Introduction to NLTE radiative transfer

…and polarization

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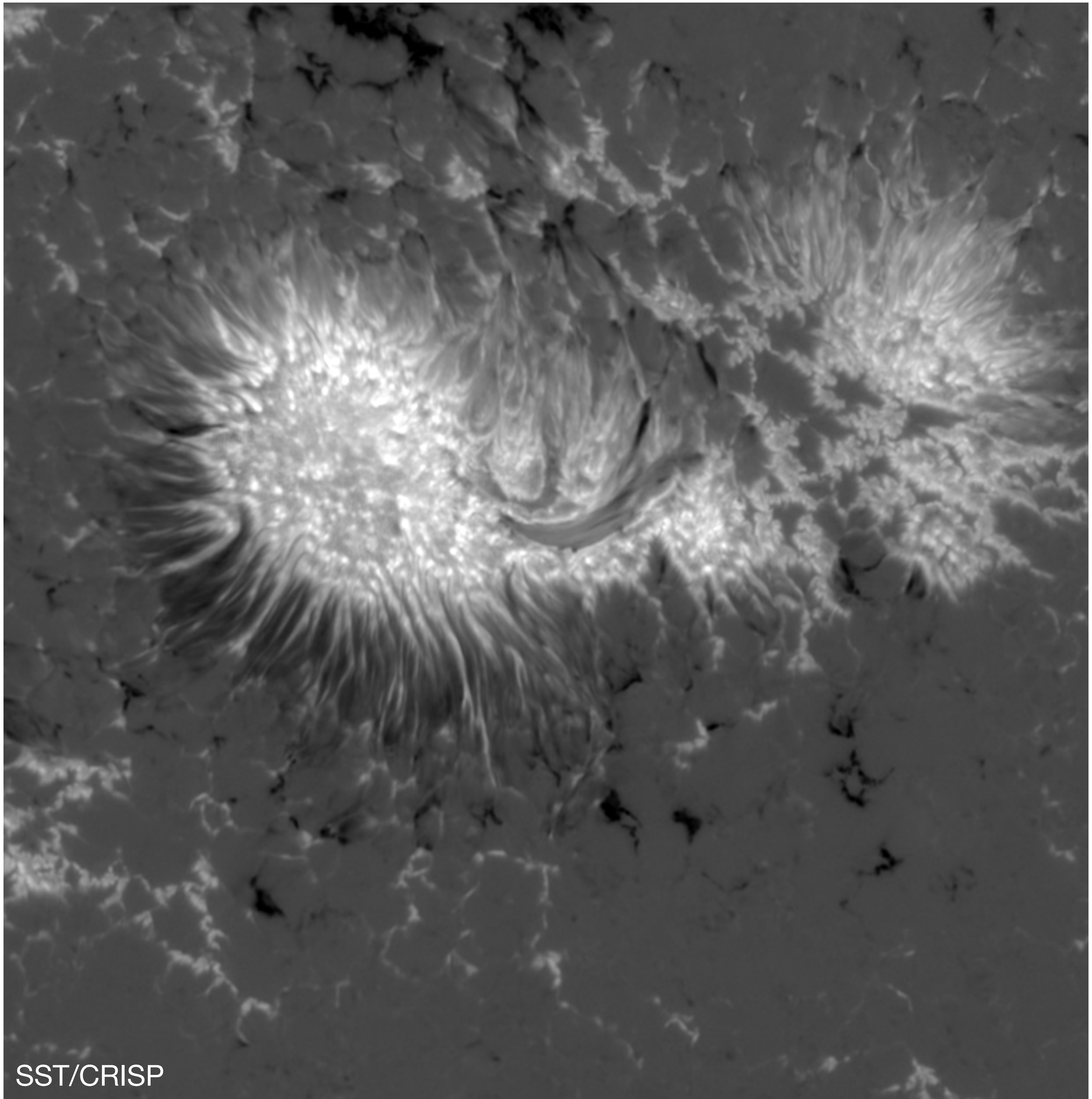
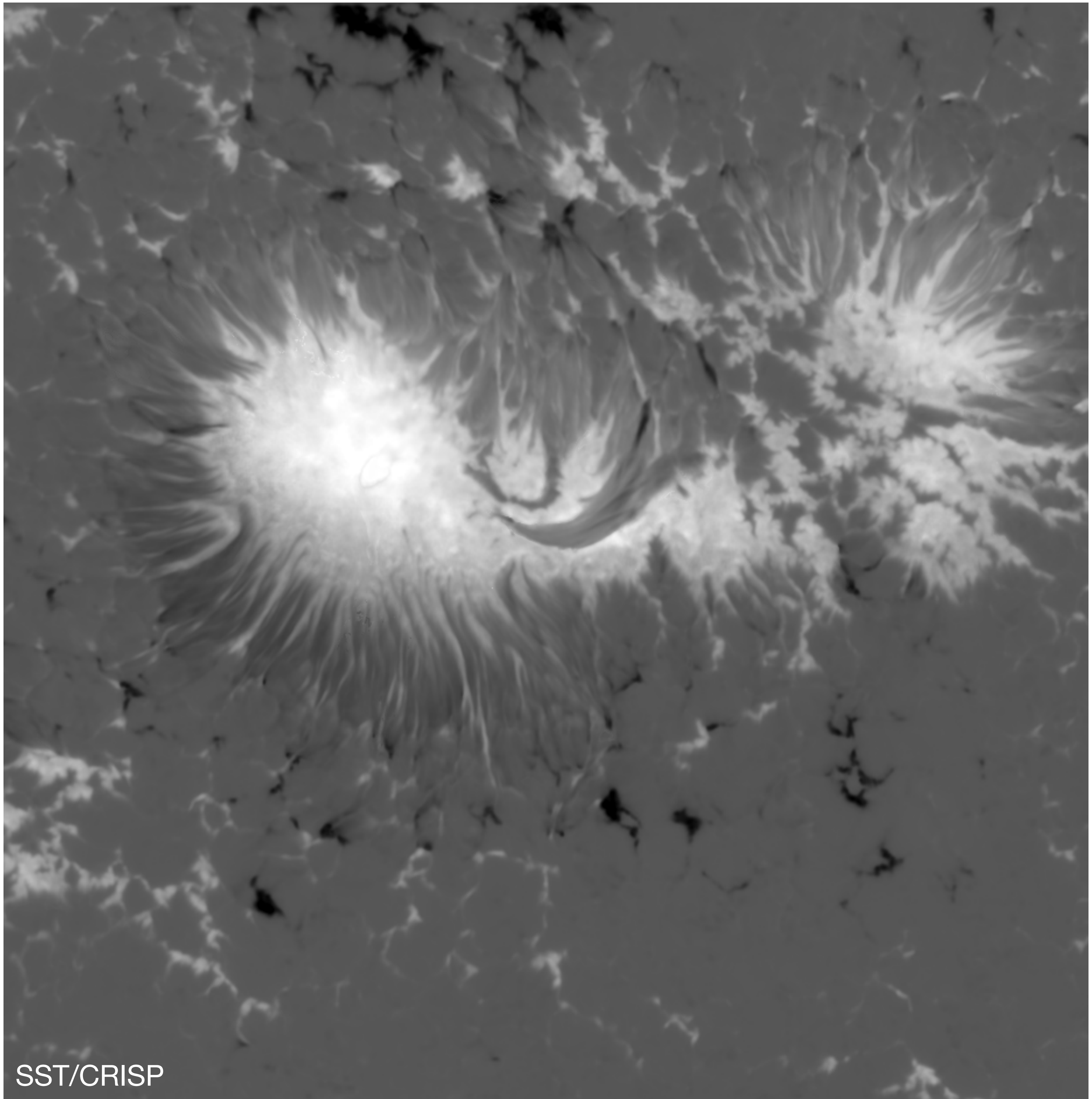
Our goals: explain observations in the photosphere

Fe I 6302 magnetogram $\sum_{\lambda} V_\lambda / I_\lambda$ (blue wing)

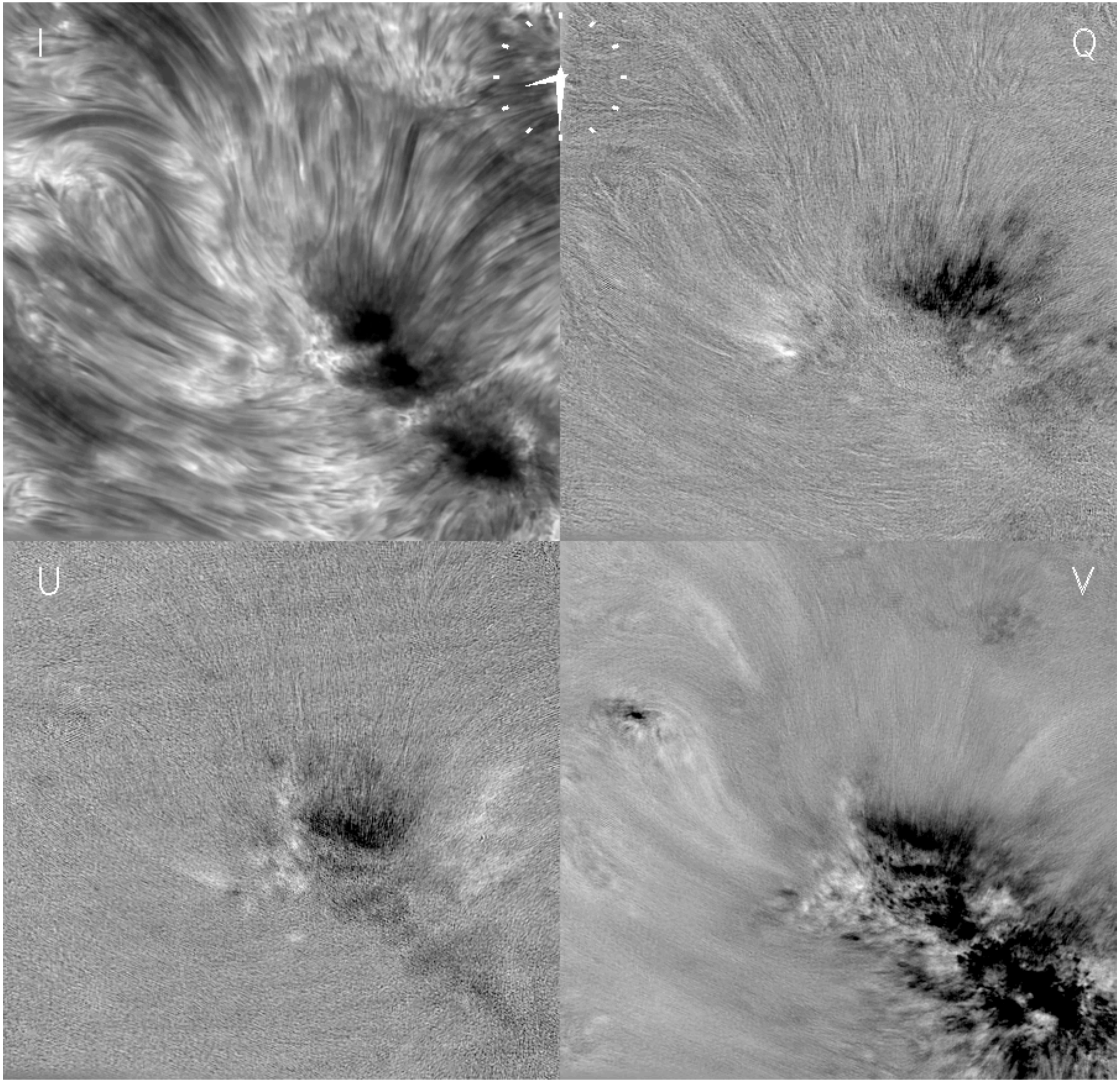


Our goals: explain observations in the photosphere

Milne-Eddington inversion: $B_{||}$



Our goals: explain observations in the chromosphere



Our goals: explain observations in the chromosphere

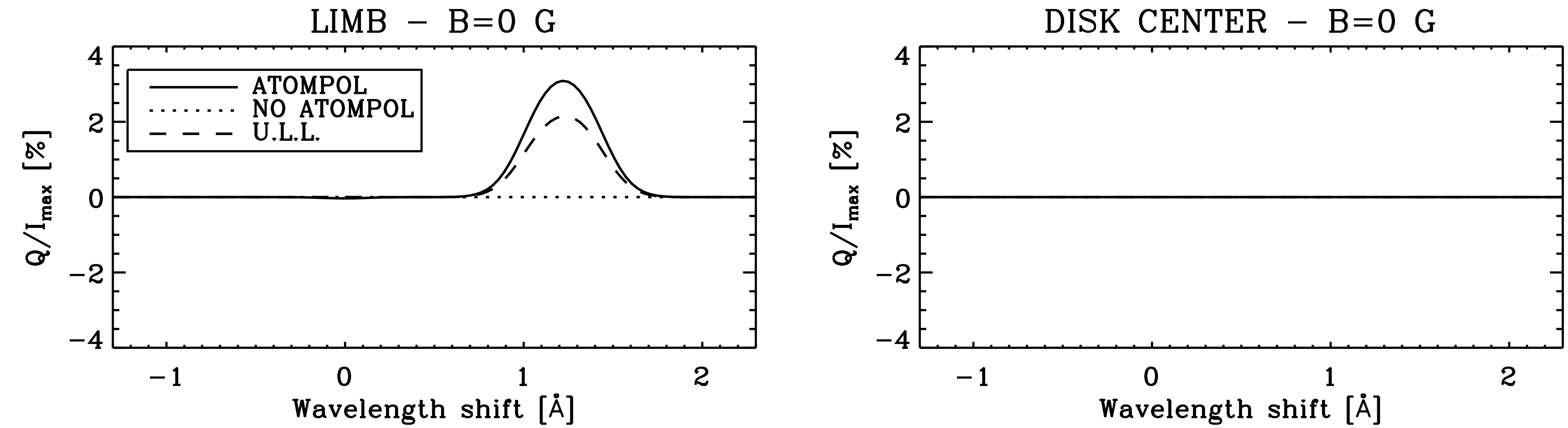
Sources of polarization: symmetry breaking situations

Magnetic fields: they point to a preferred direction

Radiation field: strong anisotropy radially, corrugation of the atmosphere…

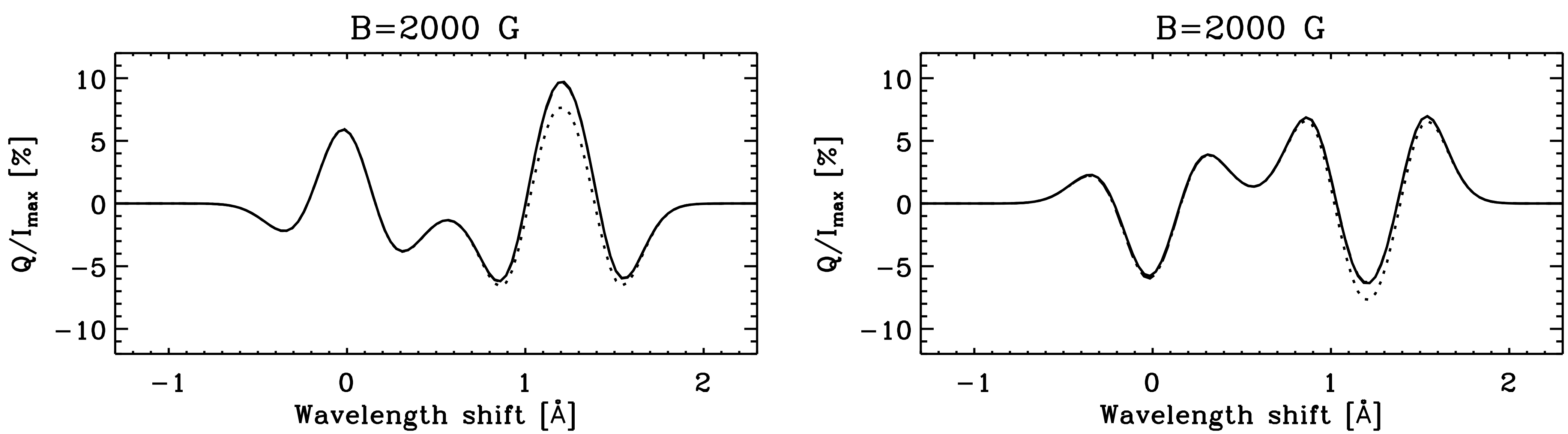
Collisions (see sec. 7.13 in “Polarization in spectral lines”)

Our goals: explain observations in the chromosphere



Let's assume:
Zeeman induced polarization (only)

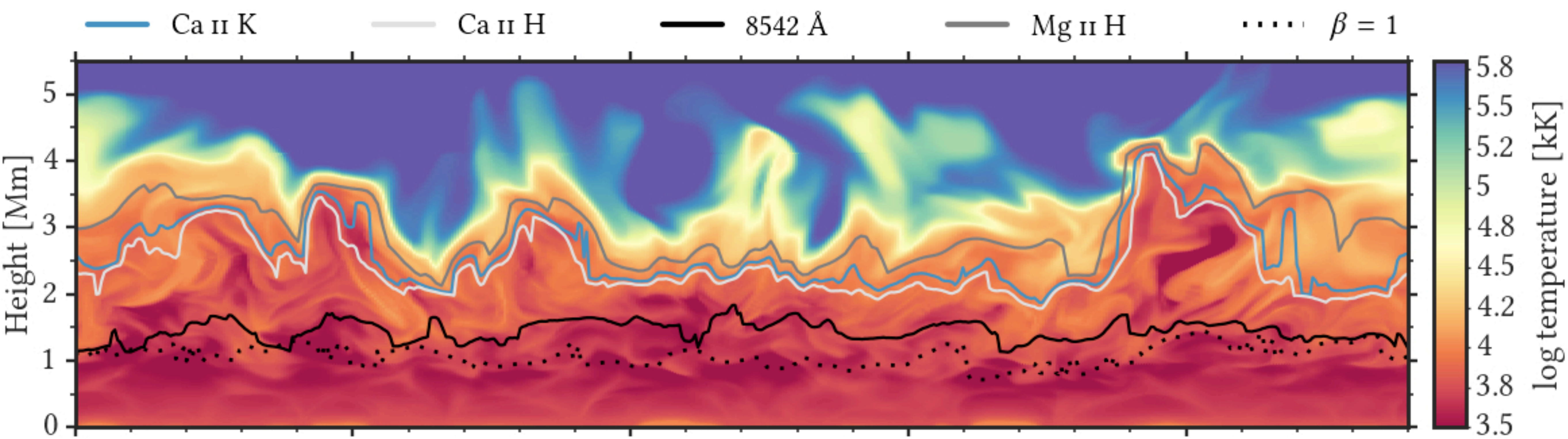
We are neglecting:
scattering/atomic polarization, Hanle effect, Stark effect…



Reproduced from Trujillo Bueno & Asensio Ramos (2007)

(some) *Chromospheric* diagnostics

Line	PRD/SE	Polarization	Max. formation
Na I D1	SE	Zeeman + atomic pol.	Upper photosphere
Mg I 517 nm	SE	Zeeman + atomic pol.	Upper photosphere
Ca II IR triplet	SE	Zeeman + atomic pol.	Lower chromosphere
H I 656 nm	SE	Zeeman + atomic pol.	Middle chromosphere
He I D3	SE	Zeeman + atomic pol.	Mid/up chromosphere
He I 1083 nm	SE	Zeeman + atomic pol.	Mid/up chromosphere
Ca II H & K	PRD	Zeeman + atomic pol.	Upper chromosphere



Bjørgen et al. (2018)

Some basic relations in radiative transfer

The unpolarized transfer equation

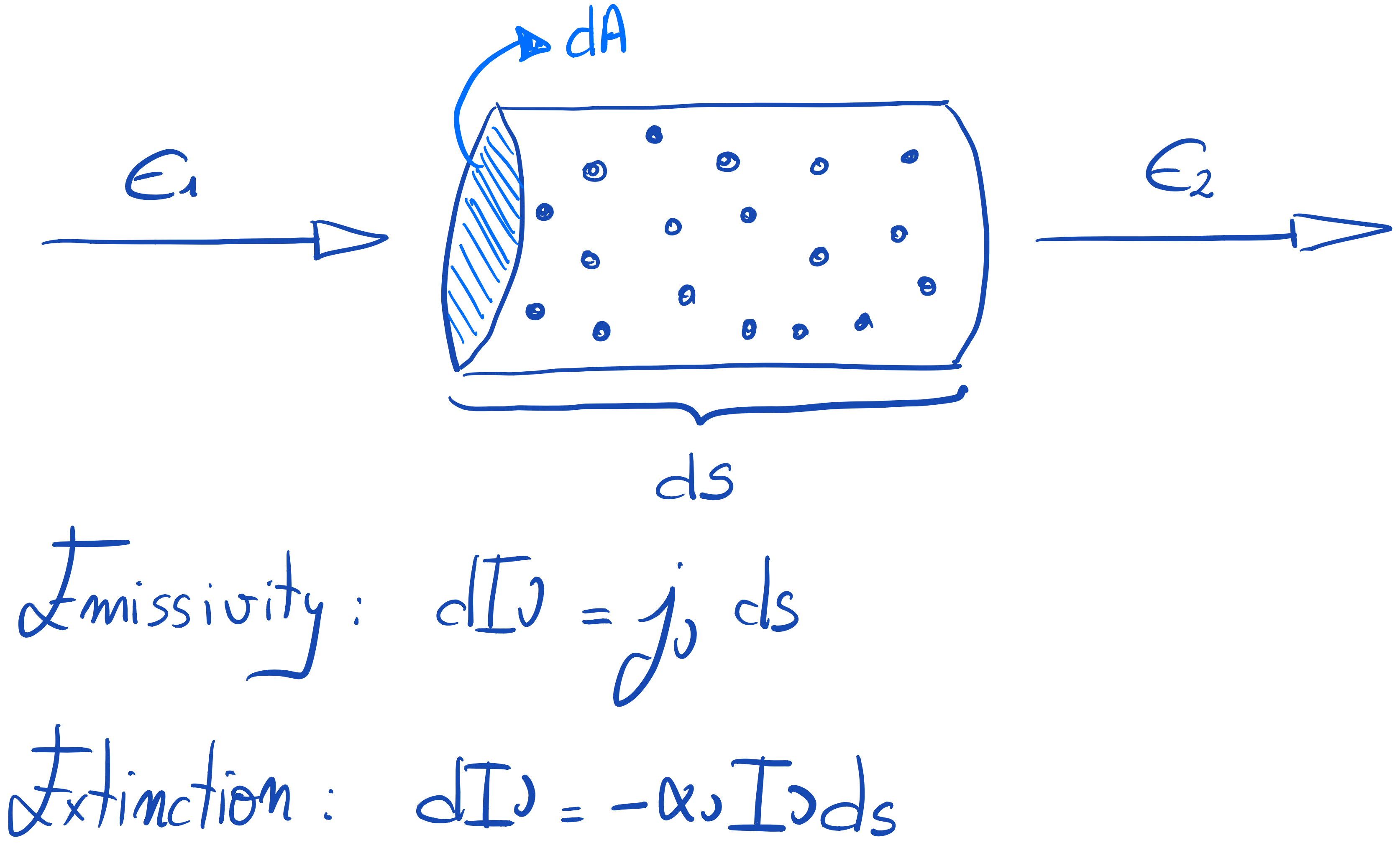
$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = j_\nu - \alpha_\nu I_\nu$$

$$\downarrow$$

$$\frac{\mathrm{d}I_\nu}{\alpha_\nu \mathrm{d}s} = \frac{j_\nu}{\alpha_\nu} - I_\nu$$

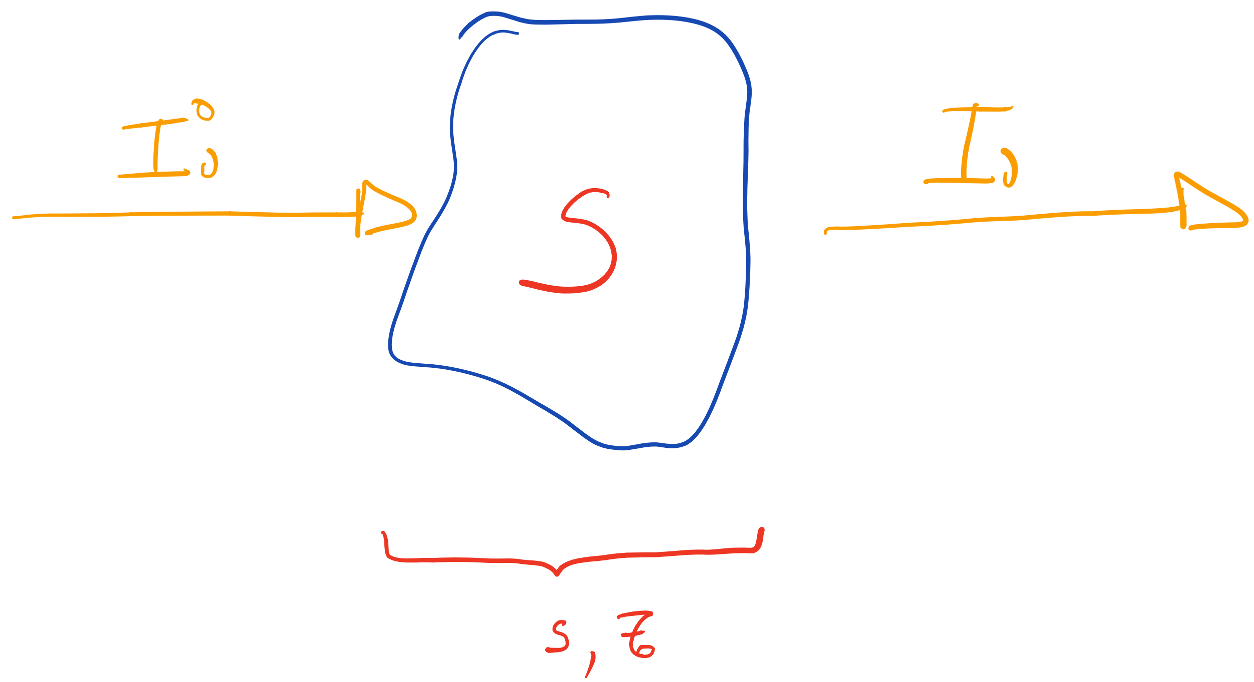
$$\downarrow$$

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = S_\nu - I_\nu$$



$$I_\nu(\tau_\nu) = I_\nu(0)\mathrm{e}^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau'_\nu)\mathrm{e}^{-(\tau_\nu - \tau'_\nu)}\mathrm{d}\tau'_\nu$$

Analytical solution: the slab of constant properties



$$I_\nu(\tau_\nu) = I_\nu(0)\mathrm{e}^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau'_\nu)\mathrm{e}^{-(\tau_\nu-\tau'_\nu)}\mathrm{d}\tau'_\nu$$

$$I_\nu(\tau_\nu) = \underbrace{I_0\mathrm{e}^{-\tau_\nu}}_{\text{Incoming radiation}} + \underbrace{S_\nu(1-\mathrm{e}^{-\tau_\nu})}_{\text{contribution of the cloud}}$$

What is the role of τ_ν in this equation?

Try do hand-wave assuming large and low values of τ_ν

The Eddington-Barbier approximation

The emerging intensity of an optically thick medium at the top of the atmosphere is:

$$I_\nu^+(\tau_\nu = 0,\mu) = \int_0^\infty S_\nu(t_\nu)\mathrm{e}^{-t_\nu/\mu}\frac{\mathrm{d}t_\nu}{\mu}$$

The intensity escaping from a stellar atmosphere is set by the source function from the top of the atmosphere ($\tau_\nu = 0$) to an optical depth where the exponential makes the integrand zero ($\tau_\nu \approx 10$). We can derive from which layer photons are scaping. Let's assume a polynomial source function:

$$S_\nu(\tau_\nu) = \sum_{n=0}^{\infty} a_n \tau_\nu^n$$

If we truncate S_ν after the first two terms, we can solve the integral and derive the Eddington-Barbier approximation:

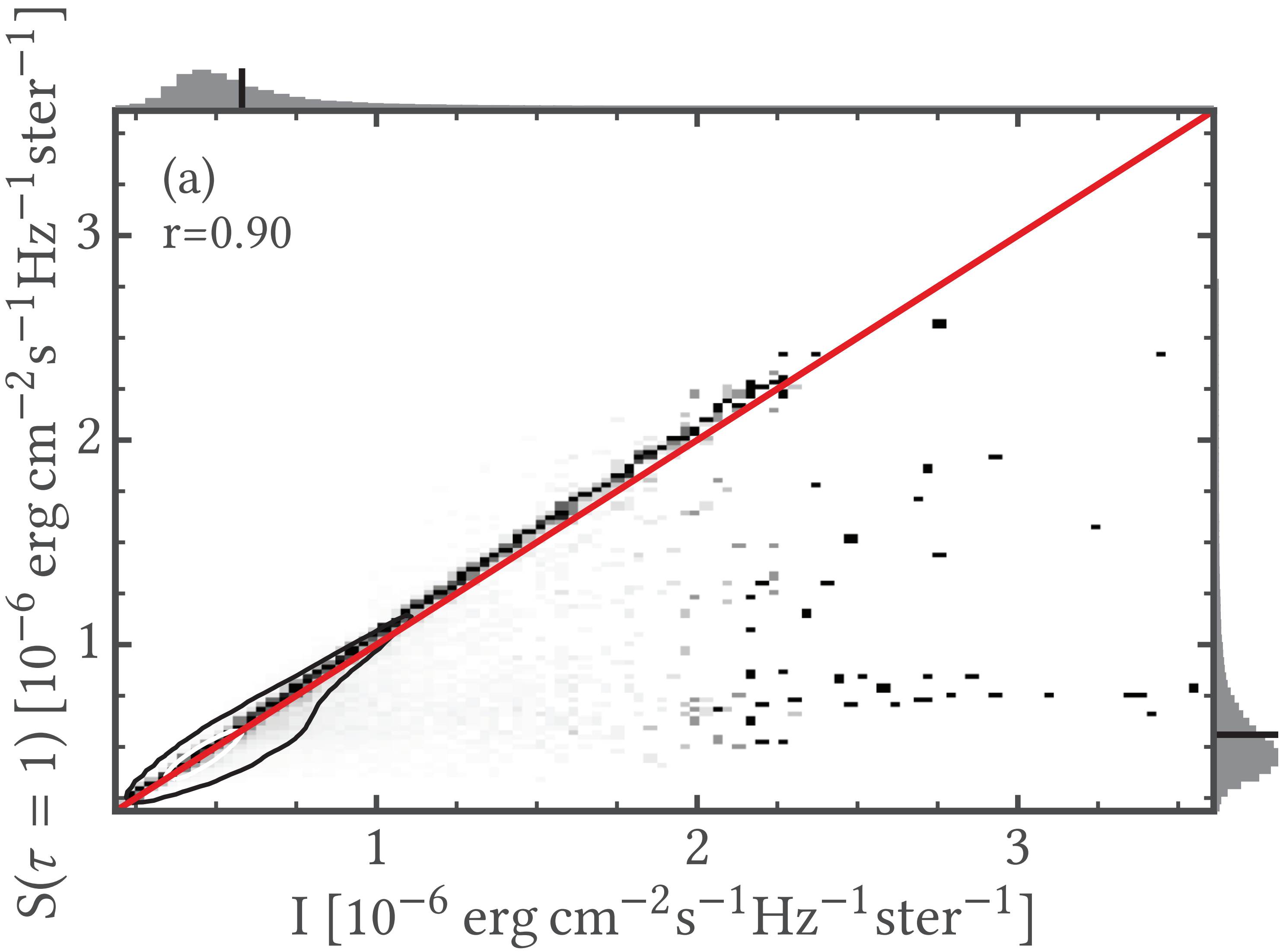
$$I_\nu^+(\tau_\nu = 0,\mu) \approx S_\nu(\tau_\nu = \mu)$$

So for vertical rays, the intensity can be approximated by the value of the source function at $\tau_\nu = 1$.

The Eddington-Barbier approximation

But how realistic is to assume Eddington-Barbier in realistic situations / chromospheric line formation?

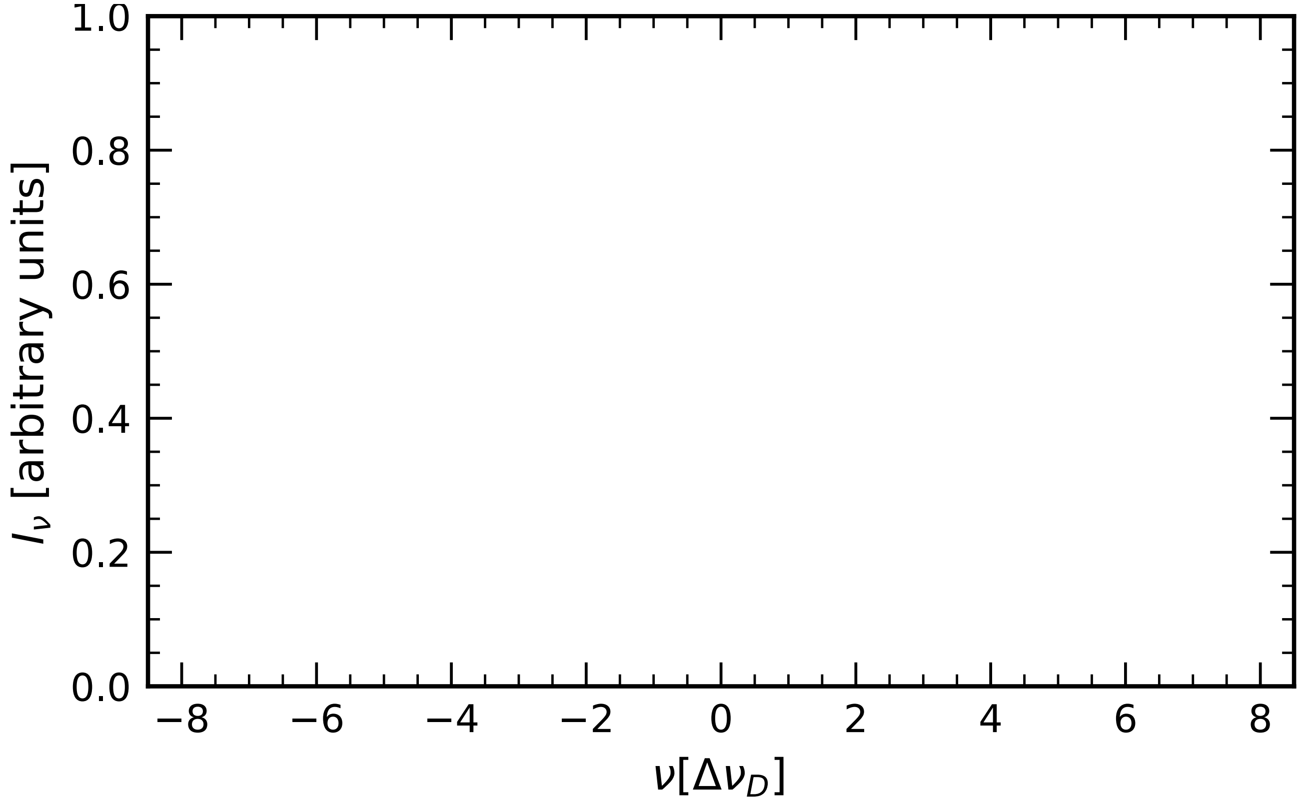
Ca II K: $S(\tau = 1)$ vs I_{k_3}

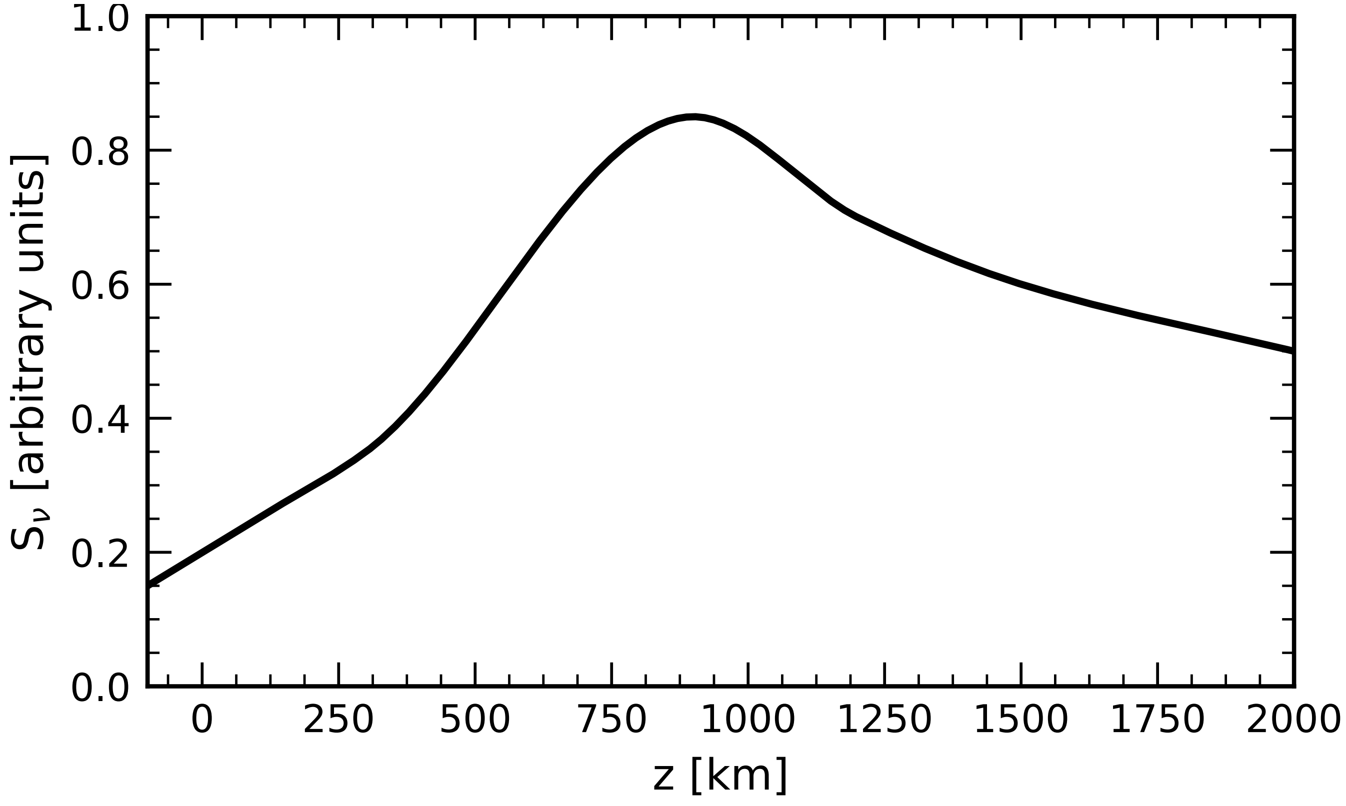


Bjørgen et al. (2018)

The Eddington-Barbier approximation

Imagine that $\tau_\nu = 1$ is reached in the continuum at $z = 0$ km and in the center of the line at $z = 1750$ km. Can you plot qualitatively the intensity profile given that you don't know the variation of the absorption coefficient with wavelength and height?





This approximation *can* hold in LTE and NLTE

Discussion:
What does NLTE mean?

In Thermodynamical Equilibrium (TE): $S_\nu = B_\nu,\ I_\nu = B_\nu,\ J_\nu = B_\nu$
(Saha-Boltzmann atom populations)

In Local Thermodynamical Equilibrium (LTE): $S_\nu = B_\nu,\ I_\nu \neq B_\nu,\ J_\nu \neq B_\nu$
(Saha-Boltzmann atom populations)

In non-Local Thermodynamical Equilibrium (NLTE): $S_\nu \neq B_\nu,\ I_\nu \neq B_\nu,\ J_\nu \neq B_\nu$

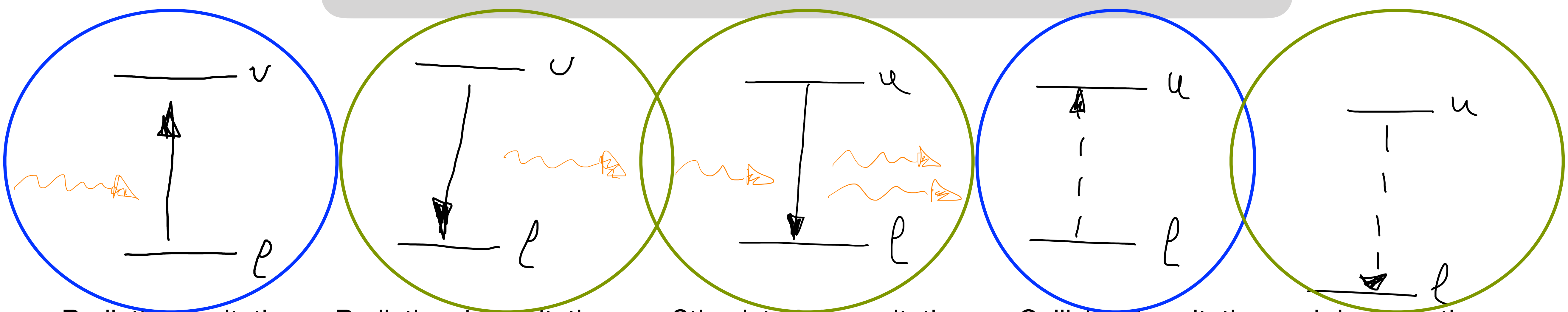
Saha: $$\frac{n^{r+1}}{n^r} = \frac{1}{n_e}\frac{2U^{r+1}}{U^r}\left(\frac{2\pi m_e kT}{h^2}\right)^{3/2} \mathrm{e}^{-\chi_r/kT}$$

Boltzmann: $$\frac{n_i^r}{n^r} = \frac{g_i}{U^r}\mathrm{e}^{-\chi_i/kT}$$

Bound-bound processes

NLTE is a very vague term!

Let's assume a bound-bound transition in a 2 level atom



Radiative excitation   Radiative de-excitation   Stimulated de-excitation   Collisional excitation and de-excitation

The rate equation for this atom in CRD is:

$$(A_{ul} + JB_{ul} + C_{ul})n_u = (JB_{lu} + C_{lu})n_l$$

$$\frac{n_u}{n_l} = \frac{JB_{lu} + C_{lu}}{A_{ul} + JB_{ul} + C_{ul}}$$

Note the dependence with J (the mean intensity) -> non-locality

Bound-bound processes

All processes that emit a photon involve an electron transition from the upper level to the lower level: the emissivity depends on the upper level population density.

$$j_\nu^{\rm spon} = \frac{h\nu_0}{4\pi} n_u A_{ul} \psi(\nu - \nu_0)$$

$$j_\nu^{\rm ind} = \frac{h\nu_0}{4\pi} n_u B_{ul} \phi(\nu - \nu_0)$$

All processes that involve the absorption of a photon involve an electron transition from the lower to the upper level: the absorption coefficient depends on the lower level population density.

$$\alpha_\nu^{\rm exc} = \frac{h\nu_0}{4\pi} n_l B_{lu} \chi(\nu - \nu_0)$$

However, in the rate equation both B_{lu} and B_{ul} are proportional to the mean intensity ($\bar{J}$), so we normally write induced deexcitation as a negative opacity. We do this to keep the form of the RT equation by grouping all terms that depend on I_ν:

$$\alpha_\nu^{\rm line} = \frac{h\nu_0}{4\pi} \left(n_l B_{lu} \chi(\nu - \nu_0) - n_u B_{ul} \phi(\nu - \nu_0) \right)$$

The source function

$$S_\nu^{\rm line} = \frac{j_\nu}{\alpha_\nu} = \frac{n_u A_{ul} \psi}{n_l B_{lu} \phi - n_u B_{ul} \chi}$$

Einstein relations

$$\frac{A_{ul}}{B_{ul}} = \frac{2h\nu^3}{c^2} \qquad \frac{B_{lu}}{B_{ul}} = \frac{g_u}{g_l} \qquad \frac{C_{ul}}{C_{lu}} = \frac{g_u}{g_l} \mathrm{e}^{(E_u - E_l)/kT}$$

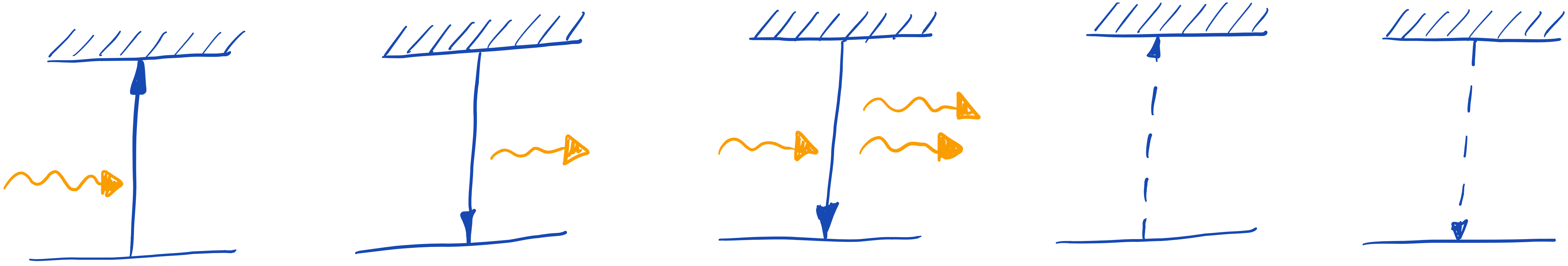
$$S_\nu^{\rm line} = \frac{2h\nu^3}{c^2} \frac{1}{\frac{g_u n_l}{g_l n_u} - 1}$$

$$S_{\nu,\rm LTE}^{\rm line} = \frac{2h\nu^3}{c^2} \frac{1}{\mathrm{e}^{-(E_u - E_l)/kT} - 1} = B_\nu$$

Where are the collisional terms?

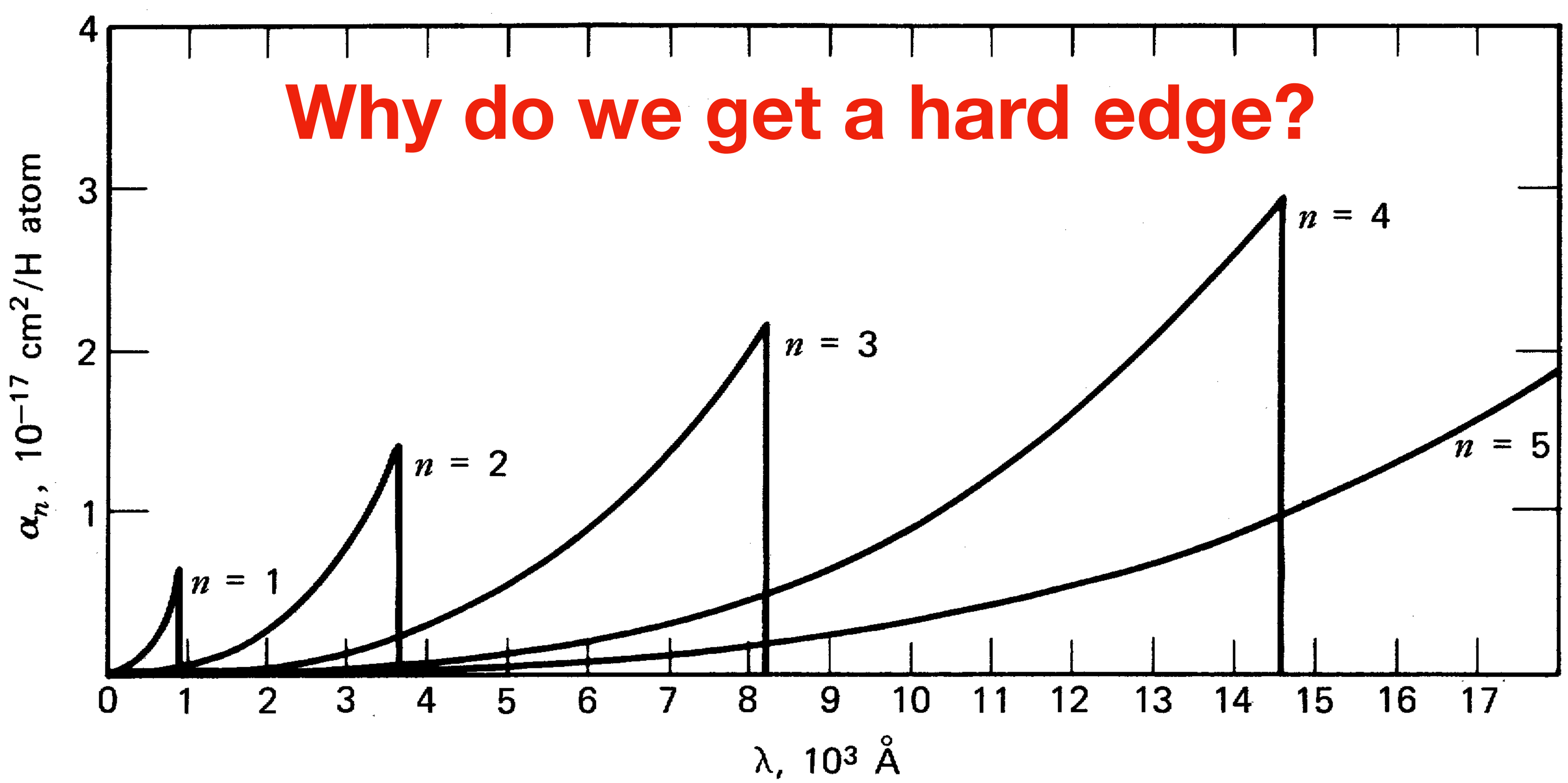
Bound-free processes

There are 5 processes that can take place between a bound level and a continuum level (ionization). These processes are analogous to those in bound-bound levels.



Radiative ionization | Radiative recombination | Induced recombination | Collisional ionization | Collisional recombination

In a complex atom, these processes must also be taken into account. The contribute regulating the electron density and the density of the species under consideration.



Reproduced from Gray (2005)

The statistical equilibrium equations

If the rates between the states of a particle are known we can set up an equation system that determines the population of the states:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \text{rates into level } i - \text{rates out of level } i$$

We can also assume that the system has reached an equilibrium state so there are no changes in time:

$$\sum_{j,j\neq i} n_j P_{ji} - n_i \sum_{j,j\neq i} P_{ij} = 0$$

By defining:

$$P_{ii} = \sum_{j,j\neq i} P_{ij}$$

We can write these equations in matrix form:

$$\mathbf{P}^T \boldsymbol{n} = \boldsymbol{0}$$

The statistical equilibrium equations

$$\mathbf{P}^T \boldsymbol{n} = \boldsymbol{0}$$

There are only $N - 1$ independent equations so impose particle conservation to close the system of equations. To do so, we replace one equation of the system with:

$$\sum_{i=1,N} n_i = n_{\text{tot}}$$

For a 2-level atom:

$$\begin{bmatrix} P_{11} & P_{21} \\ P_{12} & P_{22} \end{bmatrix} = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

And given that, $P_{11} = -P_{12}$ and $P_{22} = -P_{21}$:

$$\begin{bmatrix} -P_{12} & P_{21} \\ P_{12} & -P_{21} \end{bmatrix} = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Imposing particle conservation:

$$\begin{bmatrix} -P_{12} & P_{21} \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix} = \begin{bmatrix} 0 \\ n_{\text{tot}} \end{bmatrix}$$

The statistical equilibrium equations

Which, after expanding P_{12} and P_{21} has solution:

$$\frac{n_2}{n_1} = \frac{B_{12}\bar{J}_{\nu_0} + C_{12}}{A_{12} + B_{12}\bar{J}_{\nu_0} + C_{21}}$$

In LTE: $\left.\frac{n_2}{n_1}\right|_{LTE} = \frac{C_{12}}{C_{21}}$ (the radiative terms are negligible)

What happens if we set $\bar{J}_{\nu_0} = B_{\nu_0}$ in that population ratio?

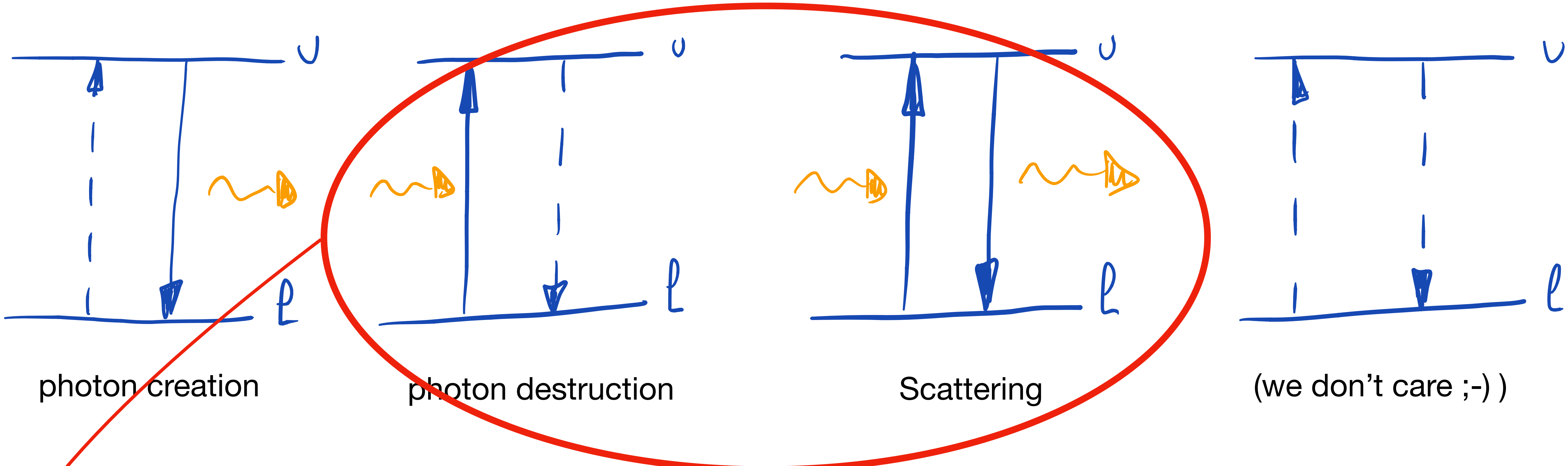
In reality we have atoms with more complex atoms: many bound-bound and bound-free transitions.

The NLTE problem: $I_\nu = I_\nu(\boldsymbol{n}(\bar{J}_{\nu_0}(I_\nu)))$

We need to iterate in order to make I_ν and $\boldsymbol{n}$ consistent with each other.

Scattering

There are 4 combinations of processes that can occur between 2 levels:



Stimulated de-excitation is a particular case because it depends on the radiation field. Let's conveniently ignore it for this explanation.

These two involve photon absorption

Scattering

When collisional rates are very low, there is no net creation/destruction of photons: There is no energy being exchanged between radiation and matter.

The photon simply *scatters* in the atmosphere until it can scape.

For a 2-level atom we can introduce the photon destruction probability:

$$\epsilon_\nu = \frac{C_{ul}}{C_{ul} + A_{ul}}$$

Collision

Scattering

…and re-write the source function based on these two contributions:

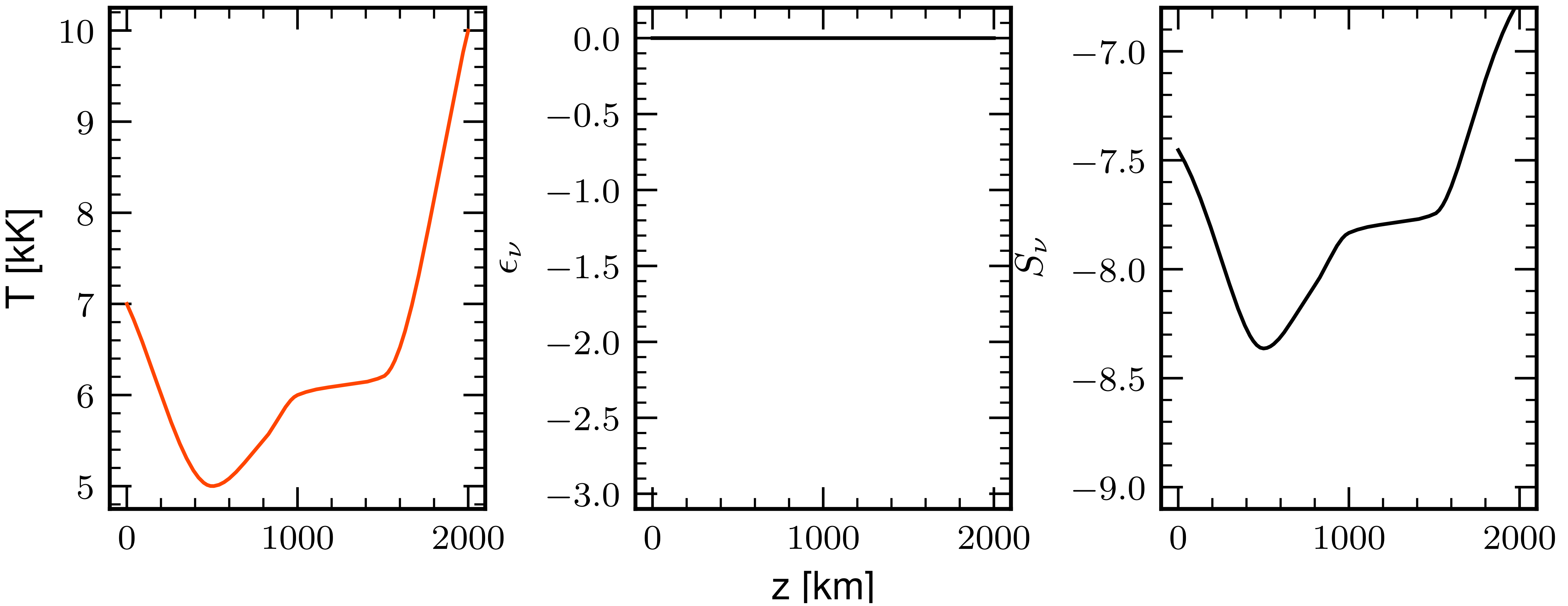
$$S_\nu = (1 - \epsilon_\nu) J_\nu + \epsilon_\nu B_\nu$$

With two extreme cases based on the value of ϵ_ν:

$$\epsilon_\nu = 1 \rightarrow S_\nu = B_\nu$$

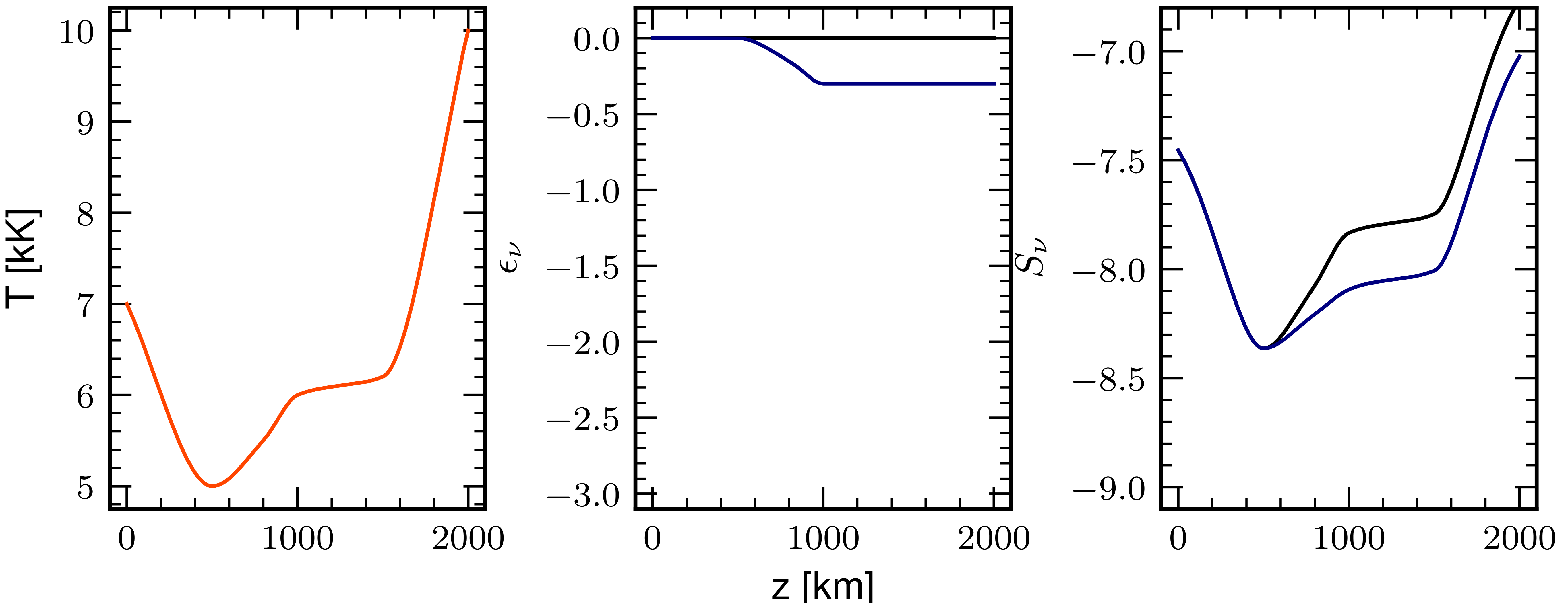
$$\epsilon_\nu = 0 \rightarrow S_\nu = J_\nu$$

Scattering



T [kK]
10
9
8
7
6
5
0
1000
2000
ϵ_ν
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
S_ν
−7.0
−7.5
−8.0
−8.5
−9.0
z [km]

Scattering



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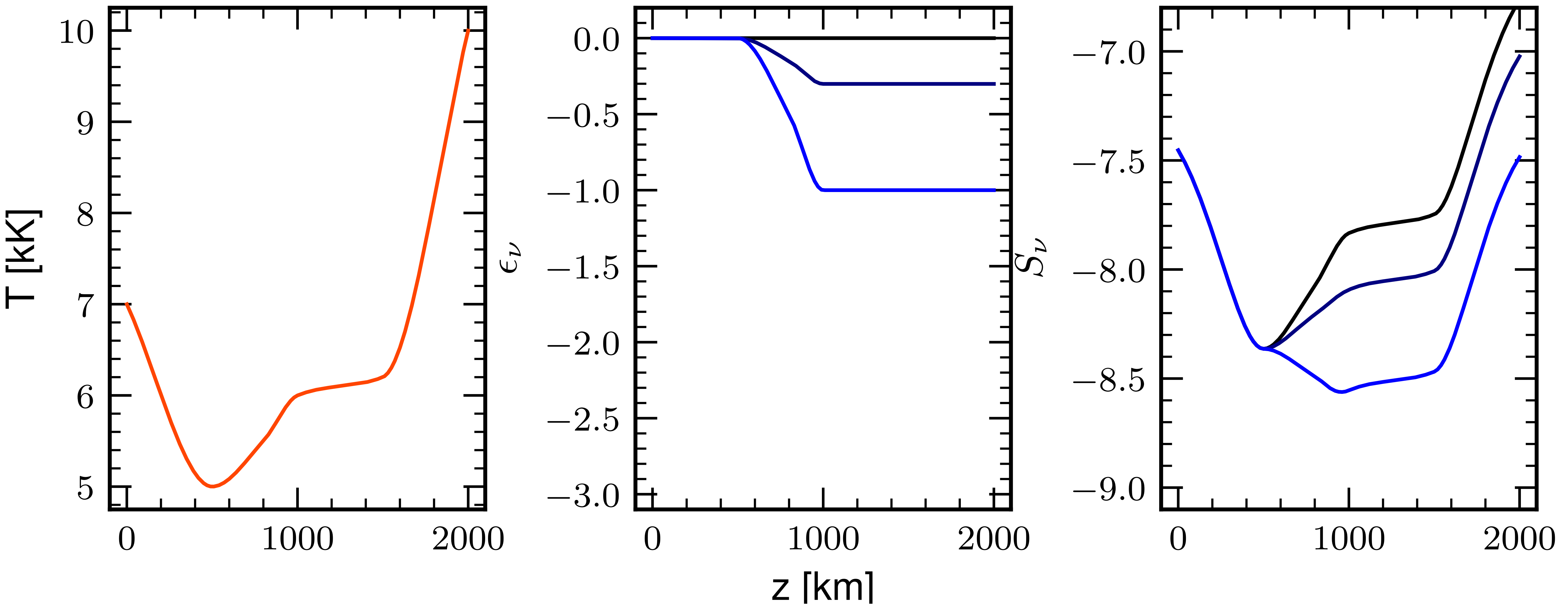
−9.0
0
1000
2000

Scattering



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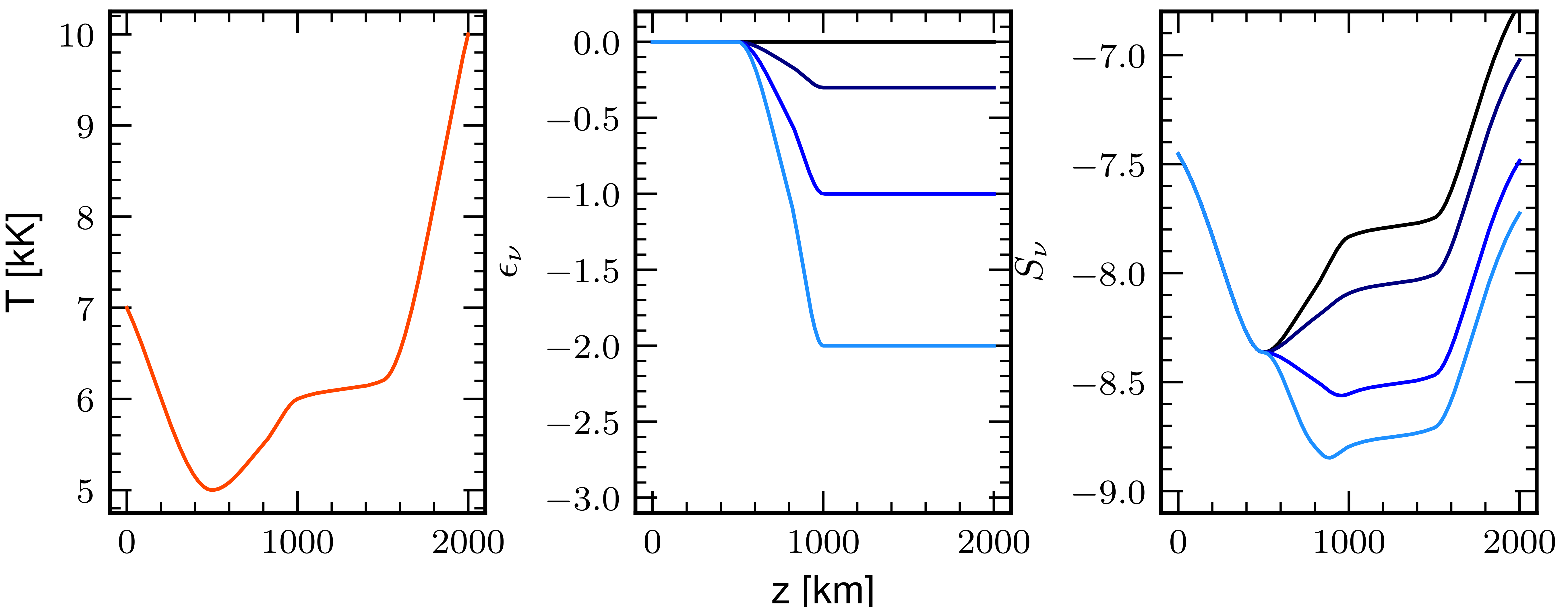
Scattering



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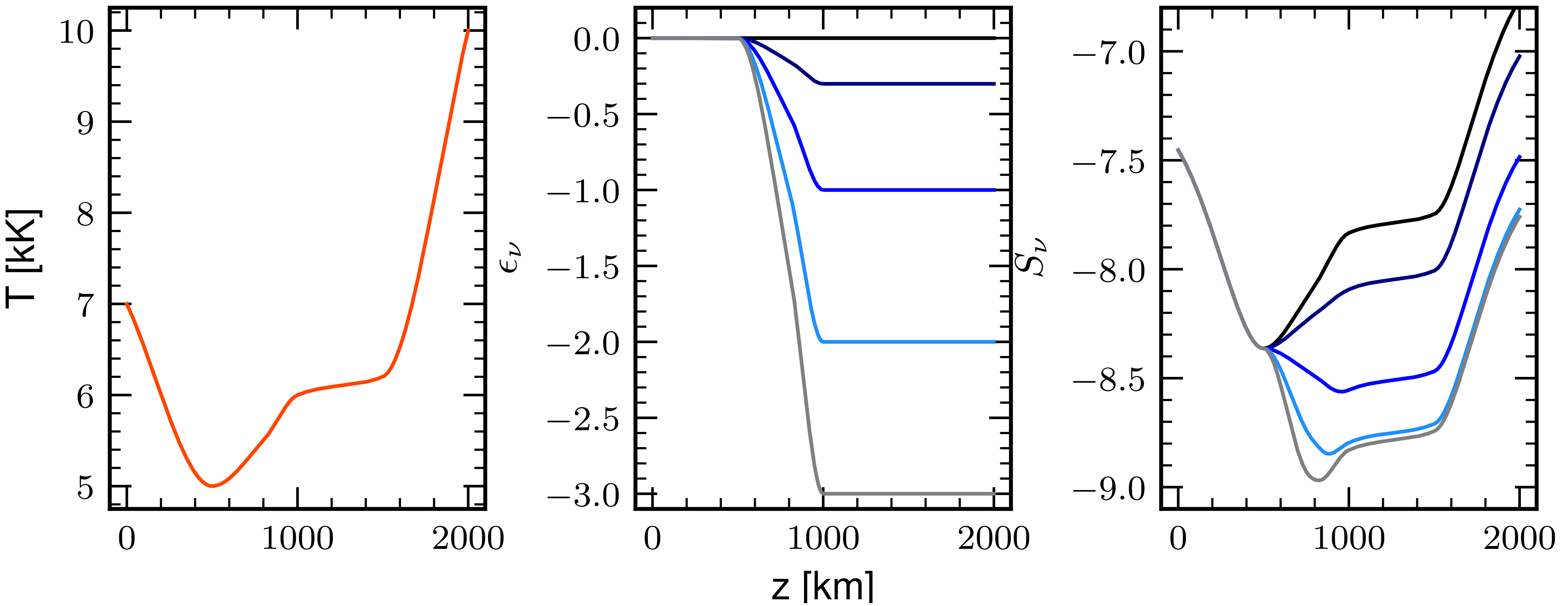
0
1000
2000
z [km]
S_ν
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000

Scattering

Remember Eddington-Babier and the relation between S and I:

$$I_\nu = S_\nu(\tau_\nu = \mu)$$



A scattering atmosphere implies no photon creation or destruction via collisions!

Solving the statistical equilibrium equations

The NLTE problem: $I_\nu = I_\nu(\boldsymbol{n}(\bar{J}_{\nu_0}(S_\nu(I_\nu))))$, but we don't now $\bar{J}_{\nu_0}$ (or S_ν).

We typically start from $\boldsymbol{n}_{\mathrm{LTE}}$ or $\boldsymbol{n}_{\bar{\mathrm{J}}=0}$ and iterate from there the **linearized** or **preconditioned** rate statistical equilibrium equations.

$$\left.\frac{n_2}{n_1}\right|_{\mathrm{LTE}} = \frac{C_{12}}{C_{21}}$$

LTE populations

$$\left.\frac{n_2}{n_1}\right|_{\bar{J}=0} = \frac{C_{12}}{A_{12} + C_{21}}$$

Zero radiation

Lambda-iteration

After each iteration we update $\bar{J}_{\nu_0}$ and recompute $\boldsymbol{n}$ until they are consistent with each other: Λ-iteration ($\bar{J}_{\nu_0} = \Lambda_\nu(S_\nu)$) $\longrightarrow$ very poor convergence and slow.

$$\boldsymbol{n}^i \rightarrow I_\nu \rightarrow \bar{J}_{\nu_0} \rightarrow \boldsymbol{n}^{i+1}$$

The main reason is that we solve individually $\bar{J}_{\nu_0}$ and then $\boldsymbol{n}$. Which translates into photons taking very small steps in each iteration ($\Delta\tau \approx 1$).

Solving the statistical equilibrium equations

Approximate Lambda-iteration

We can choose an approximate lambda operator that is easy to invert and that converges much faster at large optical depth: $\mathbf{\Lambda}_\nu = \mathbf{\Lambda}^* + (\mathbf{\Lambda}_\nu - \mathbf{\Lambda}^*)$

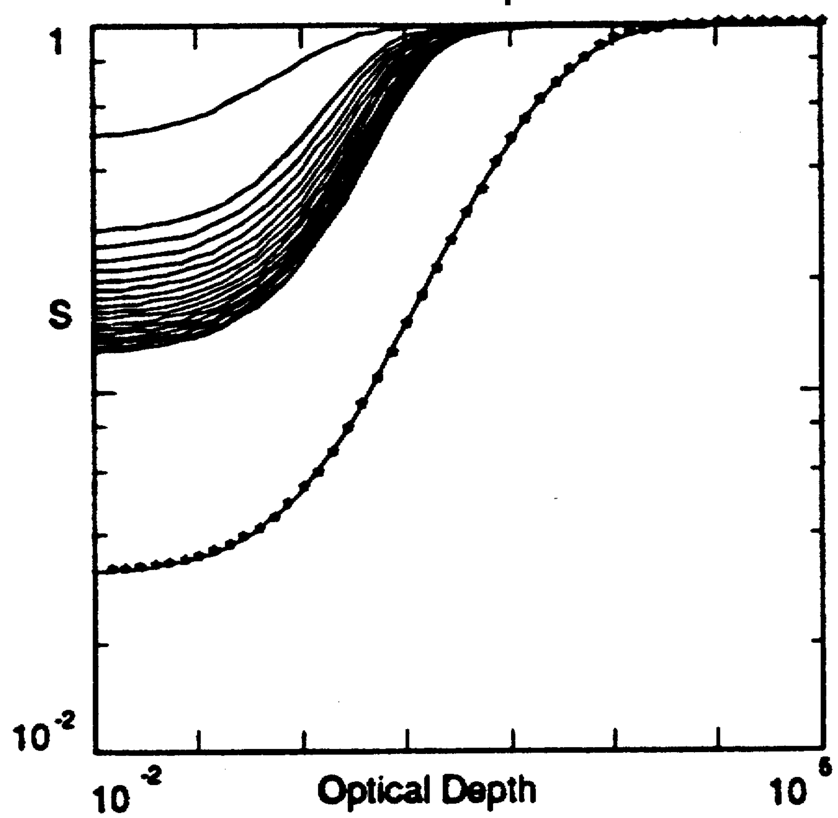
We can re-write the problem so only invert $\mathbf{\Lambda}^*$ and iterate (anyway, we had to iterate because we had linearized the problem!).

It turns out that we can choose $\mathbf{\Lambda}^*$ in such a way that it accelerates the computations at large optical depths:

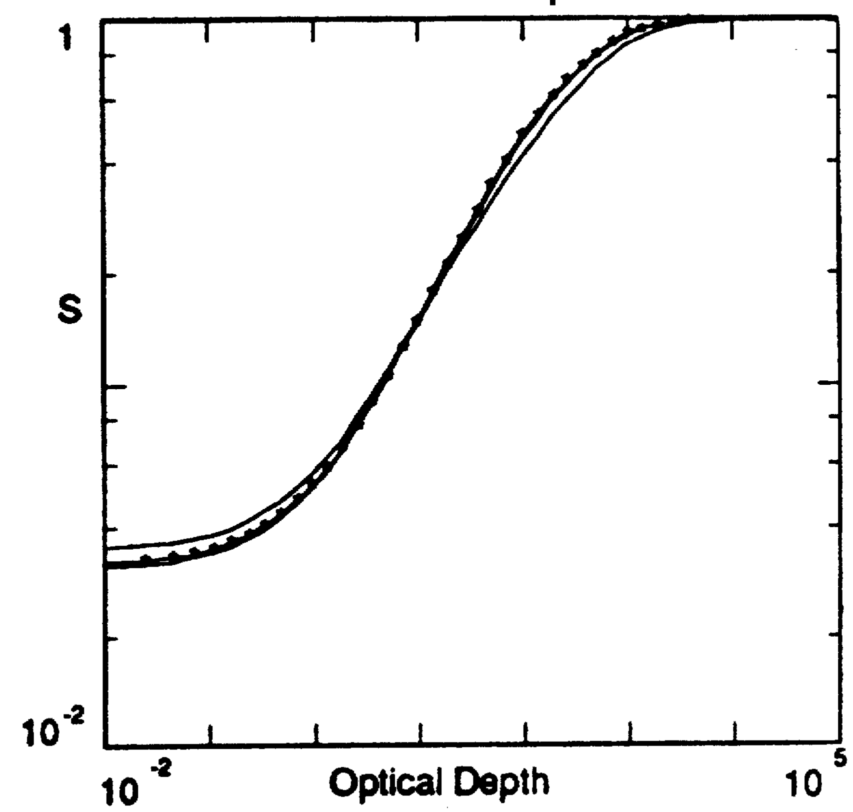
- Scharmer's global operator [MULTI]
- Diagonal operator (turns the problems into Jacobi iterations) [RH,MULTI3D,SNAPI,PORTA]
- Core saturation
- Gauss-Seidel [MULTI3D]

Solving the statistical equilibrium equations

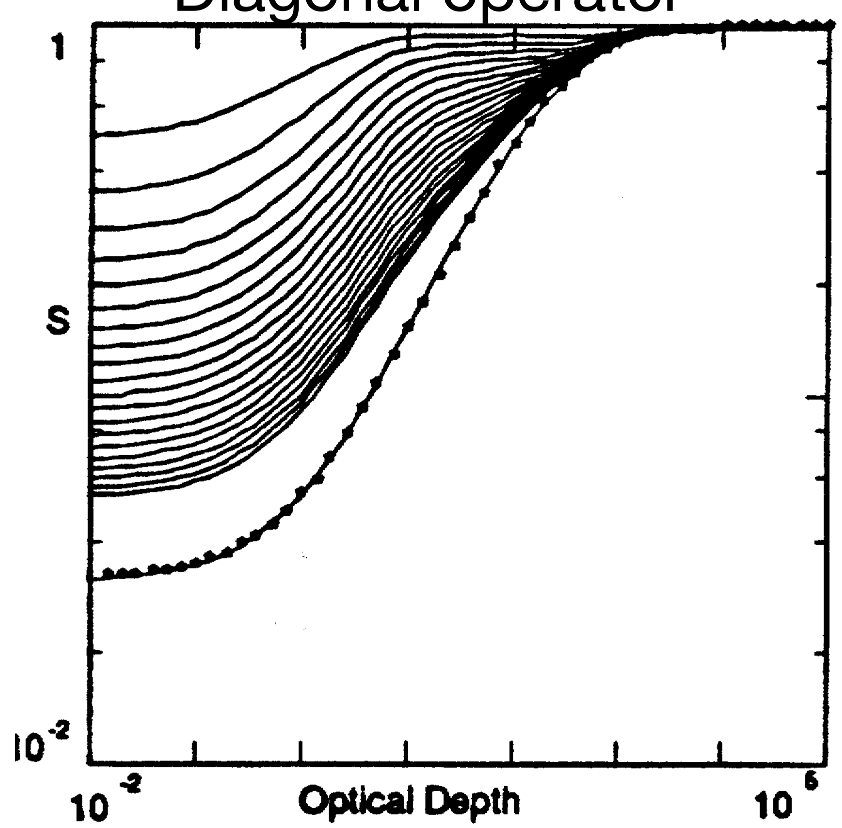
Lambda operator



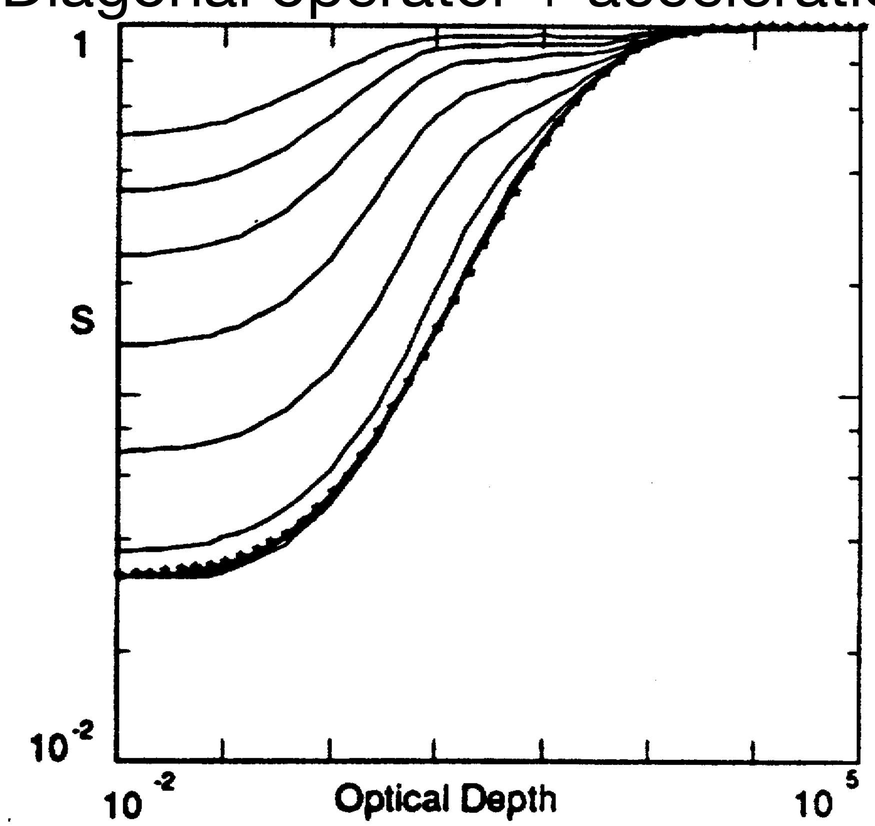
Scharmer's operator



Diagonal operator



Diagonal operator + acceleration



To take home

- Collisions allow to create and destroy photons and to transfer energy from radiation to gas and vice-versa. They are very important, even when collisional rates are very low!
- Without collisions, atoms absorb and re-emit photons until they scape (scattering).
- Coupling to the local conditions of the plasma is achieved via collisions.
- Statistical equilibrium equations are solved iteratively.