{2}\Phi^*_{ba}\left(\nu_0-\nu\right)\frac{A_{ba}}{2}\Phi_a\left(\nu-\nu_1\right)\Phi_{ba}\left(\nu_0-\nu_1\right)\right]$$

$\Phi_{ba}\left(\nu_0-\nu_1\right)$: complex profile of half-half-width γ_{ba}

$\Phi_a\left(\nu-\nu_1\right)$: complex profile of half-half-width the lower level a life-time

infinitely sharp lower level a :

$$\left[\frac{1}{2}\Phi^*_{ba}\left(\nu_0-\nu\right)\frac{A_{ba}}{2}\Phi_a\left(\nu-\nu_1\right)\Phi_{ba}\left(\nu_0-\nu_1\right)\right]=\frac{A_{ba}}{2\gamma_{ba}}\left\{\underbrace{\delta\left(\nu-\nu_1\right)\phi_{ba}\left(\nu_0-\nu_1\right)}_{r_{II}}-\underbrace{\phi_{ba}\left(\nu_0-\nu\right)\phi_{ba}\left(\nu_0-\nu_1\right)}_{r_{III}}\right\}$$

The order-4 term in the emissivity:

– its integral over one or the other of the frequencies is zero
– it redistributes the frequencies inside the emission profile
– the result is a decoupling between atom and radiation

2-level atom: Redistribution Function

The analytical solution of the statistical equilibrium reported into the emissivity

Γ_R : radiative inverse life-time

Γ_I : inelastic collisions ($b \leftrightarrow a$) inverse life-time

Γ_E : elastic collisions (in b) inverse life-time

$$\gamma_{ba} = \frac{1}{2}\left(\Gamma_R + \Gamma_I + \Gamma_E\right)$$

$$\varepsilon = \frac{h\nu}{4\pi}\frac{\nu^3}{\nu_0^3} N\rho_{aa}B_{ab}\int \mathrm{d}\nu_1 J(\nu_1)\left\{\frac{\Gamma_R}{\Gamma_R+\Gamma_I+\Gamma_E}\underbrace{\delta(\nu-\nu_1)\phi_{ba}(\nu_0-\nu_1)}_{r_{II}} + \frac{\Gamma_R}{\Gamma_R+\Gamma_I}\frac{\Gamma_E}{\Gamma_R+\Gamma_I+\Gamma_E}\underbrace{\phi_{ba}(\nu_0-\nu)\phi_{ba}(\nu_0-\nu_1)}_{r_{III}}\right\}$$

with polarization:

$$\varepsilon = \frac{h\nu}{4\pi}\frac{\nu^3}{\nu_0^3} N\rho_{aa}B_{ab}\int \mathrm{d}\nu_1 \oint \frac{\mathrm{d}\vec{\Omega}_1}{4\pi}\sum_K \left[w_{J'J}^{(K)}\right]^2 \sum_{j=0}^{3}\left[P_R^{(K)}\left(\vec{\Omega},\vec{\Omega}_1\right)\right]_{ij} S_j\left(\nu_1,\vec{\Omega}_1\right) \quad \text{Rayleigh phase matrix}$$

$$\left\{\frac{\Gamma_R}{\Gamma_R+\Gamma_I+\Gamma_E}\underbrace{\delta(\nu-\nu_1)\phi_{ba}(\nu_0-\nu_1)}_{r_{II}} + \frac{\Gamma_R}{\Gamma_R+\Gamma_I+D^{(K)}}\frac{\Gamma_E-D^{(K)}}{\Gamma_R+\Gamma_I+\Gamma_E}\underbrace{\phi_{ba}(\nu_0-\nu)\phi_{ba}(\nu_0-\nu_1)}_{r_{III}}\right\}$$

The collision rates weight the contributions of the different redistribution types (coherent or complete)