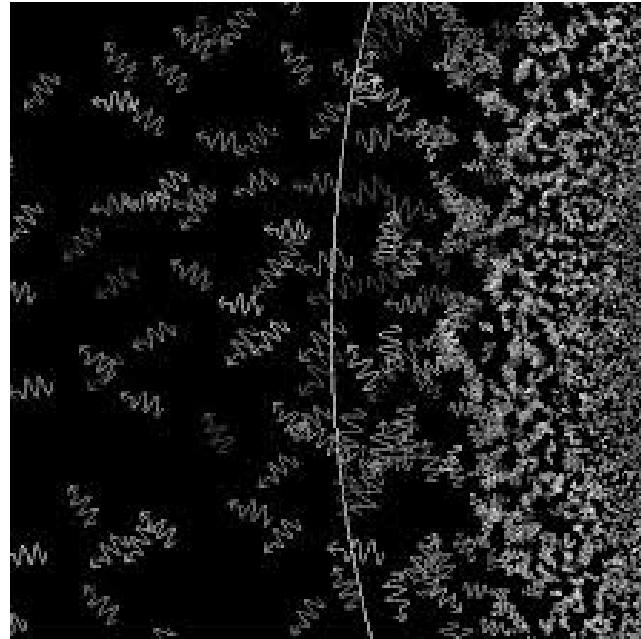


# Challenges in NLTE diagnostics



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NSO Brown Bag talk 03/10/2020

# Takeaways

- NLTE (polarized) radiative transfer is by far the most numerically demanding component of today's forward models (either standalone RT or R(M)HD)
- We (think) we understand the physics, but we don't have enough (person?) computing power to tackle the most complicated problems
- There is work to be done at all the aspects :
  - Iterative methods
  - Response functions / diagnostics**
  - Multidimensional calculations**
  - Time dependent calculations
  - PRD
- Radiative transfer and NLTE might be hard, but they are also fun!

# What is NLTE and why do we care?

*“... and the assumption of LTE no longer holds, a condition often referred to as non-LTE (NLTE), a description of what it is not rather than what it is.”*

(Michiel van Noort)

*“In contrast, by the term non-LTE or (NLTE) we describe any state that departs from LTE”*

(Ivan Hubeny & Dmitri Mihalas, Stellar Atmospheres 3<sup>rd</sup> edition)

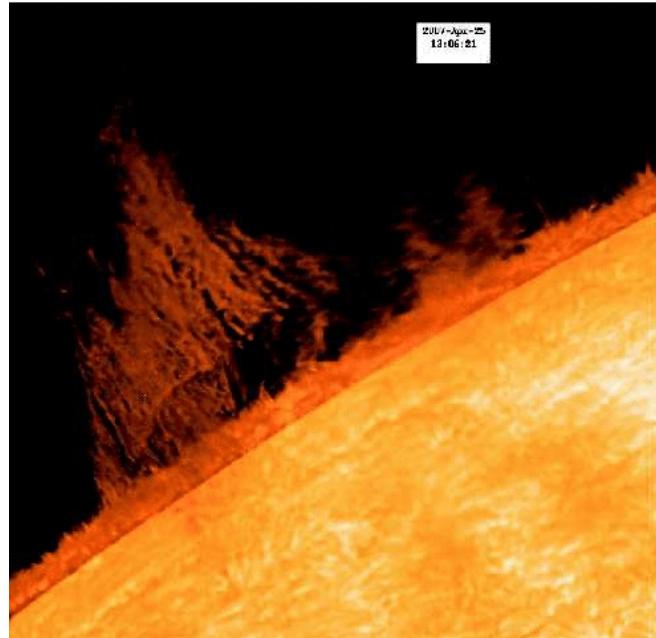
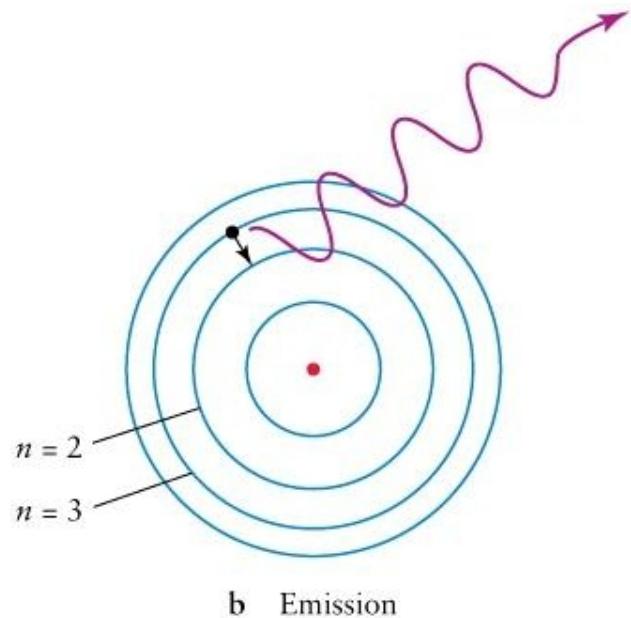
## LTE:

Ionization follows Saha distribution, excitation Boltzmann distribution, velocities Maxwellian distribution.

**We will mostly focus on the departures from the first two.**

# The core of the NLTE problem

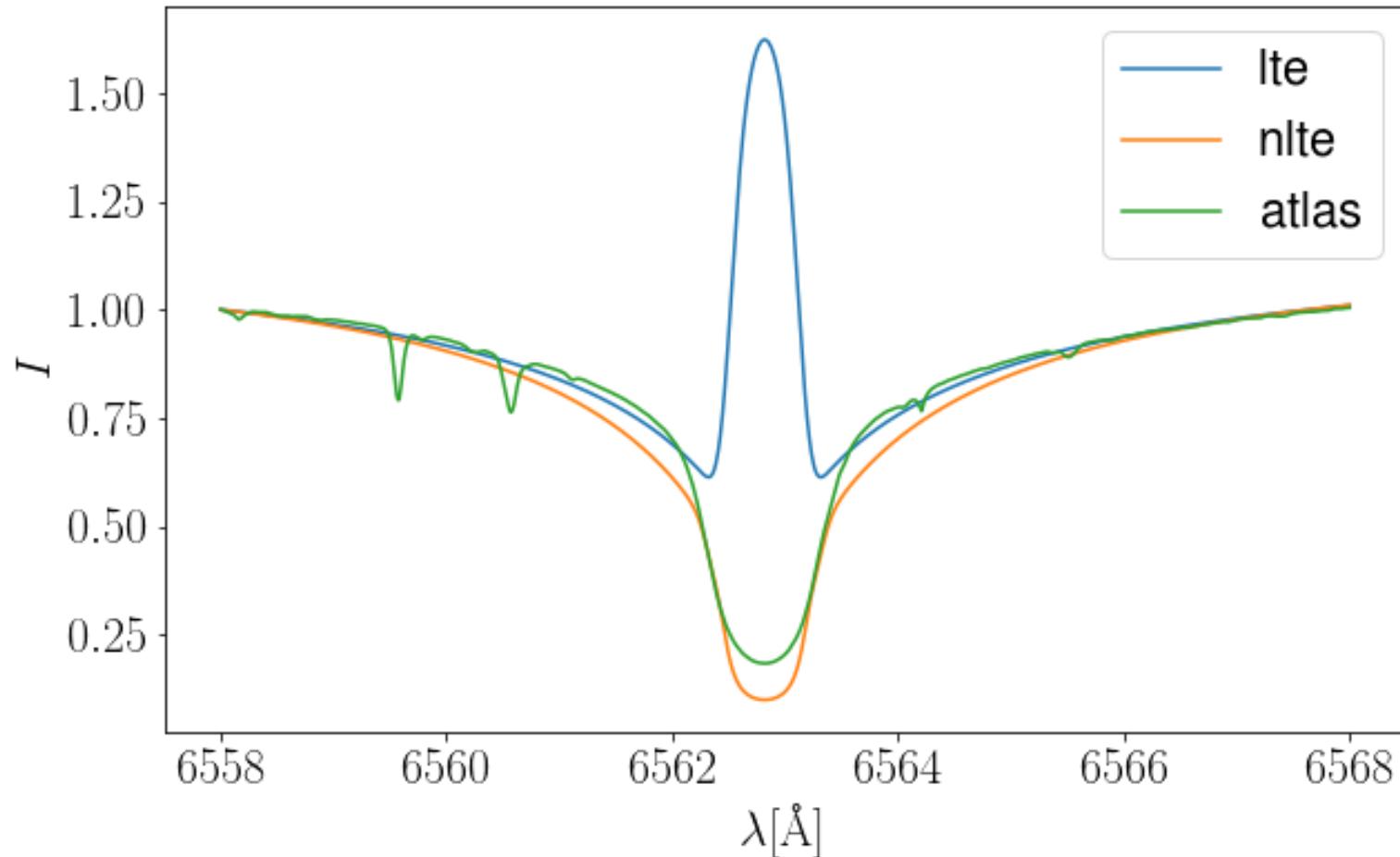
To paraphrase John Wheeler:



Credits: HINODE/SOT

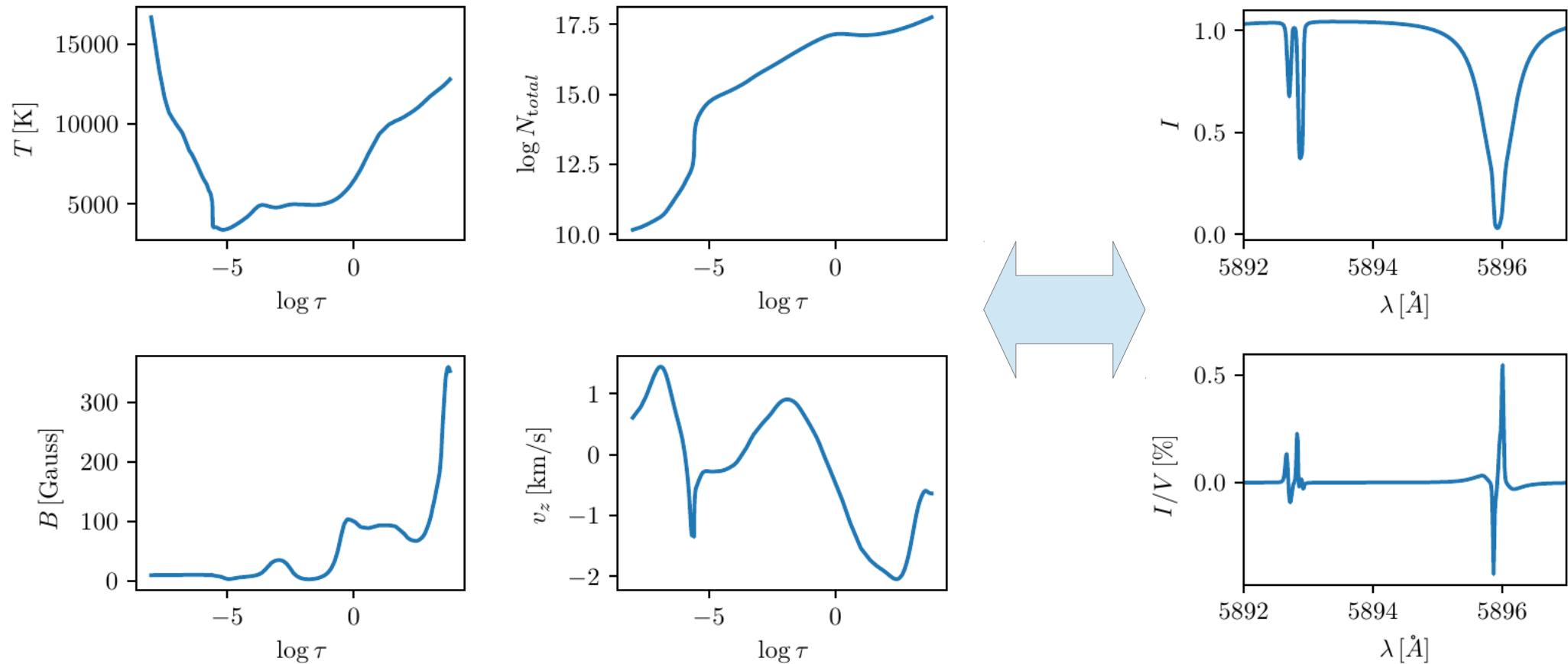
“Excitation tells the levels how many photons to emit,  
photons tell the levels how to excit(e).”

# Is NLTE important?

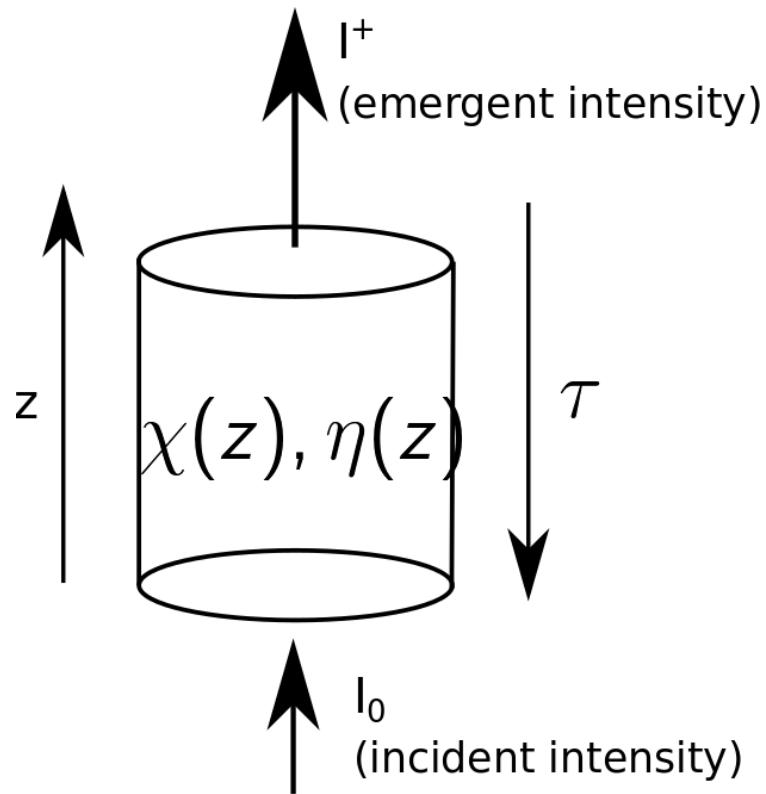


Why does this specific line (H-alpha) turn from emission to absorption?  
What is the mystery behind this?

# Step by step – how do we calculate the spectrum?



# Step by step – how do we calculate the spectrum?



$$\frac{dI_\lambda(z)}{dz} = -\chi_\lambda(z)I_\lambda(z) + j_\lambda(z)$$

$$\frac{dI_\lambda}{d\tau_\lambda} = I_\lambda - S_\lambda$$

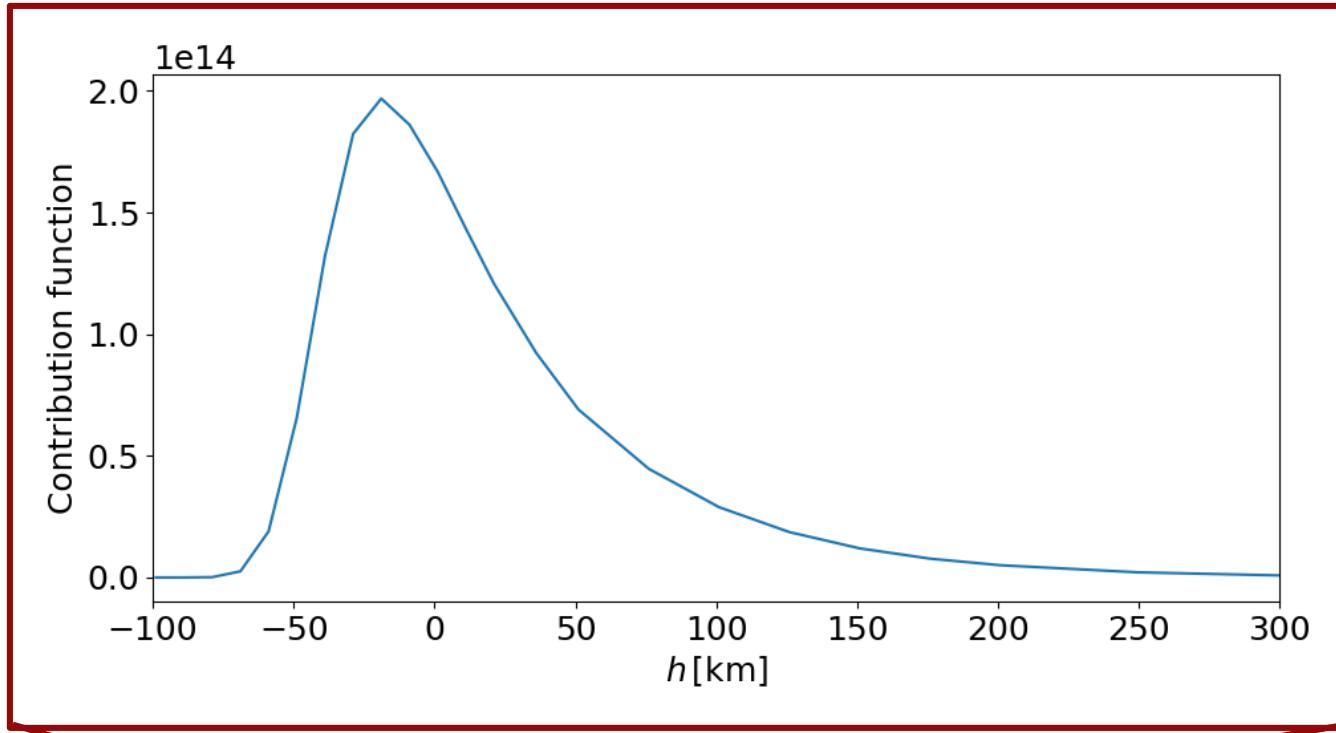
$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

**Given:** boundary conditions, physical parameters  
→ opacity / emissivity → **SPECTRUM**.

**Inverse problem:** Much harder

Ok, well that does not sound so bad...

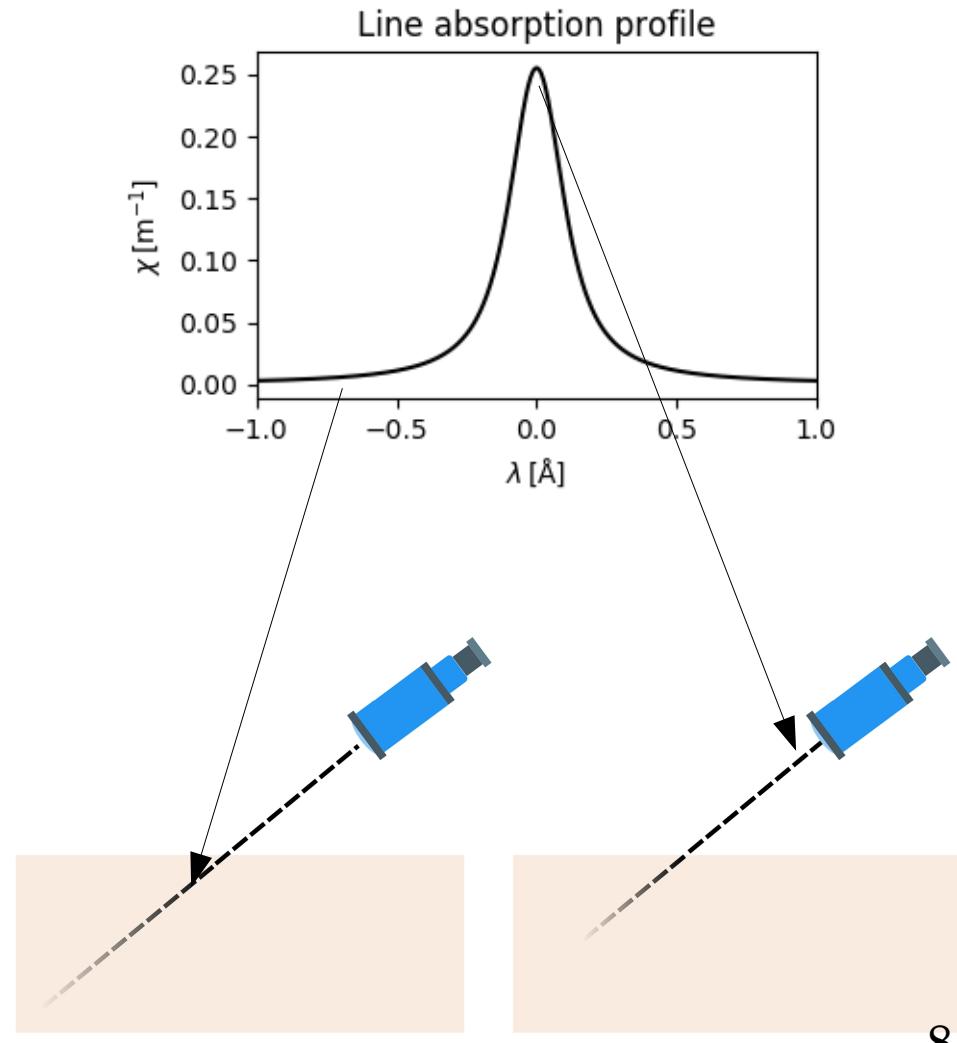
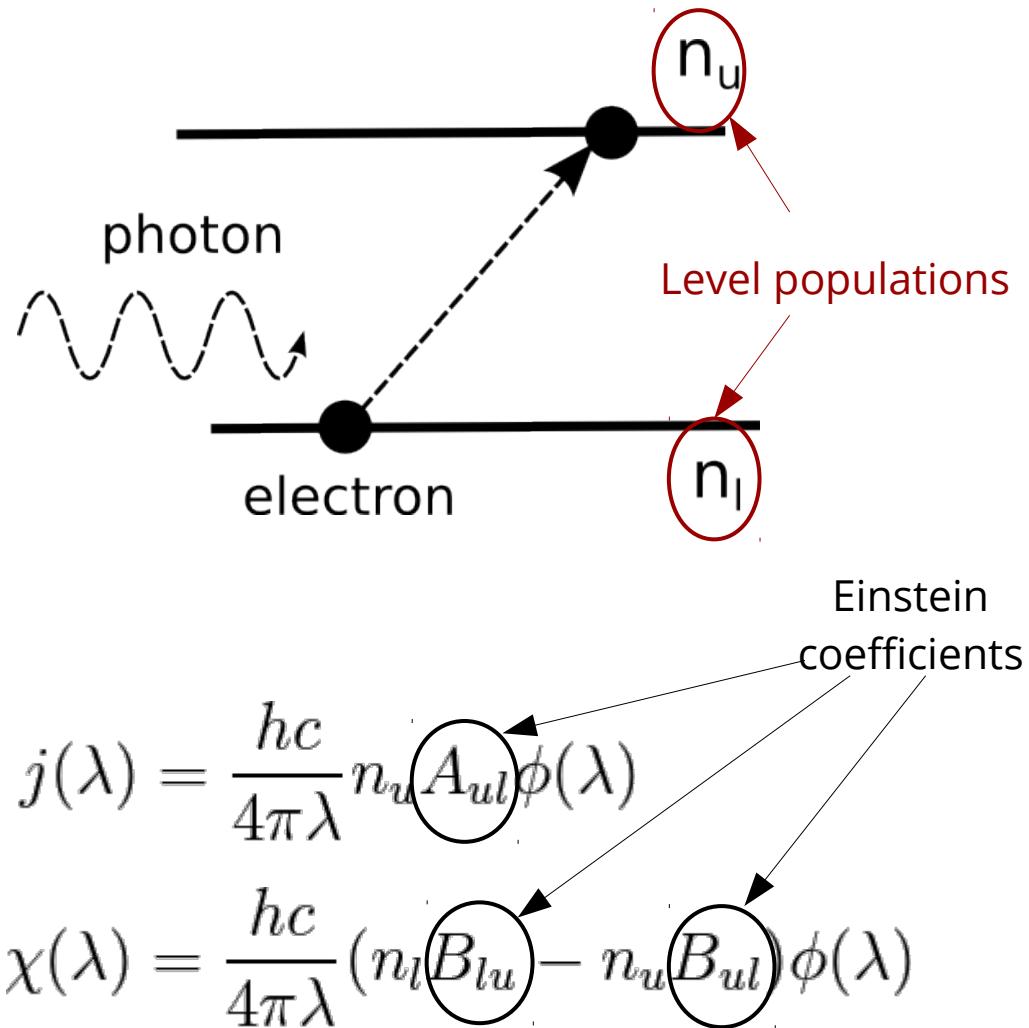
Well, it is, because this makes our problem non-local.



$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

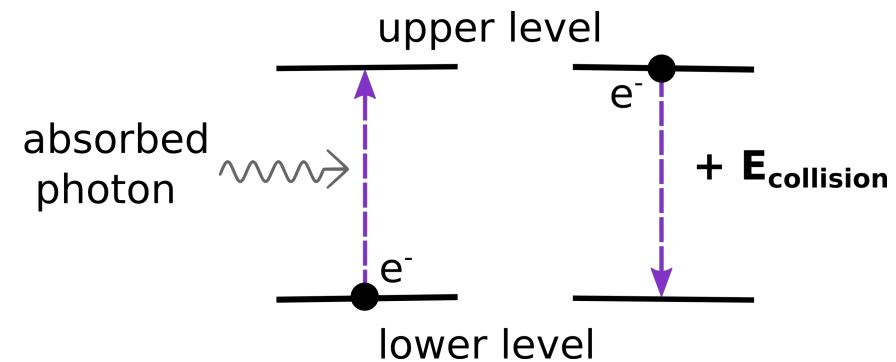
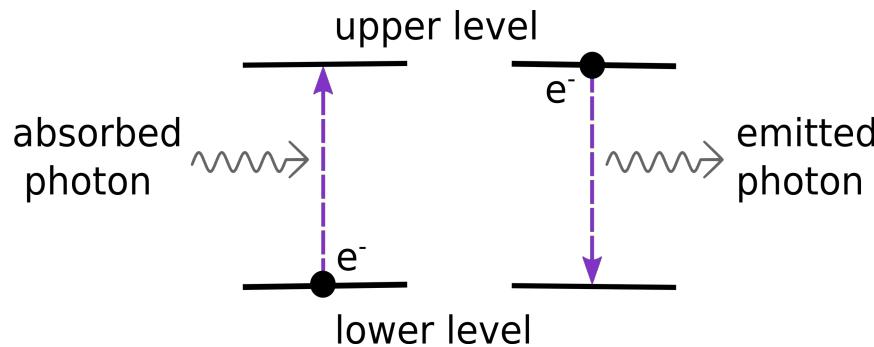
Strictly speaking, everything “upwind” from the point in question contributes.

# Let's focus on spectral lines for the moment



# NLTE complicates the calculation of the level populations

**Radiation** can alter the level populations (e.g. photoinization, optical pumping)



We replace Saha-Boltzmann with statistical equilibrium equation:

$$\frac{dn_i}{dt} = \sum_j n_j T_{ji} - n_i T_{ij} = 0$$

$$T_{ij} = R_{ij} + C_{ij}$$

$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

$$j(\lambda) = \frac{hc}{4\pi\lambda} n_u A_{ul} \phi(\lambda)$$

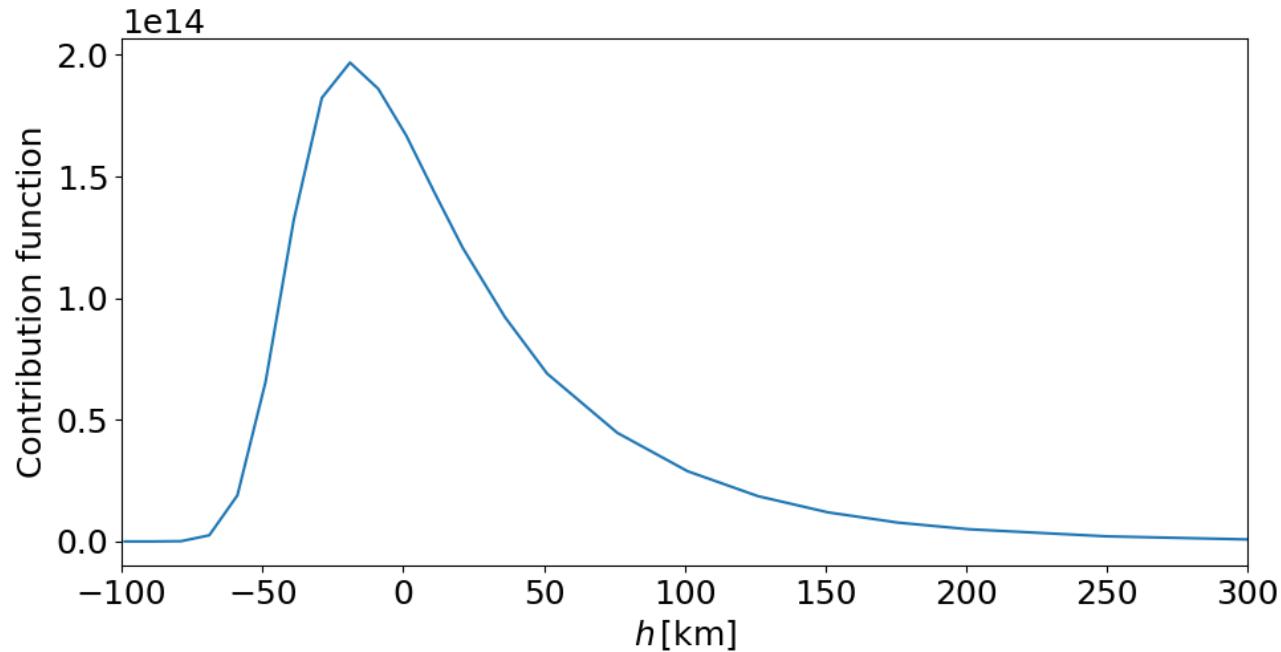
$$R_{ij} = A_{ij} + B_{ij} \oint \int I(\lambda, \Omega) \frac{d\Omega}{4\pi} \phi(\lambda) d\lambda$$

Ok, well that **still** does not sound so bad...

Well, it is, because this makes our problem non-local. **And non-linear.**

This is where the level populations are hiding.

$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$



Strictly speaking, everything “upwind” from the point in question contributes.

# Now we have a non-local and non-linear problem

- Intensity in a given point depends on the level populations everywhere.
- Level populations in the given point depend on the local intensity.
- **Level populations in the given point depend on the level populations everywhere: Coupling.**
- To solve it, we need to calculate all the relevant intensities for:

$$R_{ij} = A_{ij} + B_{ij} \oint \int I(\lambda, \Omega) \frac{d\Omega}{4\pi} \phi(\lambda) d\lambda$$

- For a 1D atmosphere with 100 points, 10 directions, 20 wavelenghts per line, 5 lines atom (i.e. Ca II 8542): **100 000 unknowns**.
- Or, said in another way:  $5 \times 20 \times 10 \times 20$  (iterations) = **20 000 formal solutions** .

# The simplest example – 2 level atom.

This is statistical equilibrium

This is radiative transfer

$$S = \epsilon B + (1 - \epsilon) \int \oint I(\lambda, \hat{\Omega}) \frac{d\Omega}{4\pi} \phi_\lambda d\lambda \quad I_d = \sum_0^{ND} w_{d,d'} S_{d'}$$

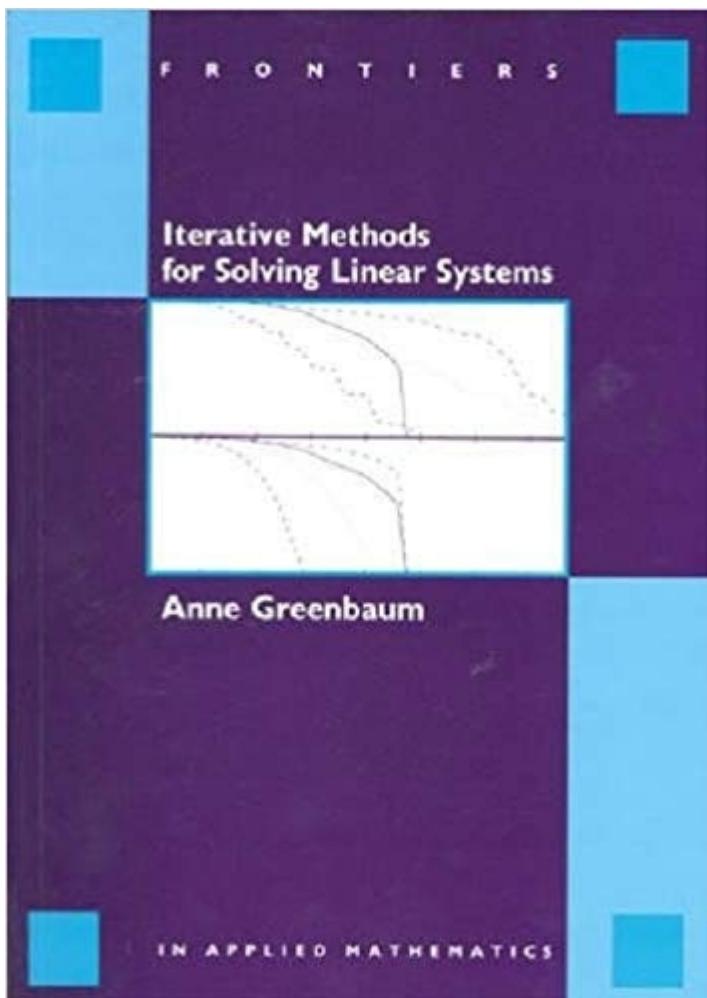
Let's merge them into one:

$$S_d = \epsilon_d B_d + (1 - \epsilon_d) \sum_{d'=0}^{ND} \Lambda_{d,d'} S_{d'}$$

Which is actually good old:

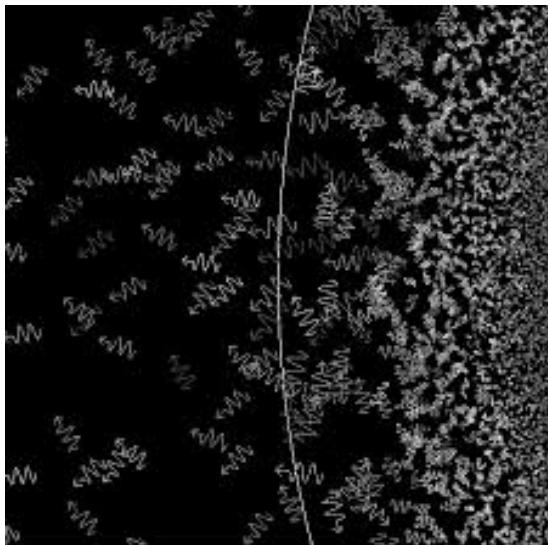
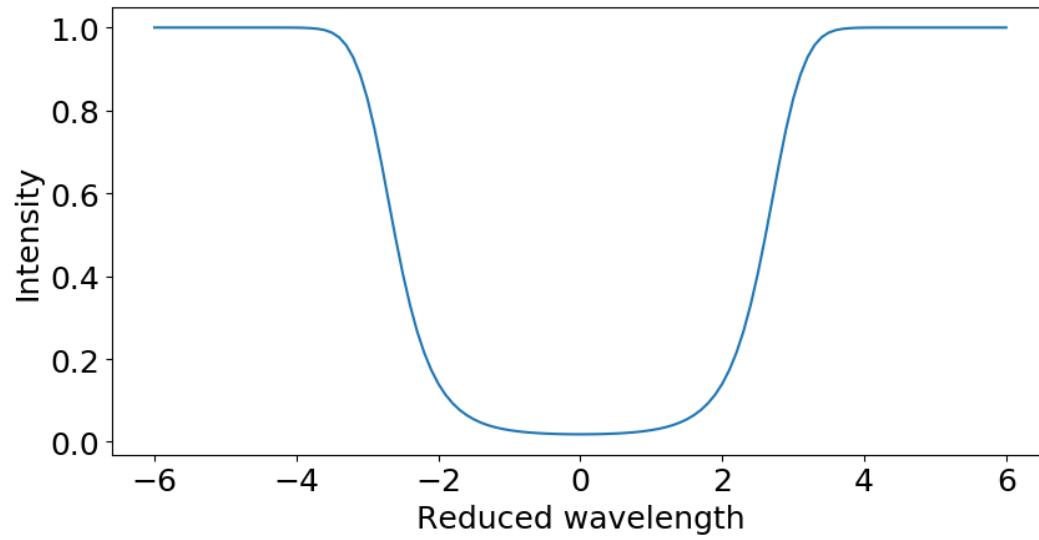
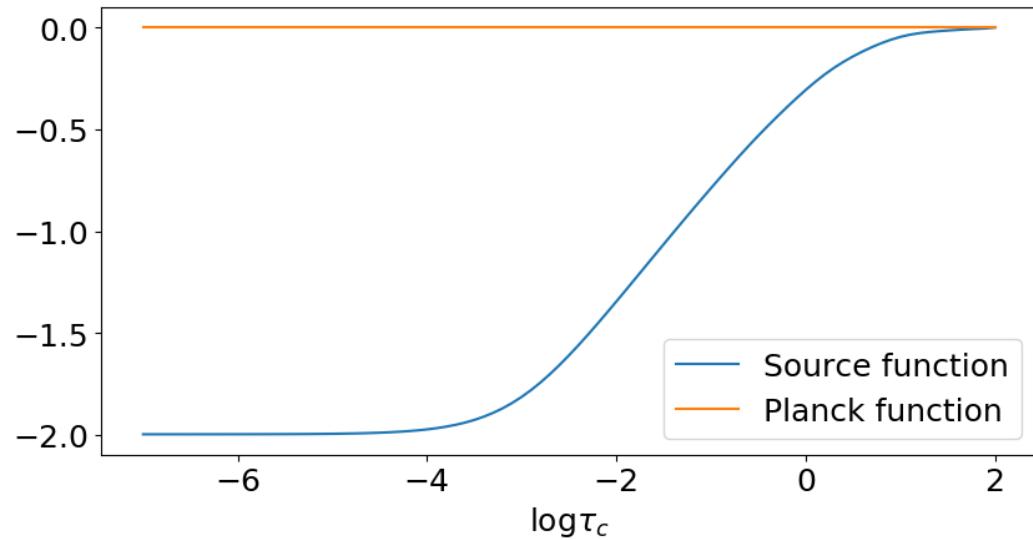
$$\hat{A}\vec{x} = \vec{b}$$

In 99.9% cases solved by iteration:



- ALI (Rybicki & Hammer) : easy, robust, well-tested. But, there are (much) faster ones:
- Gauss Seidel + SSOR (Trujillo Bueno & Fabiani Bendicho)
- Implicit lambda iteration (Atanackovic & Milic)
- Multigrid (Steiner, Stepan & Trujillo Bueno)
- Bi-conjugate Gradient (Anusha, Paletou)
- ***Something new?***  
(especially for 2-level atom like lines)

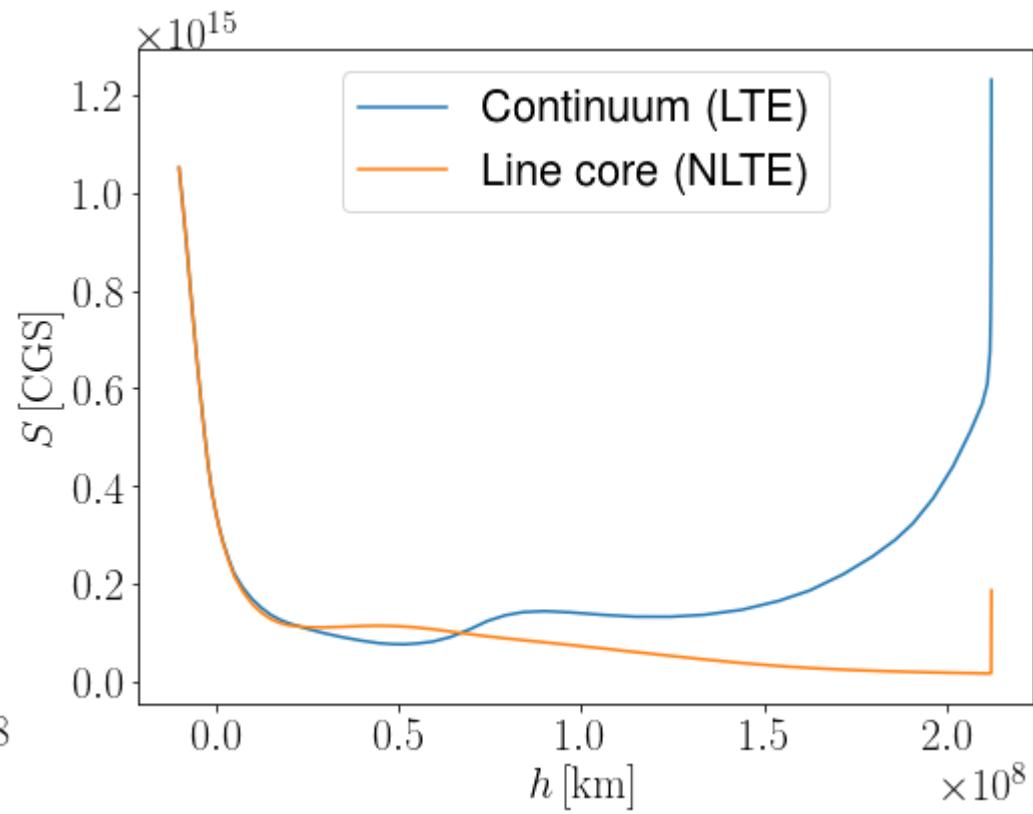
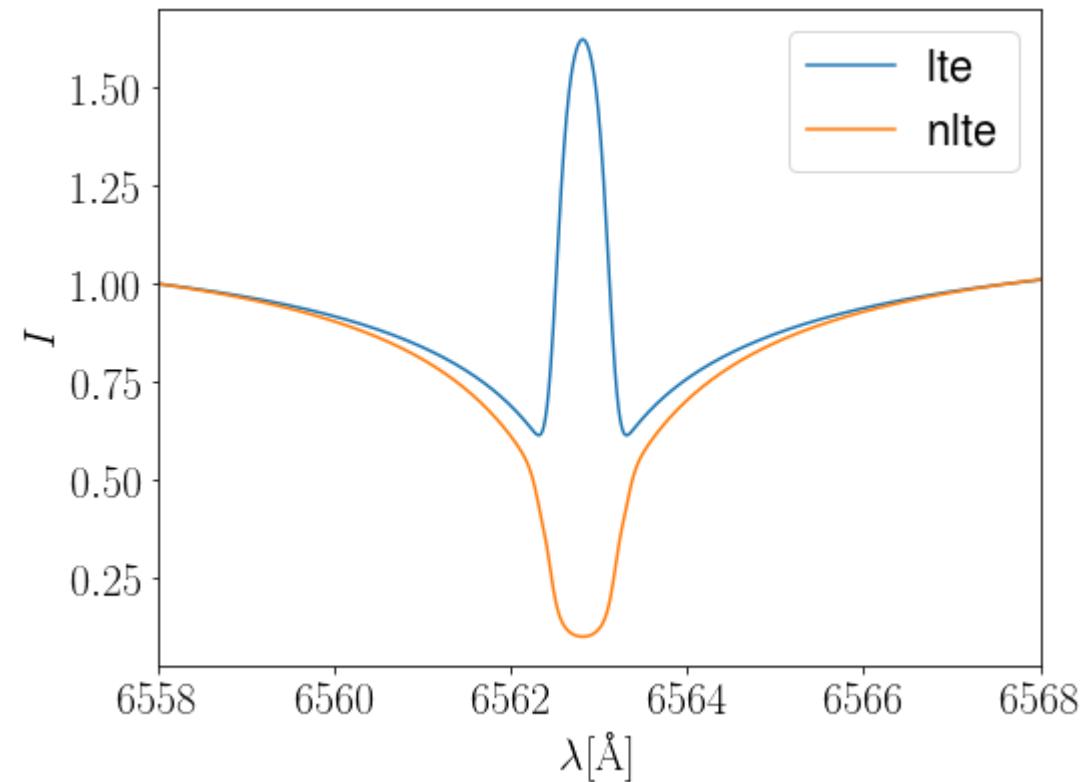
# So what happens then?



- Photons “leak” from the surface, there are few collisions, so upper level is under-populated.
- Source function decoupled from the local temperature (Planck function).
- Line appears even in an isothermal atmosphere.

Credits: Mats Carlsson

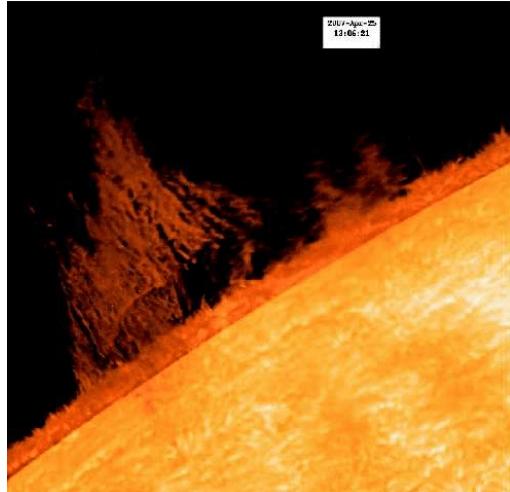
# How does it look for our beloved H alpha?



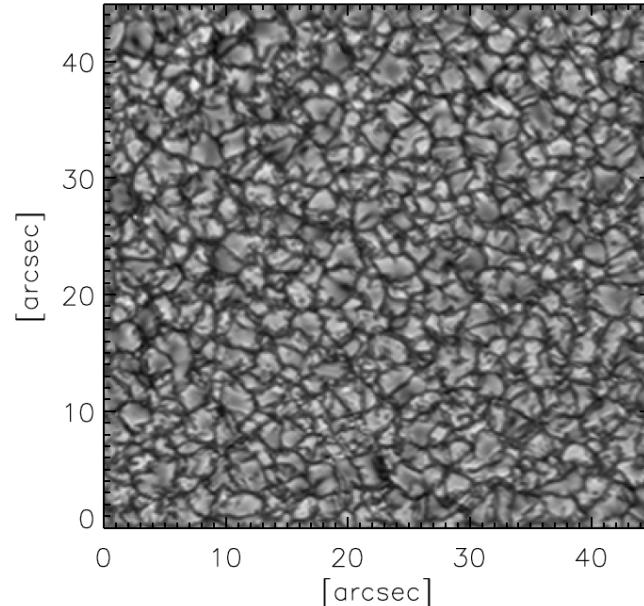
Line shape tracks the depth run of the source function (wavelength maps to height!)

# So, to recap

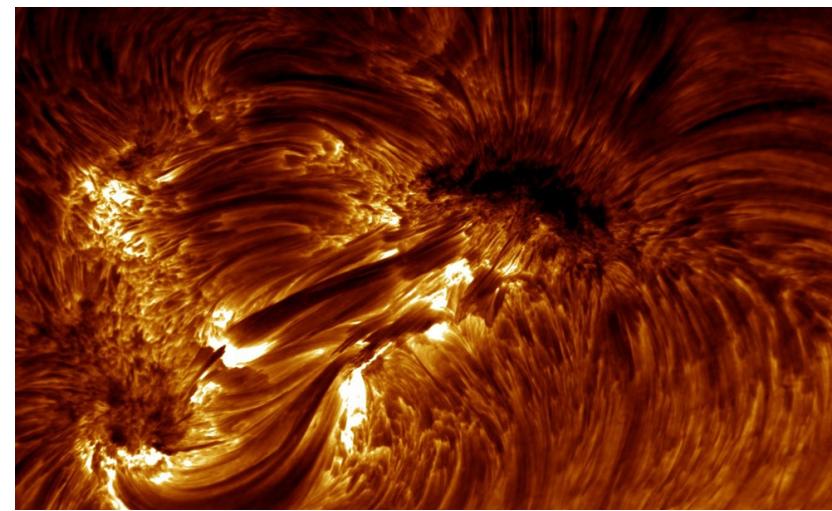
- Coupling between the intensity (photons), and level populations (atoms).
- Numerically demanding
- Non-local (radiation can travel a looot)
- **Quiz:**



Credits:  
HINODE / SOT



SUNRISE/IMAX (Danilovic et al, 2010)



Credits: SST

# Where does a spectral line form?

- Well, strictly speaking it depends on a model atmosphere.
- We can model the spectrum, and extract some relevant quantities.
- **Tau = 1 point (surface)** : the simplest measure of the “height” of formation
- **Contribution function:** how much does each layer contribute

$$I_{\lambda}^{+} = \int_0^{\infty} S(\tau_{\lambda}) e^{-\tau_{\lambda}} d\tau_{\lambda}$$

- **Response function:** how sensitive is the spectra to the changes in a layer

$$R_{\lambda}(q, h_d) = \frac{\partial I_{\lambda}^{+}}{\partial q_d}$$

# Let's apply it to our academic 2-level atom problem

This is statistical equilibrium

$$S_d = \epsilon B_d + (1 - \epsilon) \sum_m \sum_l w_m w_l I_{d,l,m}$$

This is radiative transfer

$$I_d = \sum_0^{ND} w_{d,d'} S_{d'}$$

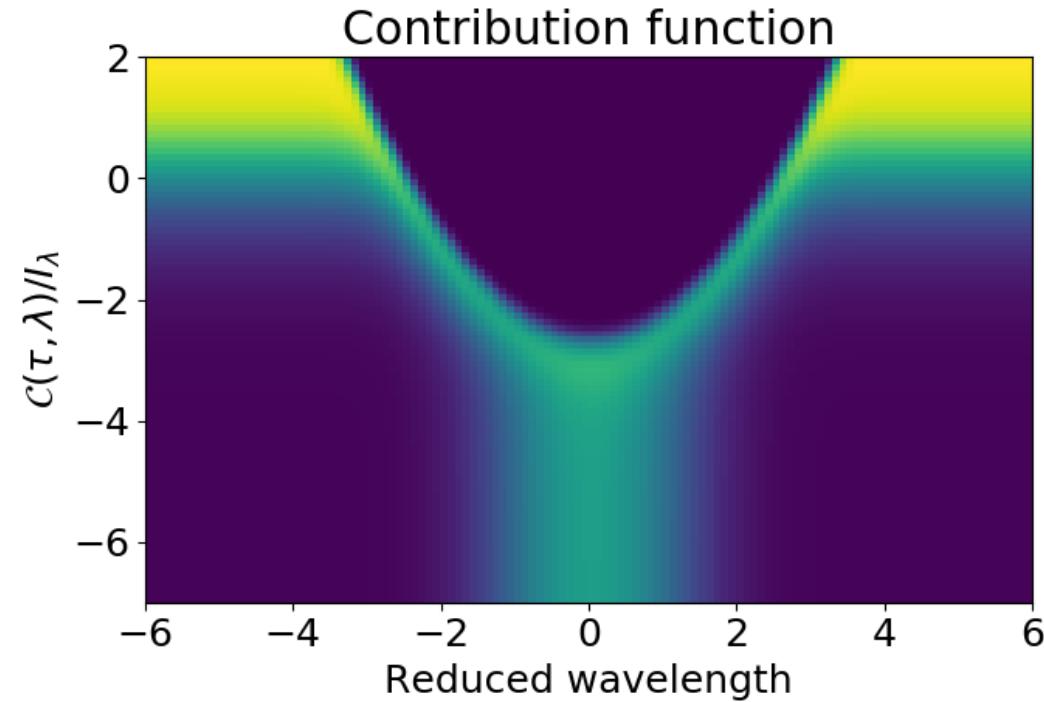
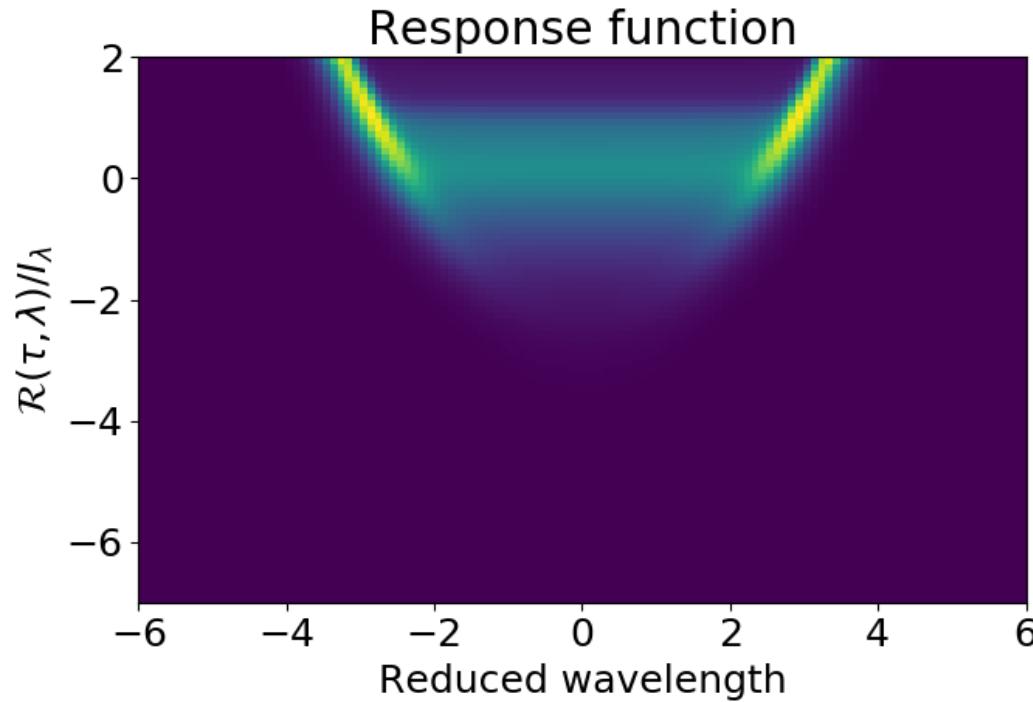
Let's merge them into one:

$$S_d = \epsilon_d B_d + (1 - \epsilon_d) \sum_{d'=0}^{ND} \Lambda_{d,d'} S_{d'}$$

This is the contribution function

To get the response function, we need to calculate derivative of the last equation to each  $B$  and plug it back into the formal solution

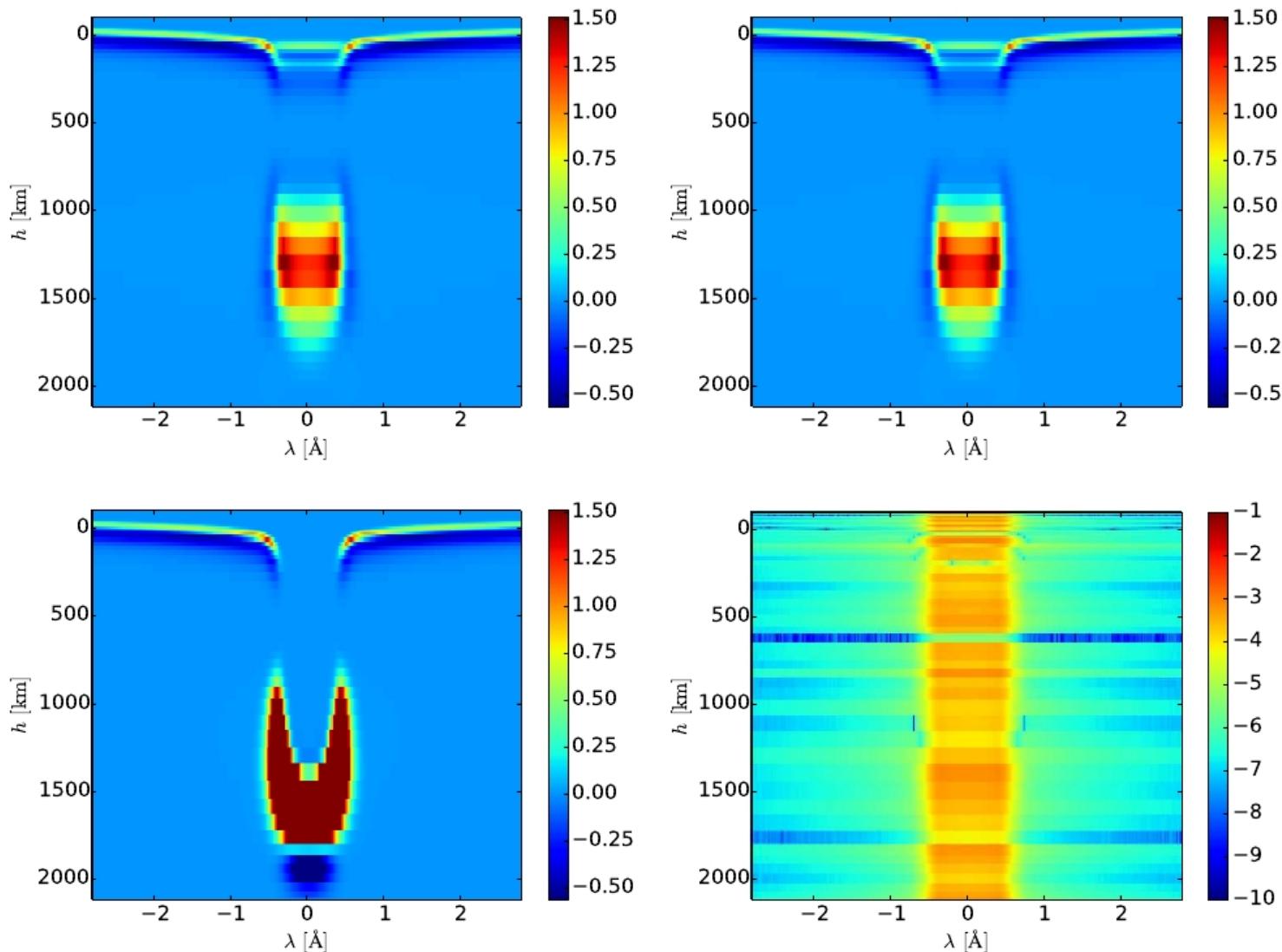
# Let's do it!



$$S = \epsilon B + (1 - \epsilon) \hat{\Lambda} S$$
$$(I - (1 - \epsilon) \hat{\Lambda}) S = \epsilon B$$
$$\frac{dS_d}{dB_{d'}} = (I - (1 - \epsilon) \hat{\Lambda})^{-1} \epsilon \delta_{d,d'}$$

- This algebra shows us how the Source function responds to temperature
- From there we can easily calculate intensity response function

# Real life example (well, sort of): H alpha - like 2 level atom



- Generalization of the method presented above to multilevel problems
- We can capture exactly all the spatial and inter-level dependencies
- Note the double peak of the RF

## More on the response functions

- An essential ingredient of inversion codes
- They also tell us something about line formation
- That is, after solving this problem we know:

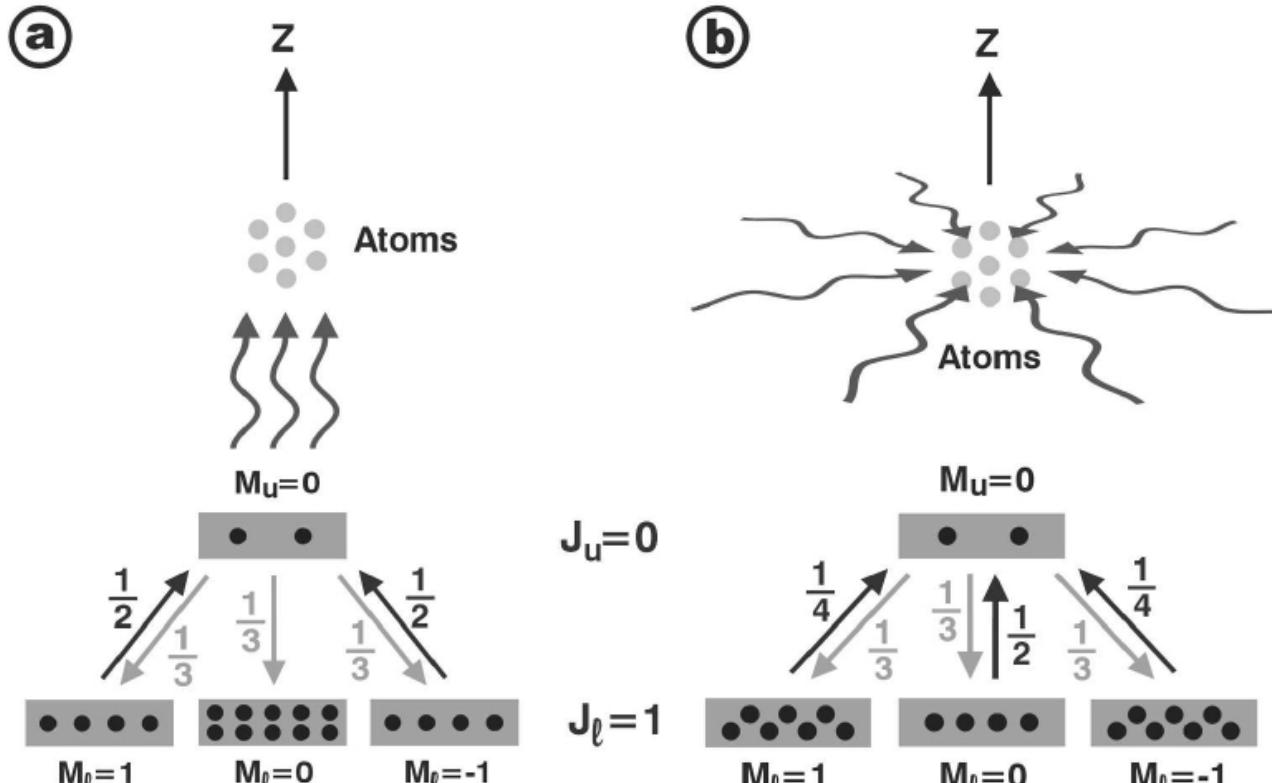
$$\frac{\partial I_d(\Omega, \lambda)}{\partial T_{d'}}$$

everywhere in the atmosphere.

- Now can also calculate the response of any moment of the intensity to T
- For example the anisotropy? It determines the scattering polarization

$$J_0^2 = \frac{1}{2\sqrt{2}} \int \oint I(\lambda, \hat{\Omega}) (1 - 3\mu^2) \frac{d\Omega}{4\pi} \phi \lambda d\lambda$$

# Before we go to play, lets look into this



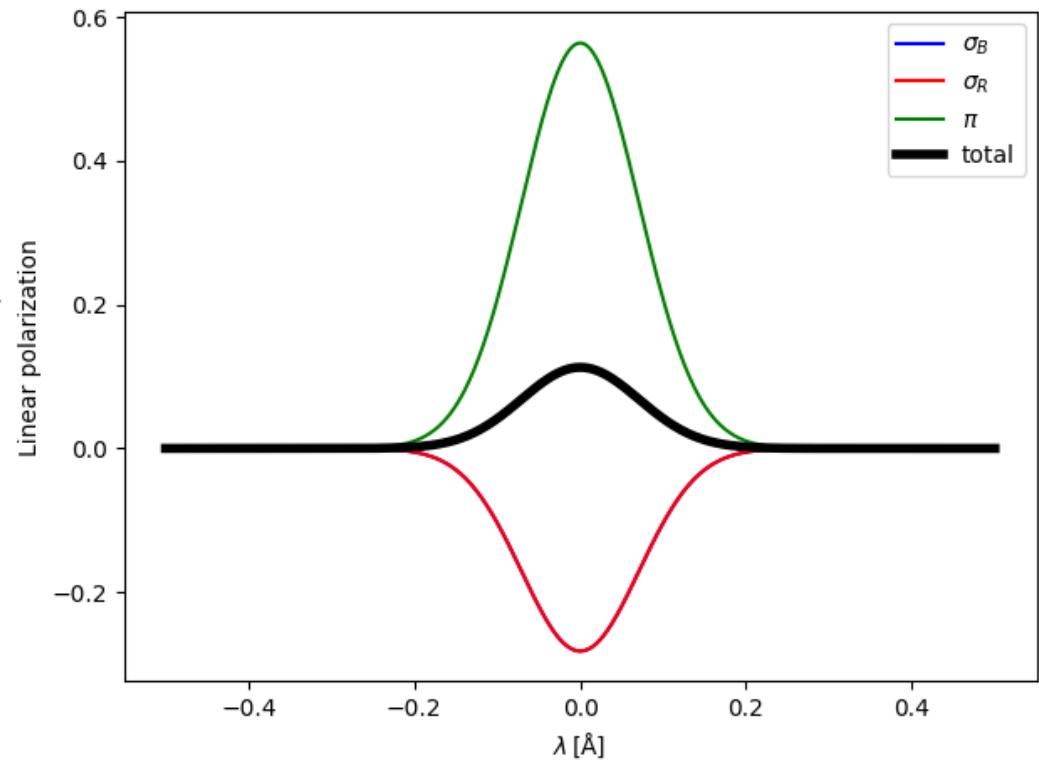
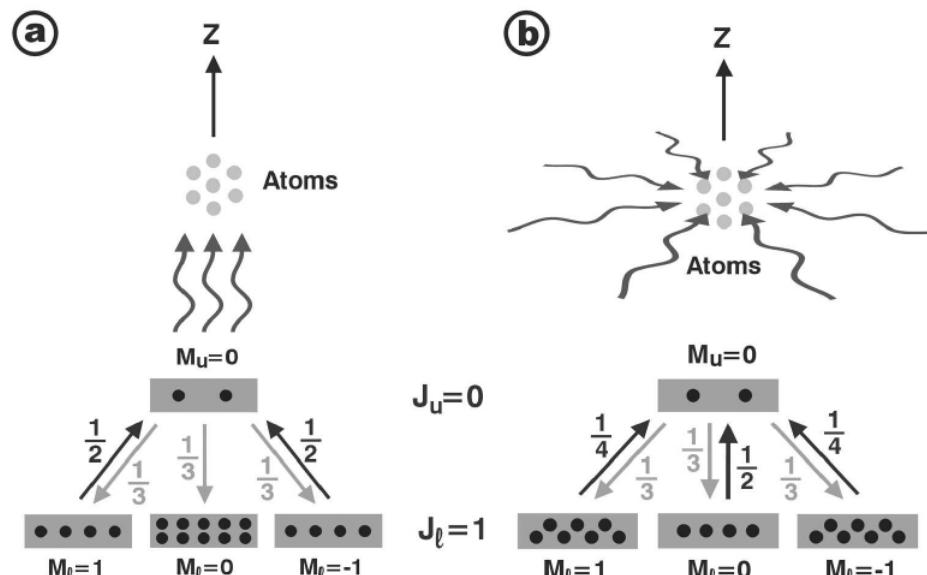
„Selective absorption“

Uneven population of  
Zeeman subl-levels  
leads to the  
“polarization” of the  
atomic levels.

This leads to the net  
linear polarization of the  
light.

from Trujillo Bueno (2003)

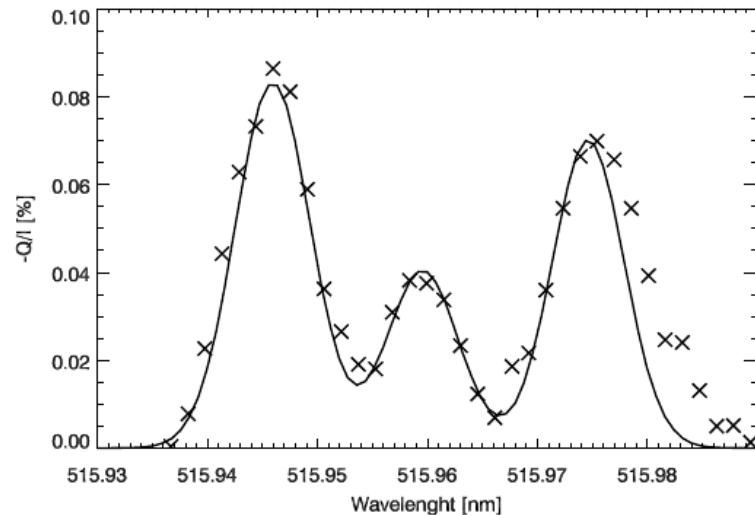
# Scattering line polarization – comparison with Zeeman



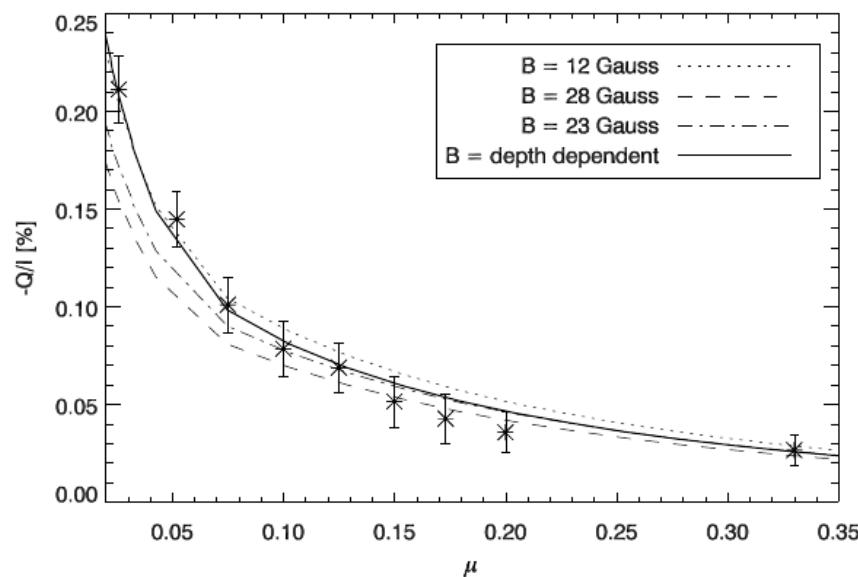
from Trujillo Bueno (2003)

# Scattering polarization

- Inherently a NLTE effect (what gave it away?)
- Depends on a proper modeling of the radiation anisotropy (Solar atmosphere is something between the two cases we just saw).
- Further influenced by the magnetic field – **Hanle effect**
- No typical inversions so far for the “atmospheric” lines (i.e. ones formed in a stratified atmosphere) – only fitting the mean spectra

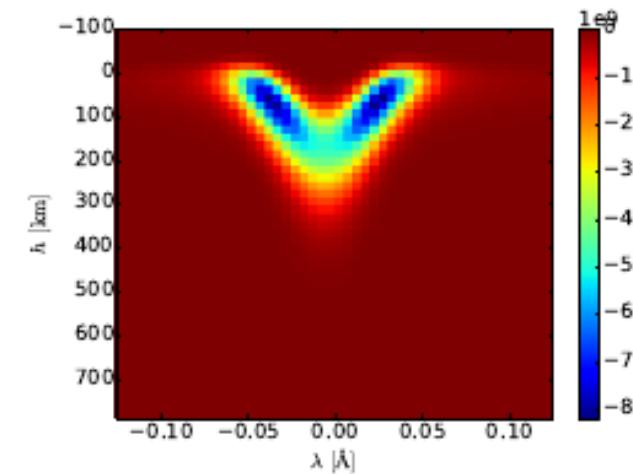
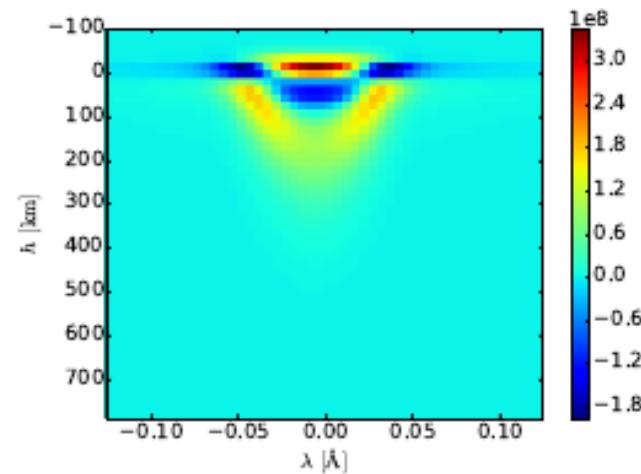
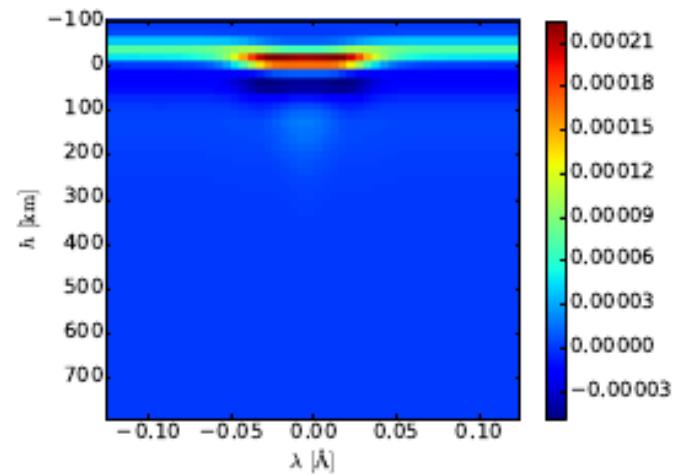
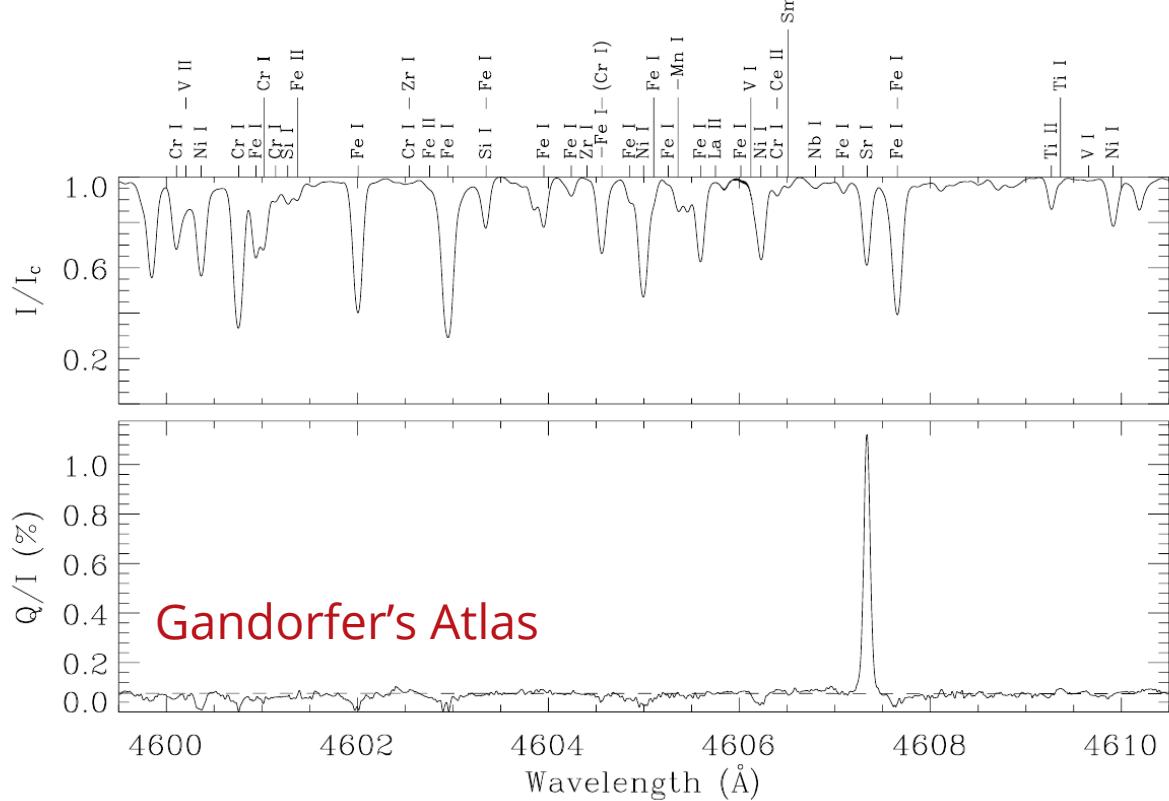


Milic & Faurobert (2012)

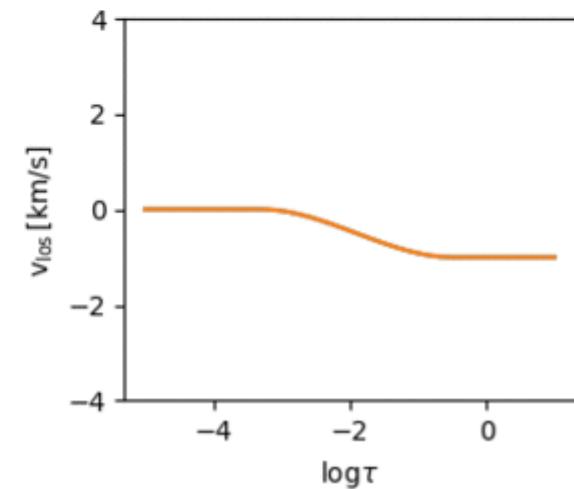
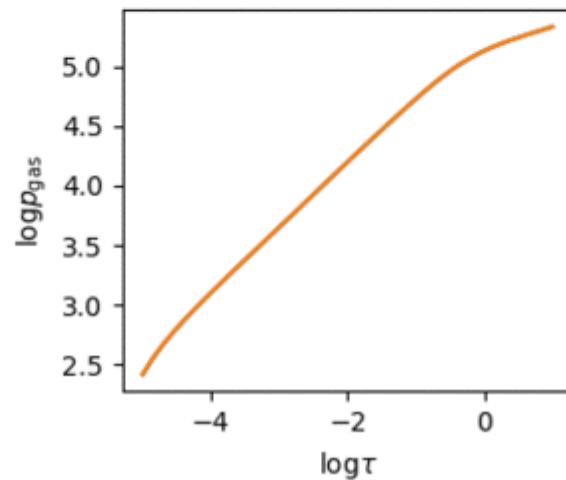
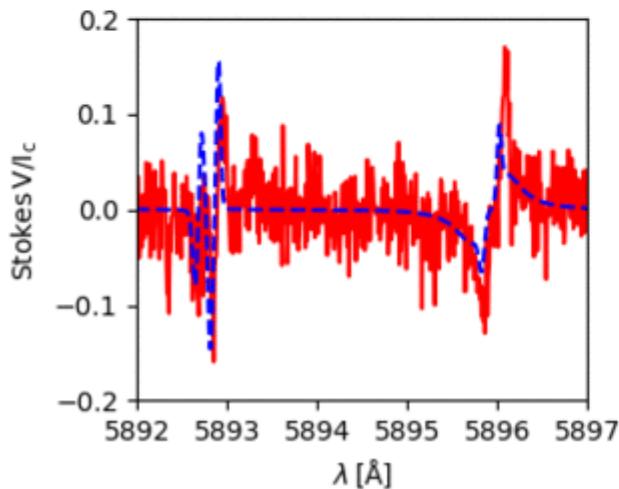
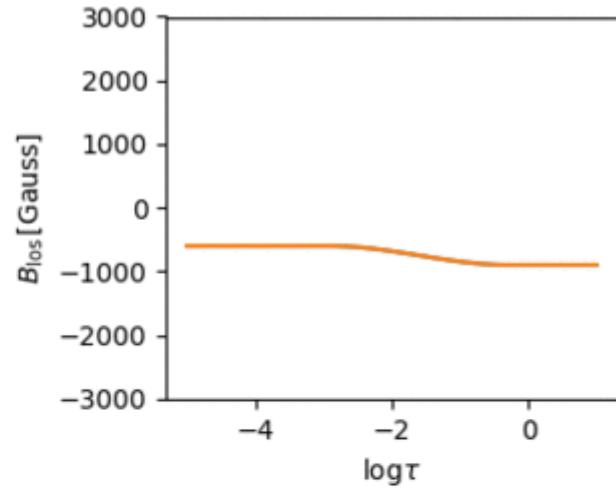
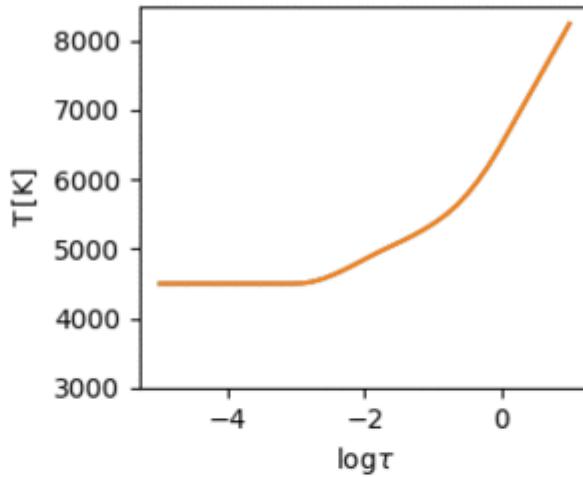
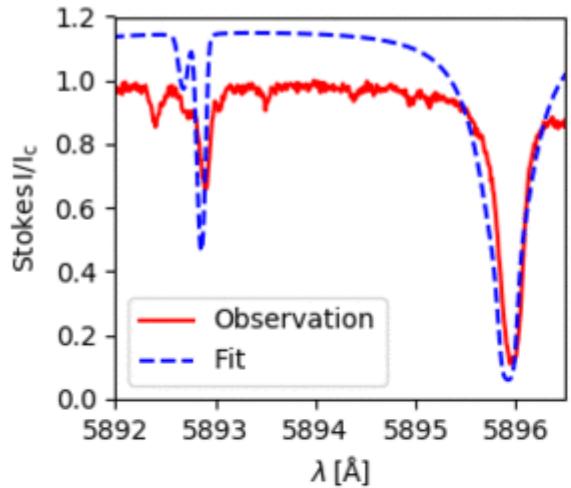


# Response functions for scattering polarization

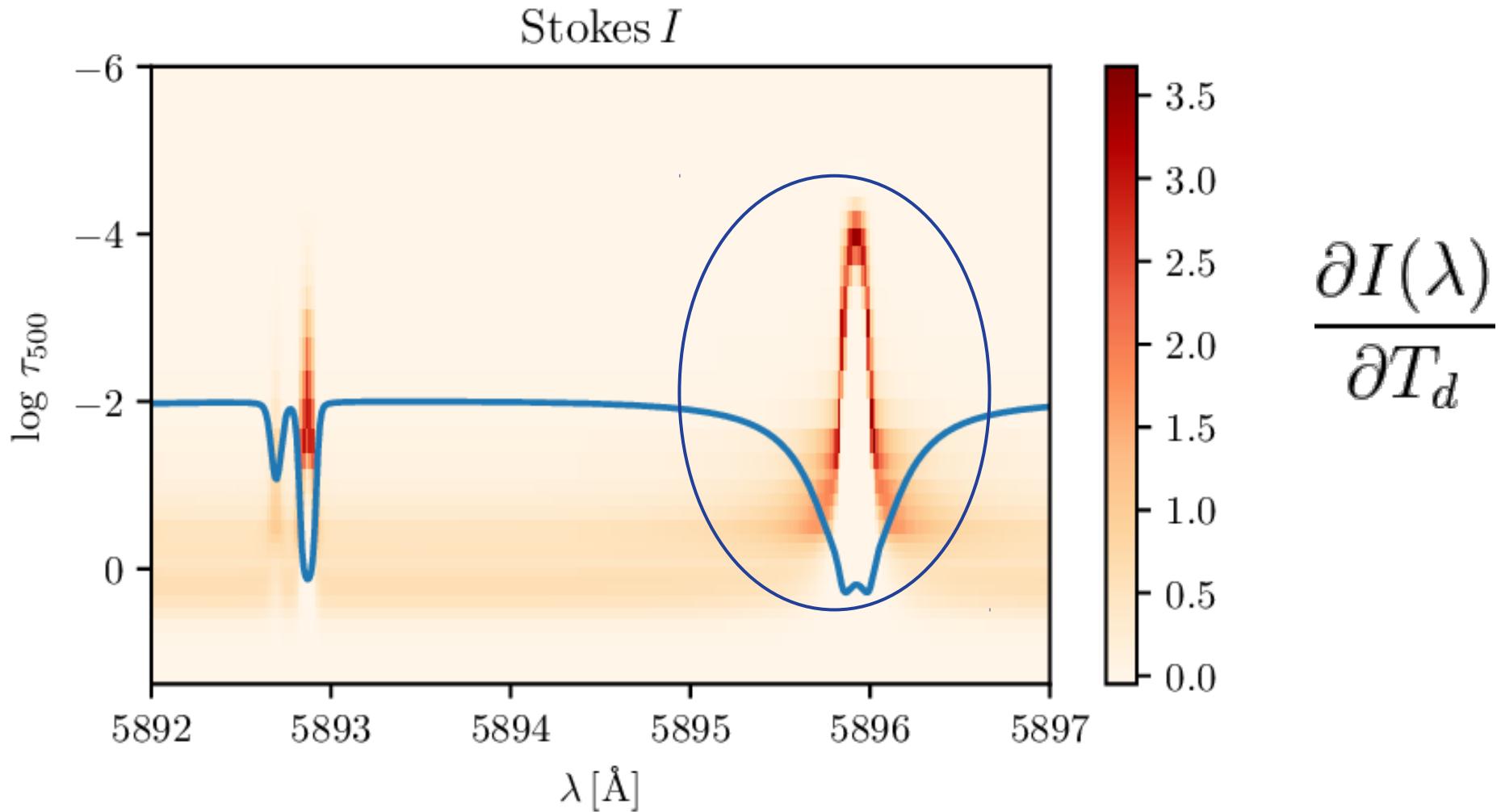
- Beloved Si I 4607 line.
- Modeled as 2lvl + continuum
- A promising tool for quiet Sun magnetism (DKIST target)
- Complements Fe I 6300 lines



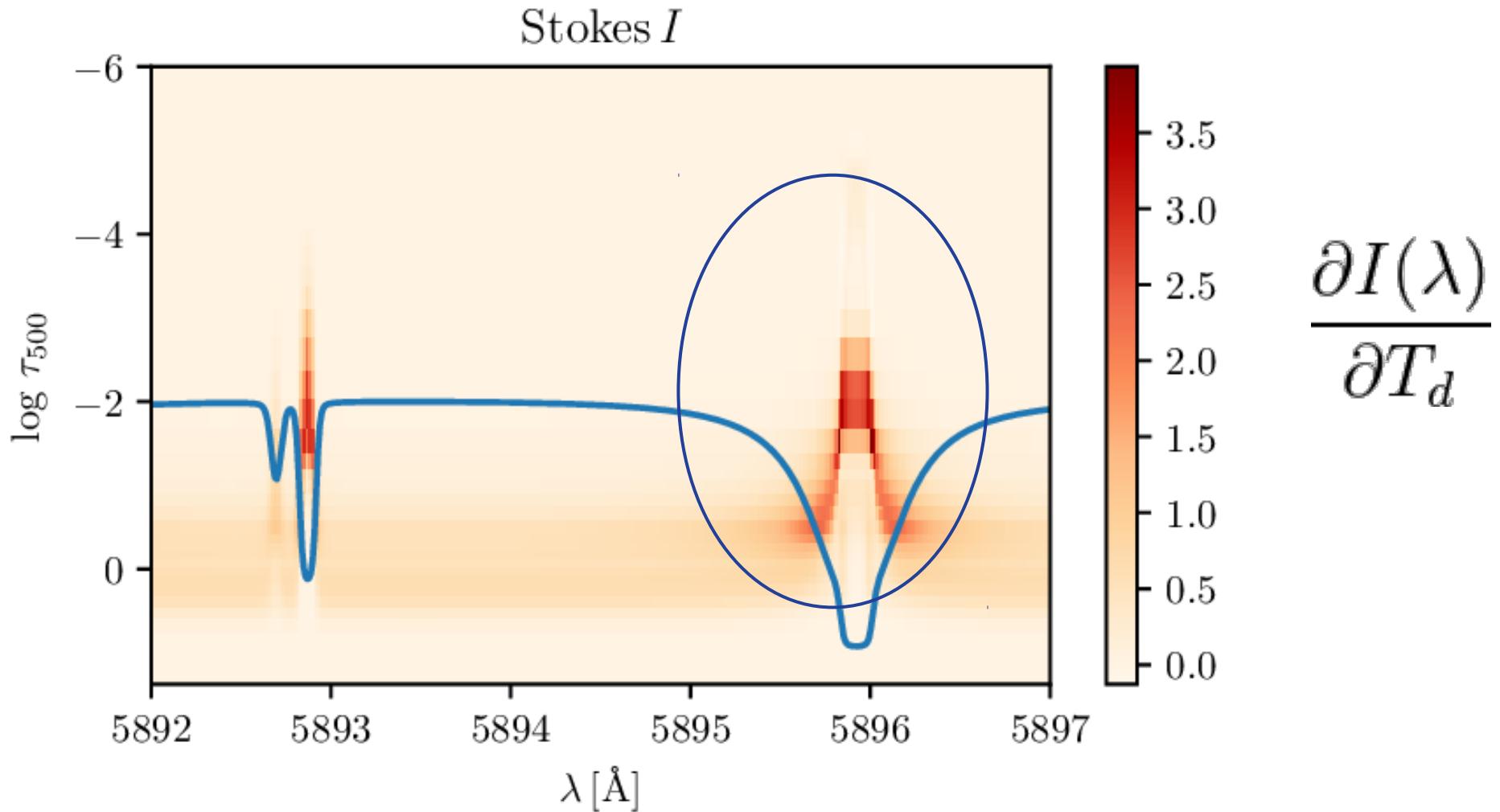
# What do we use these response functions for? - Inversion



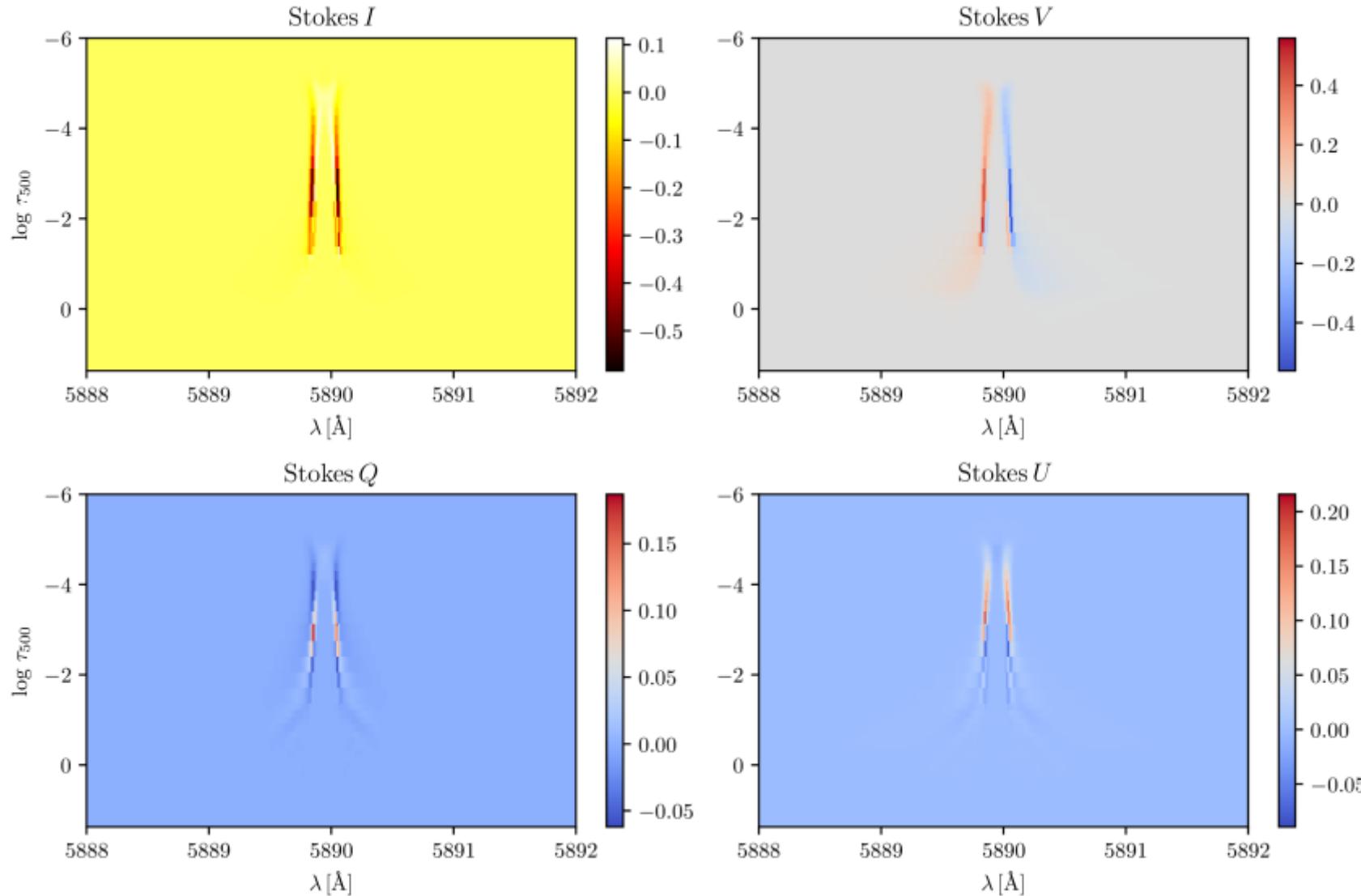
Wait wait wait, something is not correct here!



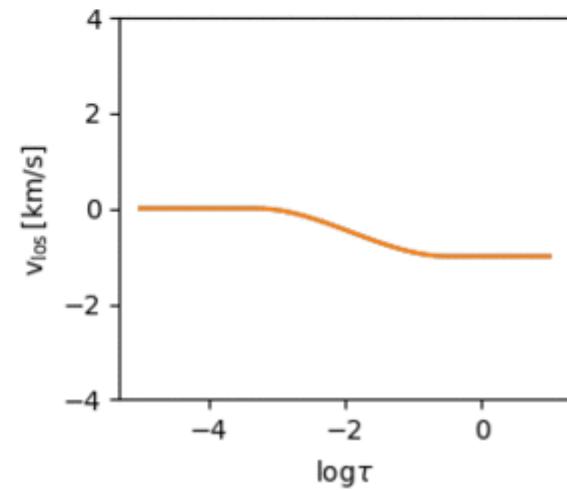
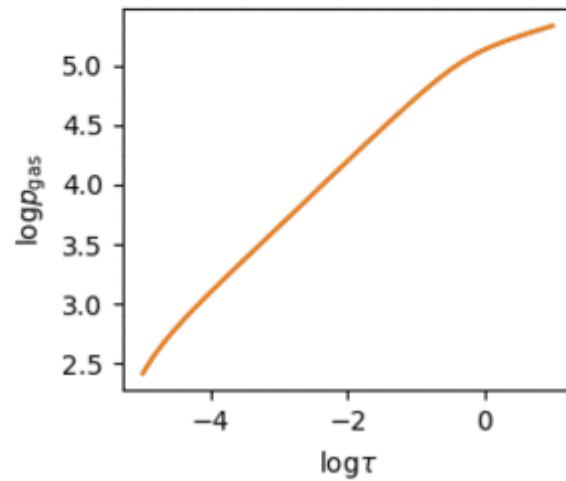
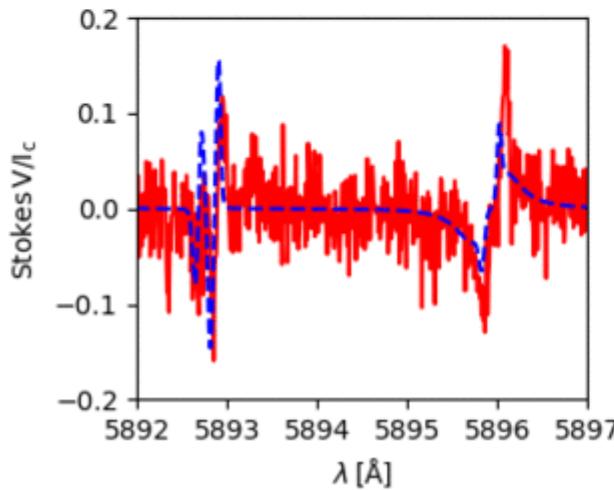
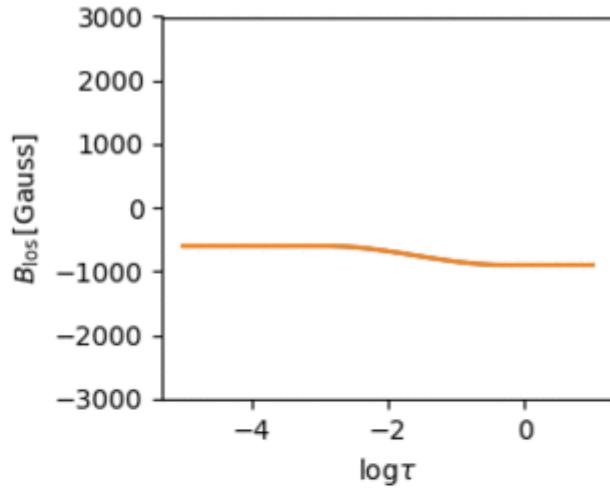
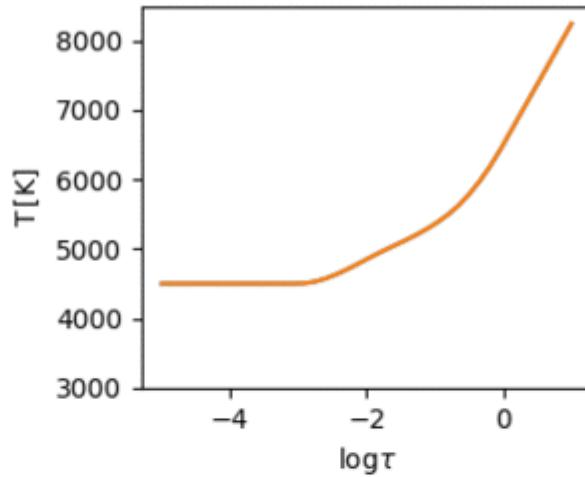
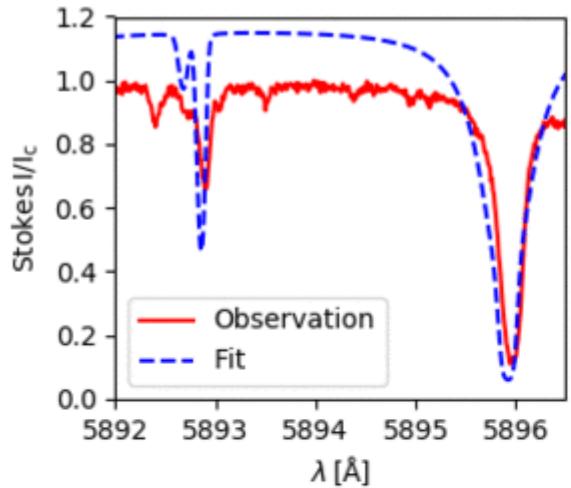
Ah sweet, this NLTE stuff actually **is** important

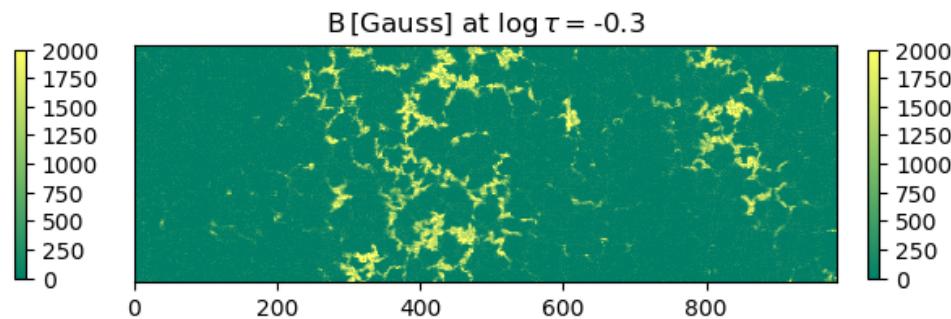
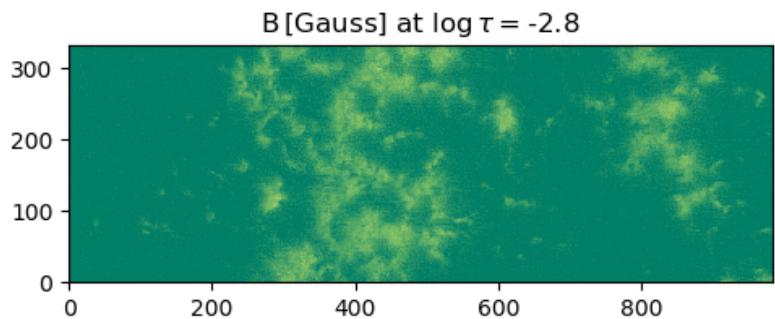
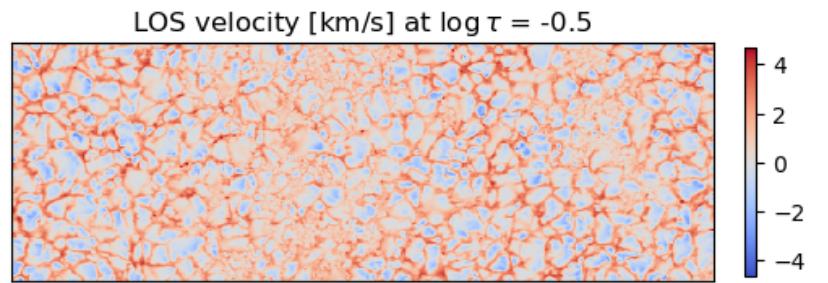
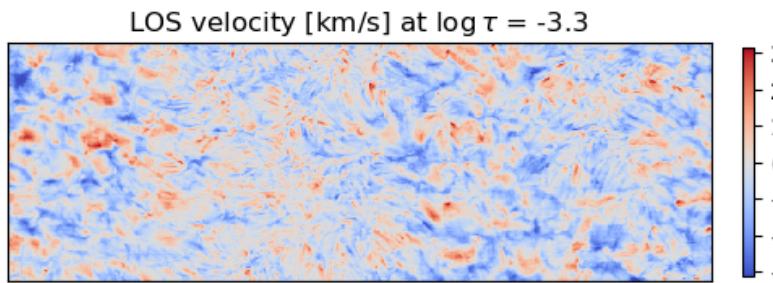
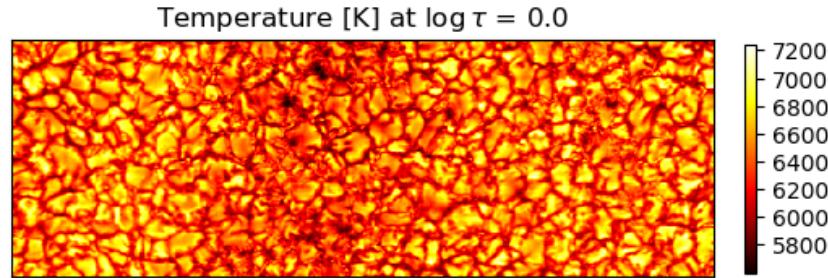
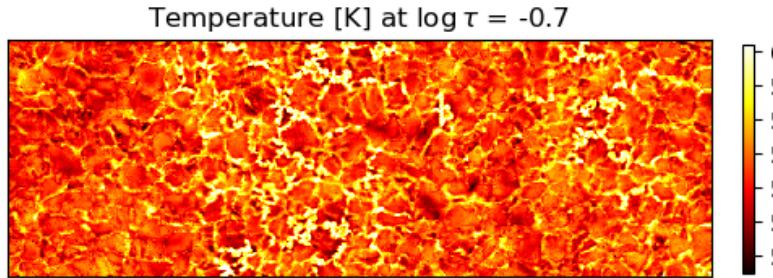
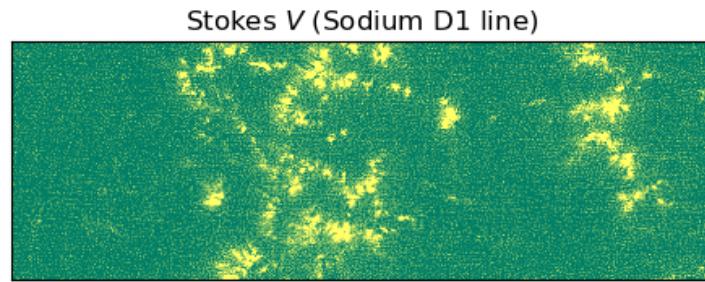
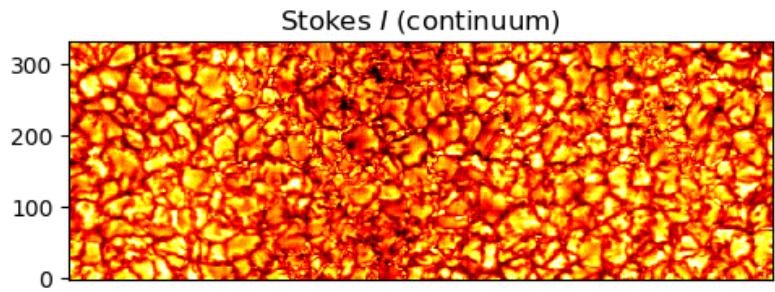


# Response functions to the magnetic field - why do they still exist high in the atmosphere?



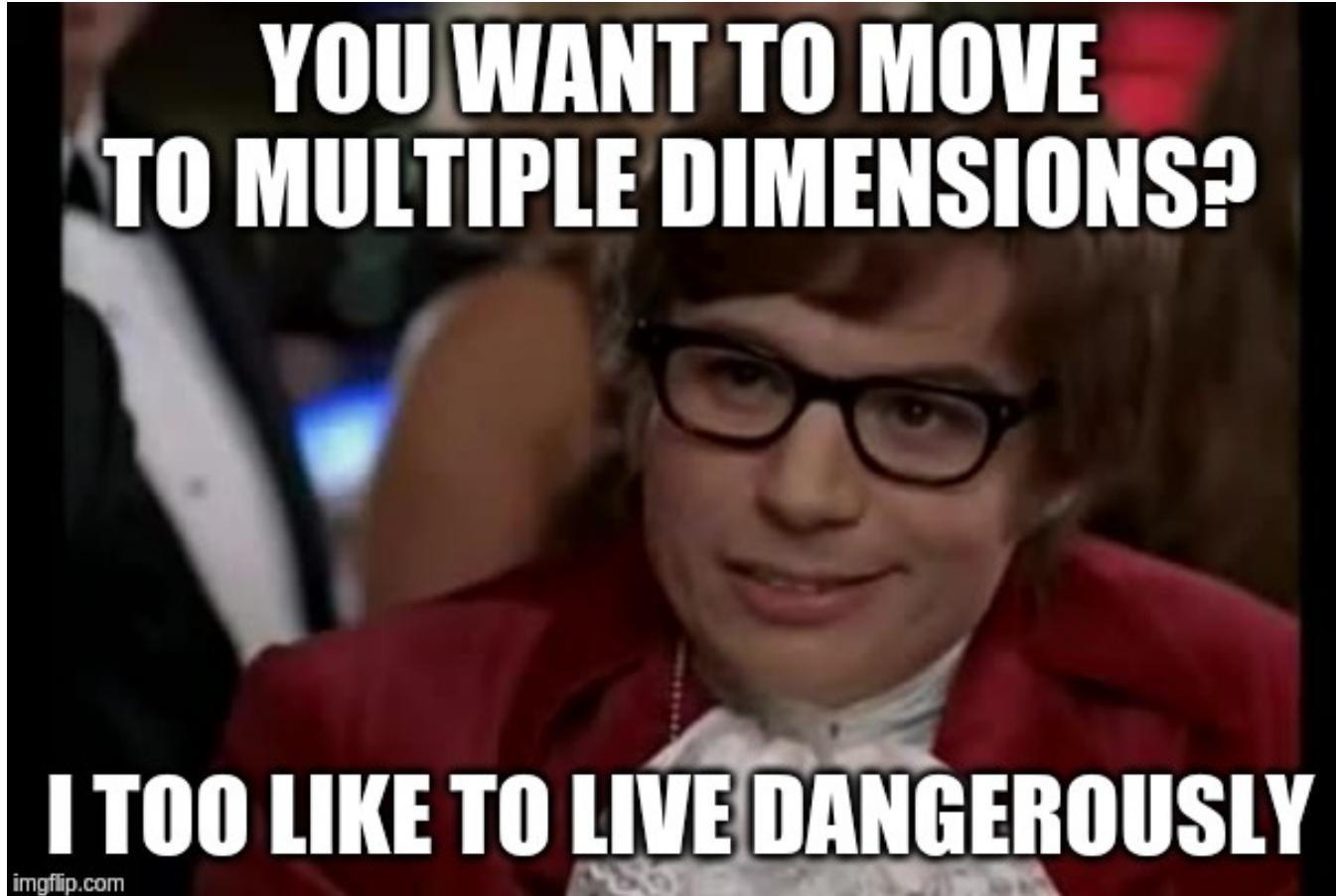
# What do we use these response functions for? - Inversion



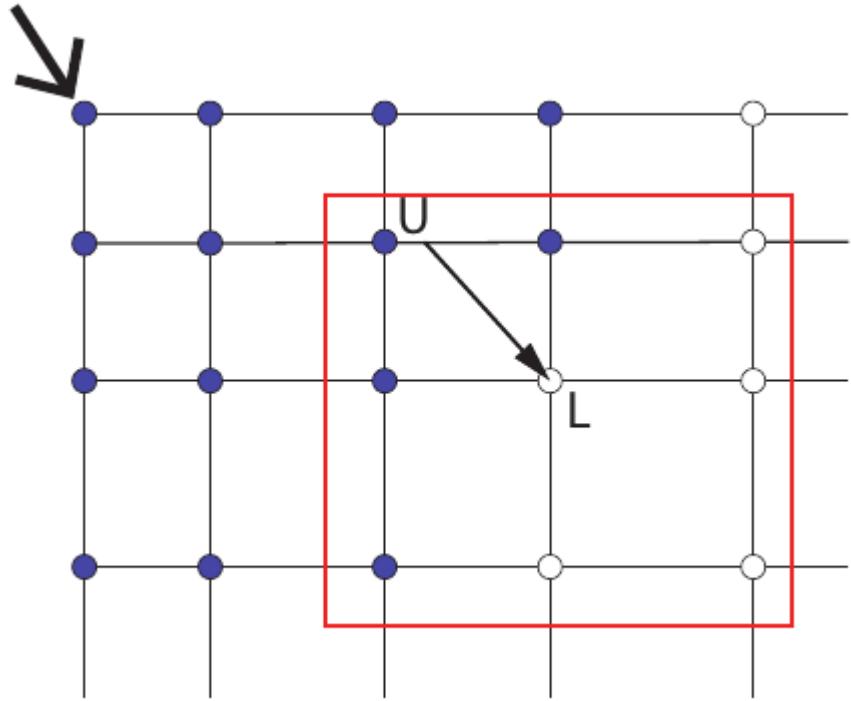


Wait Ivan, you said RT is non-local, that means...

- That we also need to think about the light that travels laterally!



# Multidimensional NLTE radiative transfer



- Increased number of spatial points (100-10000 times more).
- Additional angle dependence
- “Upwind” point does not lie on the grid, we need to interpolate quantities there.

$$I_L = I_U e^{-\Delta} + \int_0^{\Delta} S(t) e^{-t} dt$$

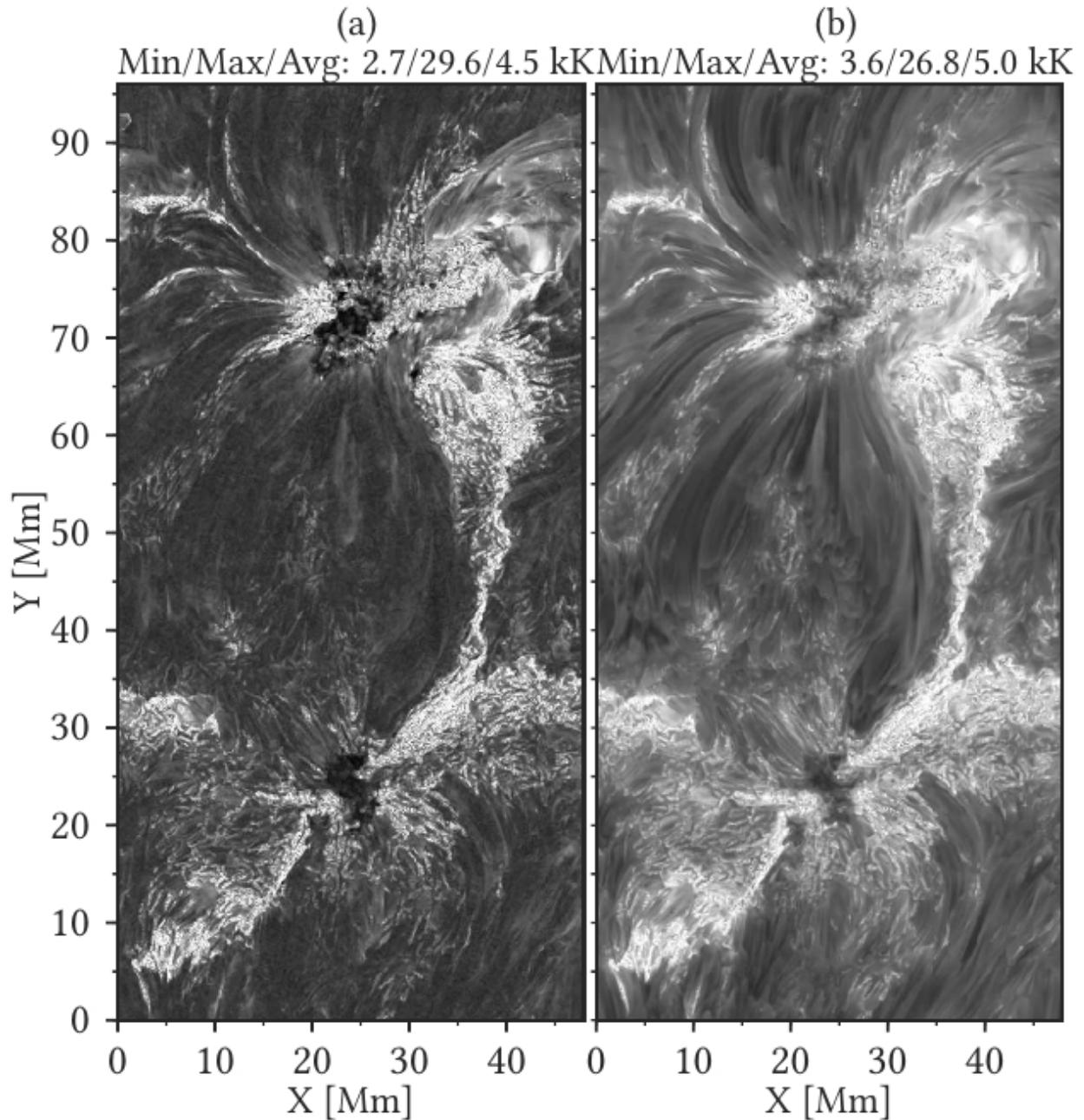
Milic, PhD thesis

$$I_L = I_U e^{-\Delta} + w_L S_L + w_U S_U + \dots$$

# Couples the atmosphere – smooths the source function

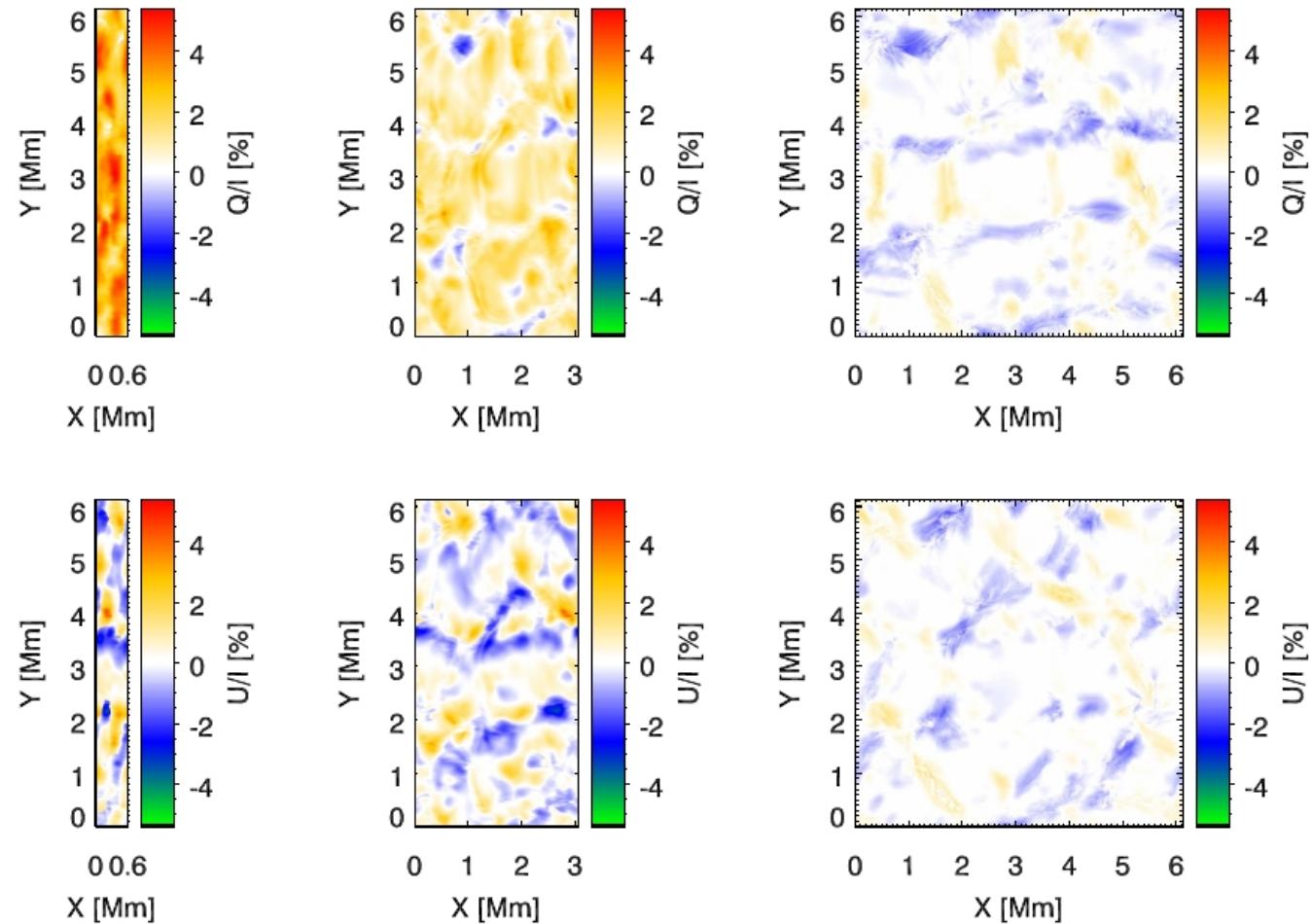
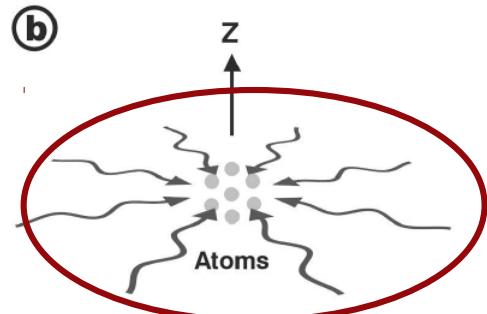
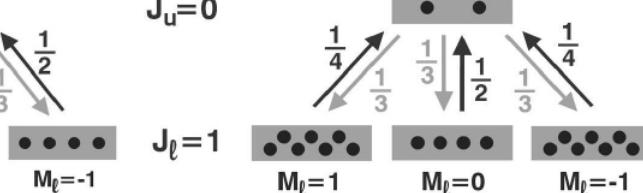
- 3-level Hydrogen atom, with CRD, and nlte ionization
- MHD simulation similar to Cheung et al (2018)
- NLTE solution and synthesis using Multi3D
- Note lower contrast by higher average brightness in 3D!

Halp<sub>a</sub> line core,  
calculated by Bjorgen  
et al. 2019



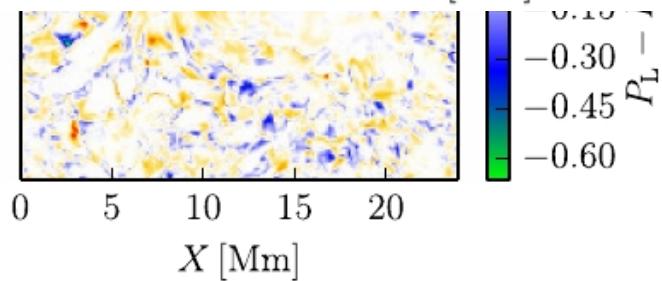
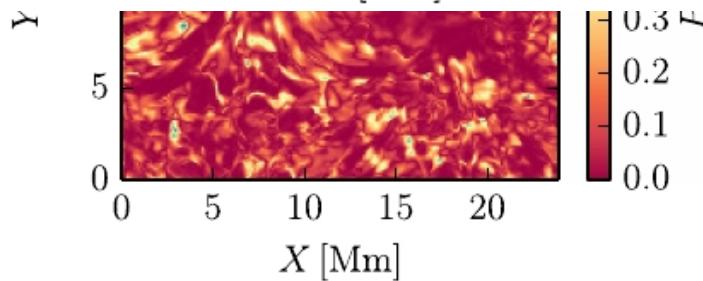
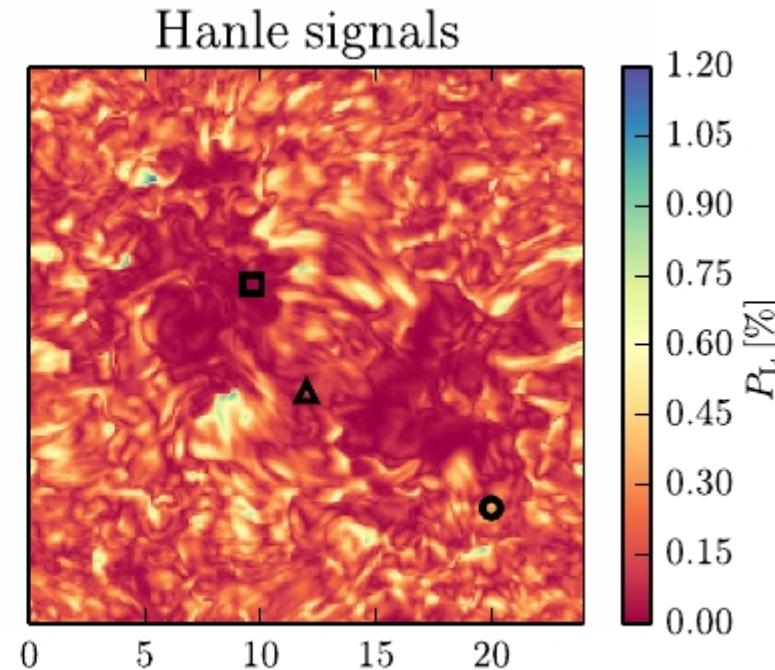
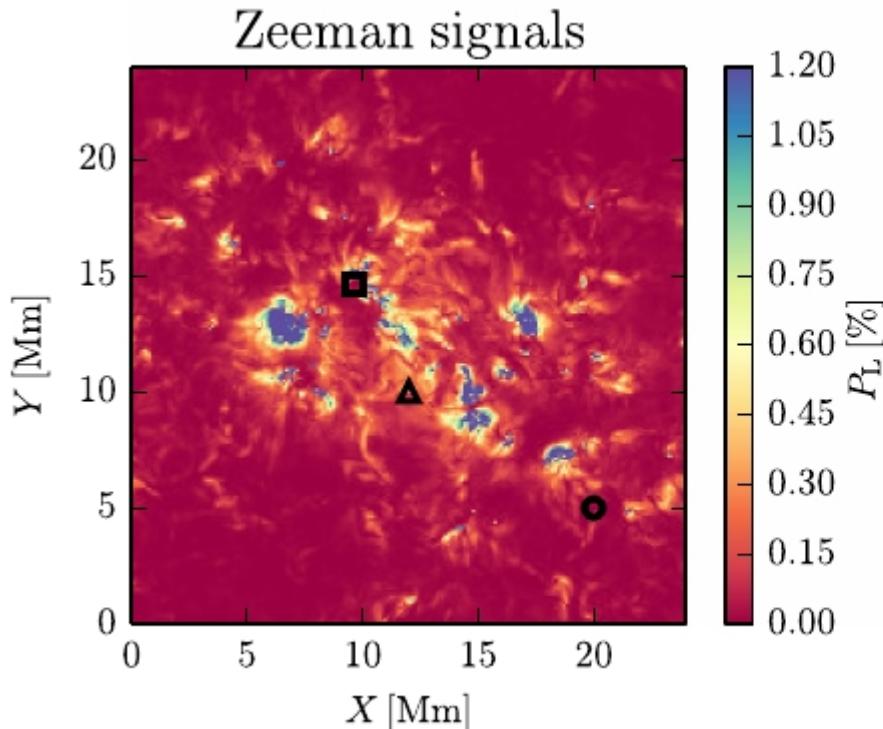
# Since the atmosphere is multi-dimensional

Atoms



Sr I 4607 polarization  
from del Pino Aleman  
et al (2018)

And modifies the radiation anisotropy



Stepan and Trujillo  
Bueno (2016)

# How hard are these calculations?

*"I am writing a new 3D NLTE code right now, I think it is going to be a good practice."* - Every enthusiastic PhD student, ever

- It is a great practice! But, there are a number of things to think about:
- Typical MHD simulation is, say  $512 \times 512 \times 100$  points. We need typically 50 angles and some 100 wavelengths:

**10E11 quantities (intensities) per iteration.**

- This must be done in parallel, using efficient techniques and robust codes.
- Radiative Transfer calculations are always going to be orders of magnitude slower than (M)HD ones, because we have **3 extra dimensions** (wavelength, direction)
- Calculation of a self-consistent 3D NLTE RT problem takes days if not weeks.

## 3D Diagnostics (future):

- Spectropolarimetric inference in 1D:

$$\mathcal{F}_{1D}[T(z), v(z), B(z)\dots] = \hat{I}_\lambda$$

- Inference in “2D” (actually 3D, e.g. van Noort, 2012)

$$PSF(x, y) \star \mathcal{F}_{1D}[T(x', y', z), v(x', y', z), B(x', y', z)\dots] = \hat{I}_\lambda(x, y)$$

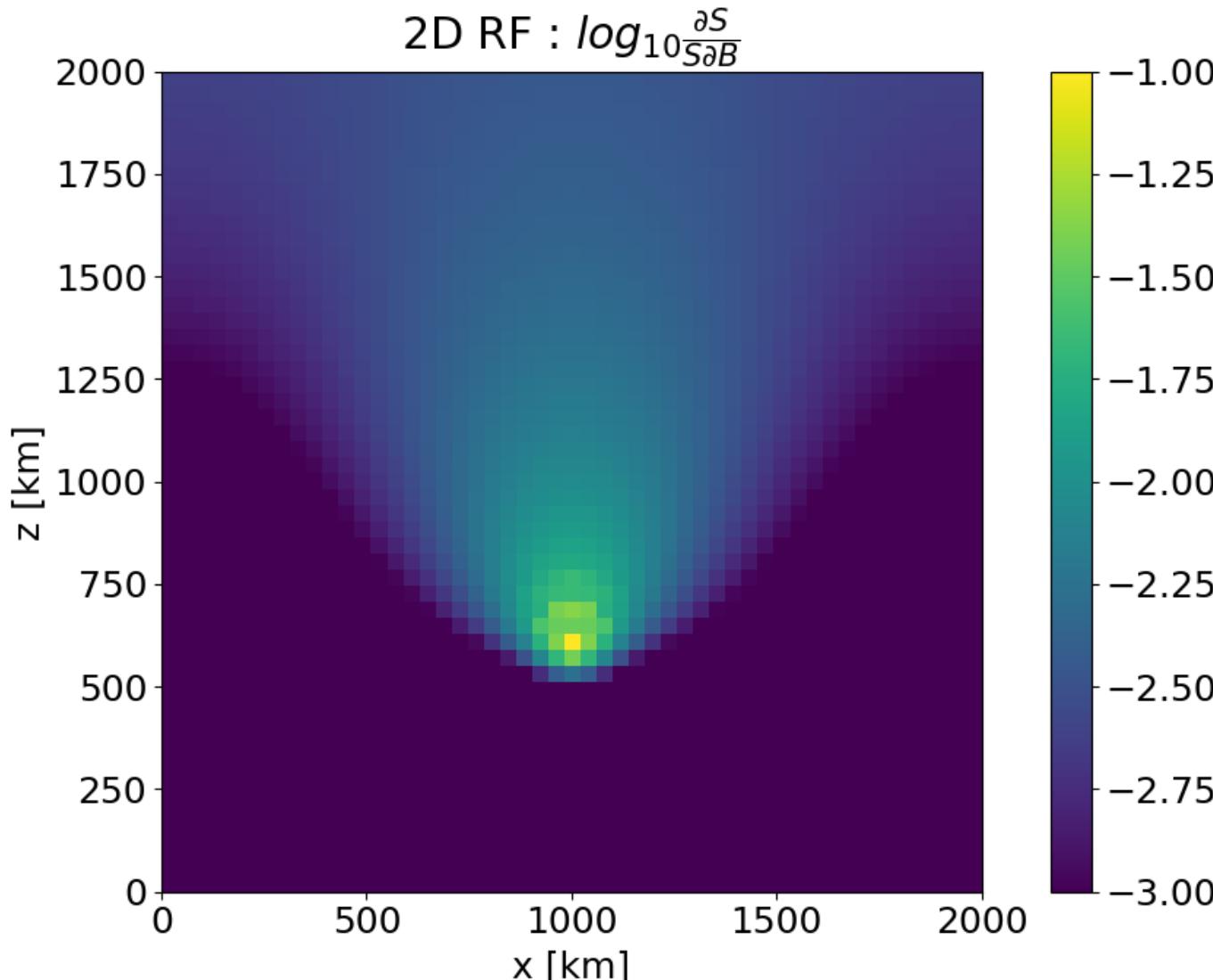
- Inference involving 3D radiative transfer (we do not have it **yet**):

$$\mathcal{F}_{3D}[T(x', y', z'), v(x', y', z'), B(x', y', z')\dots] = \hat{I}_\lambda(x, y)$$

- This would be a response function in 3D ( $\sim 1E15$  quantities)

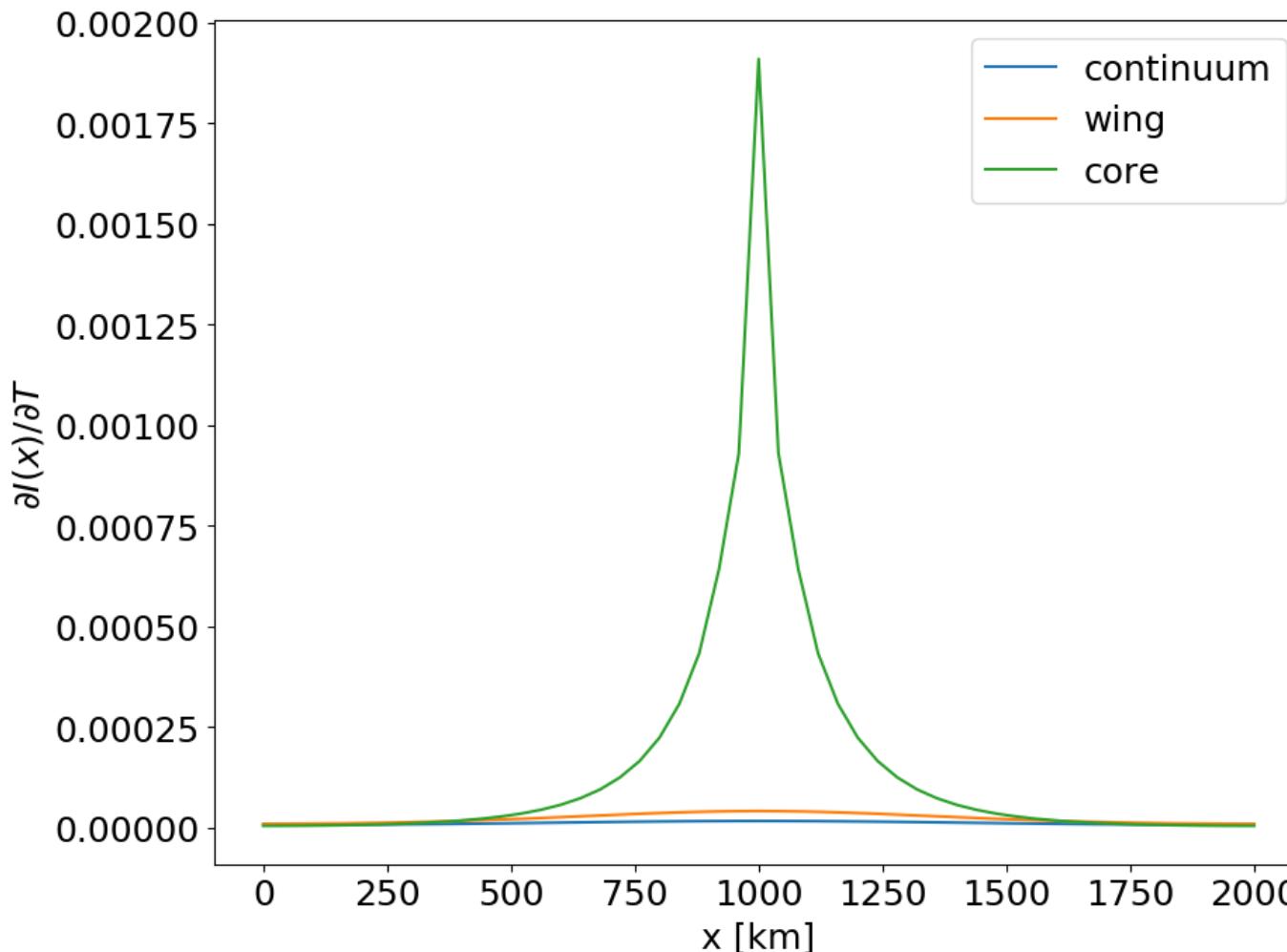
$$\frac{\partial I_\lambda(x, y)}{\partial T(x', y', z')}$$

# Multidimensional response functions:



- 2-level prototype line with total line-center optical depth of  $10^5$
- Isothermal atmosphere, perturbed at various depths (recall NLTE Rfs)
- This plot illustrates how temperature perturbation “diffuse” because of the line scattering

# Multidimensional response functions:



- 2-level prototype line with total line-center optical depth of  $10^5$
- This is how the emergent intensity responds to the perturbation.
- Width of the response ~ **few 100s of km!**
- Easily resolvable by DKIST!

## What is there to be done:

- We need a way to understand how 3D scattering influences the observable in the real-life examples.
- This is especially true for scattering polarization.
- Even without 3D, having a way to “invert” or diagnose spatially resolved “atmospheric” (i.e. not 10830) scattering polarization is needed.
- Finding a way to, at least statistically, compensate for 3D scattering, would be a huge step forward.
- We still need to work on faster and more stable self-consistent NLTE solutions, if we want to use realistic atom and atmosphere models.
- **Questions? Comments? Critics? Suggestions?**