Part II : Radiative transfer and Spectropolarimetry

Solving NLTE problem and NLTE in spectral lines

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Quick Summary

- In our synthesis and analysis until now, we have assumed that the matter is in so called Local Thermodynamic Equilibrium (LTE).
- This is good assumption for spectral lines formed in the photosphere, but for very strong lines that are opaque enough to sample the chromosphere, it seems to fail.
- Why? Because scattering becomes important.
- Scattering = NLTE

NLTE in the continuum

NLTE is already noticeable in the continuum, say in scattering on free electrons.

$$\frac{dI}{\mu\, d\tau} = I - S$$

$$S = \varepsilon B + (1-\varepsilon)\frac{1}{2}\int_{-1}^{1} I(\mu) d\mu$$

This is the essence. The coupling between the matter and the radiation.

In LTE: matter $\rightarrow$ radiation.

In NLTE: matter $\leftrightarrow$ radiation.

LTE vs NLTE

LTE: emission follows from the thermal state of the gas: i.e. hot gas emits a lot.

NLTE: emission follows from the illuminating radiation: gas can be cold but emit a lot because there is a lot of illuminating radiation that is scattered.

Important quantity is the **photon destruction probability:** ε.

$$\begin{aligned}\varepsilon &= \frac{p(\mathrm{scattering})}{p(\mathrm{absorption}) + \mathrm{p}(\mathrm{scattering})} \\ &= \frac{\sigma}{\sigma + \alpha}\end{aligned}$$

Nowadays we solve this numerically (and we will do it in that way today).

However, Chandrasekhar solved it semi-analytically in his “Radiative Transfer” period using discrete ordinate method.

Numerical solution - direct

$$\frac{dI}{\mu\, d\tau} = I - S$$

$$S = \varepsilon B + (1-\varepsilon)\frac{1}{2}\int_{-1}^{1} I(\mu) d\mu$$

Write the derivative as the finite difference, and the integral as the sum. Let's restrict to only two "rays".

$$\frac{I^+_{i+1} - I^+_{i-1}}{\tau_{i+1} - \tau_{i-1}} = I^+_i - \varepsilon_B - (1-\varepsilon)\frac{1}{2}(I^+_i + I^-_i)$$

$$\frac{I^-_{i+1} - I^-_{i-1}}{\tau_{i+1} - \tau_{i-1}} = I^-_i - \varepsilon_B - (1-\varepsilon)\frac{1}{2}(I^+_i + I^-_i)$$

This is total of $2 \times ND$ equations for $2 \times ND$ unknowns. Linear system, so solvable.

In practice, it is done differently, see: **"Feautrier method."**

Numerical solution - direct

The direct solution is possible because the system is linear in $I(\tau, \mu)$.

We will see that, in the case of spectral lines, it is not.

The non-linear systems **have to** be solved iteratively because for vast majority of those there is not a direct solution.

For example, for ionization equilibrium where only hydrogen is involved, we can solve directly.

For anything more complicated we cannot.

Numerical solution - iterative

Every iterative solution starts with a guess, that we we improve upon.
Examples:

- Solving transcedental equations.
- Non-linear fitting.
- Solution of huge systems (both non-linear and linear).

Reminder - transcedental equations

How do we solve $e^x + x = 3$? (For example)

We write it as $x = \ln(3 - x)$ and we start from a guess, say $x = 1.0$:

$$x = 0.6931471805599453$$

Then again:

$$x = \ln(3 - x) = 0.8358841797746195$$

$$x = 0.7720118809130998$$

...

$$x \approx 0.7920584794997764$$

(satisfies the original equaton to sixth decimal).

How do we apply this to our problem?

$$\frac{dI}{\mu d\tau} = I(\mu, \tau) - S(\tau)$$

$$S(\tau) = \varepsilon B(\tau) + (1 - \varepsilon) J(\tau)$$

$$J(\tau) = \frac{1}{2} \int_{-1}^{1} I(\mu, \tau) d\mu$$

In real life, you *discretize* $I(\mu)$ dependence, in order to turn the integral over angles into a quadrature sum:

$$J = \sum_{m} I_m(\tau) w_m.$$

Where you use, e.g. Gaussian weights. We won't go that far today.

“Two stream” iterative solution

We will consider outgoing and incoming radiation. If we know the source function, we can solve for intensity(use the hands-on code, but remember to change the direction).

We now need the boundary condition for incoming itensity as well. It is zero.

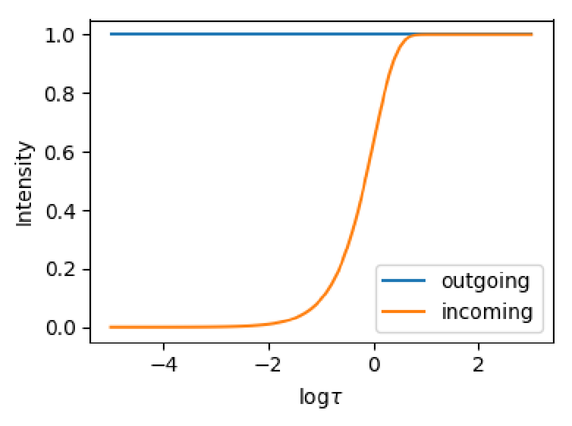
So, we will start from a value for the source function, calculate intensity and see what we got.

Start from what value? Something simple, say: $S = B$.

A common test problem is $B = const$, $\varepsilon = const$.

"Two stream" iterative solution

We start by doing one formal solution outward and one inward.

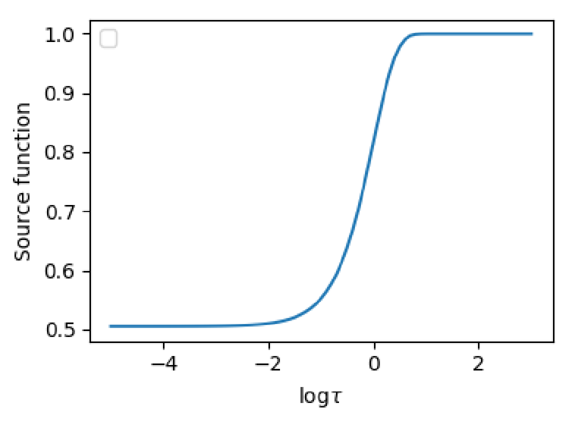


At the surface, there is a lack of photons!

“Two stream” iterative solution

Then we can calculate new value of the source function:

$$S = \varepsilon B + (1 - \varepsilon)\frac{1}{2}(I^+ + I^-)$$



“Two stream” iterative solution

So now we have a new value for the source function, different than the old one.

Obviously the original source function is not “self-consistent” as it does not satisfy both RTE and equation for S.

Is the new one self-consistent? - Probably not.

But what we can do is what we did in the case of transcedental equation - keep going.

“Two stream” iterative solution

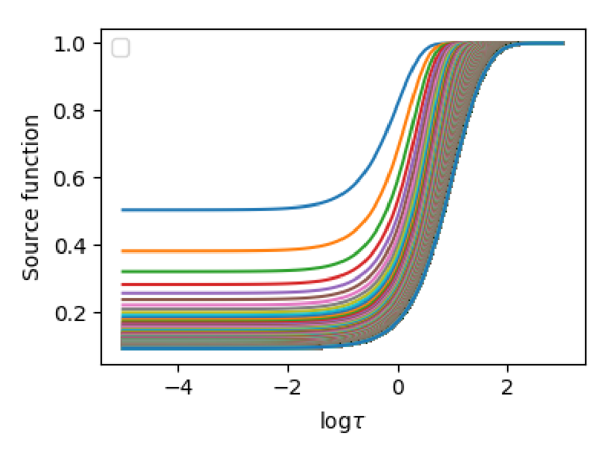


Figure 1: Change of the source function throughout the iterative proces

"Two stream" iterative solution

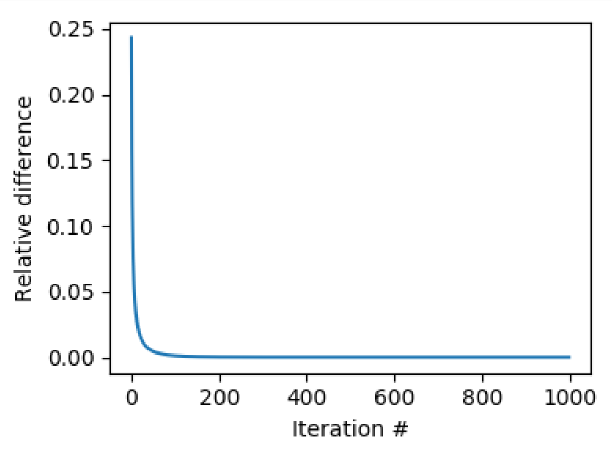


Figure 2: Convergence of the method

“Two stream” iterative solution

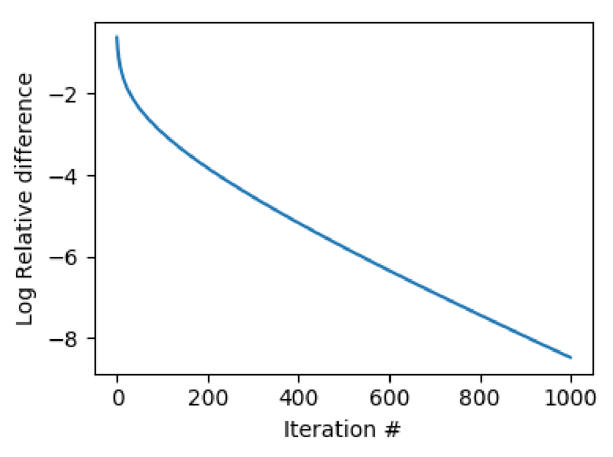


Figure 3: Convergence in log scale - very poor

Λ iteration

This iterative method is known as Λ iteration, after Schwartzschild's (1906) notation:

$$J = \Lambda[S]$$

Figure 4: Karl Schwartzschild (1873-1916)

Λ iteration

Technically, this method works.

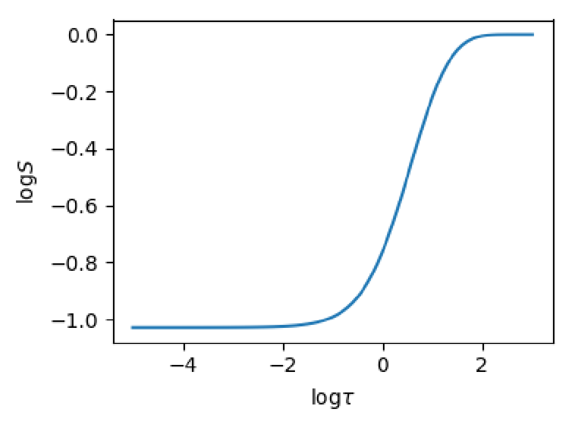
It is, however, extremely slow, and in the end converges linearly, which means that for an increase in magnitude in accuracy, we need an order of magnitude increase in number of iterations. This is not feasible.

Some ways to do this faster:

- Accelerated Lambda Iteration (ALI) / Approximate Lambda Operator (ALO)
- Gauss-Seidel iteration
- Multi-grid methods

Source function distribution

Although $B = const$, source function is decreasing with height.



Emergent intensity is 0.16, instead of 1!!!

Spectral lines

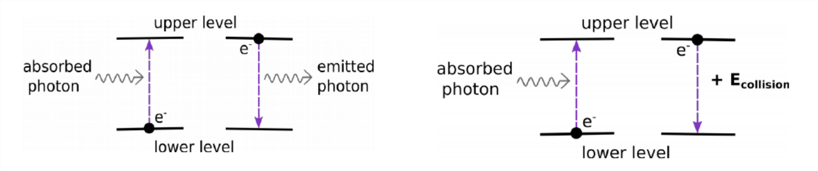
Great! So this happens in spectral lines, source function drops at the surface and we have lower intensity than anticipated, we solved everything!

Well, not really... This would assume that spectral lines scatter light *coherently* (wavelength of the light does not change in the scattering process).

Wait, wait, wait, what do you mean, lines scatter?

Spectral line scattering

Spectral line scattering is absorption followed by emission, without inelastic collision in between.



This tells us a bit *why* scattering breaks LTE.

Scattering versus collisions

Let's consider emission in LTE. Upper level is populated by the collisions and miniscule amount of these excitations will de-excite radiatively, others - collisionally.

Collisions are in balance.

Radiation proportional to the upper level population, which means proportional to collisions.

Example: Cold gas does not emit a lot because collisions have low energy.

Scattering versus collisions

In scattering **Photons are "preserved"**, so the emission of the gas does not depend on the collisions only, but also the radiation.

Radiative processes compete with the collisional processes. LTE will not be valid.

What happens with the wavelength of the photon

Although inelastic collisions are scarce, there is a plenty of elastic ones. These prevent the scattering process from being coherent. There is a *redistribution*.

Even though the photon is absorbed in the wing of the line, it has higher probability of being emitted in the line core.

And vice versa: although photons are absorbed mostly in the core, they have some chance of being emitted in the wings.

Complete redistribution

Assumption that photon completely forgets at which wavelength it was absorbed is called *complete frequency redistribution* - CRD.

We can't solve NLTE problem wavelength at the time. We need to solve all wavelengths now simultaneously. Wavelenghts are coupled too.

Size of the system increases by a factor of N_λ.

Scattering integral

In the continuum case, the quantity that determined our source function was mean intensity:

$$J = \frac{1}{4\pi} I(\hat{\Omega}) d\hat{\Omega}$$

In the line case we use angle, and profile averaged intensity, akka **scattering integral**:

$$\overline{J} = \frac{1}{4\pi} \int_0^\infty \oint I(\hat{\Omega}, \lambda) \phi_\lambda d\lambda d\hat{\Omega}$$

or, in 1D, axially symmetric case:

$$\overline{J} = \frac{1}{2} \int_0^\infty \int_{-1}^{1} I(\mu, \lambda) \phi_\lambda d\lambda d\mu$$

Radiative rates

Scattering integral will help us calculate *radiative rates* for radiative transitions in the line.

$$R_{ul}^{\text{spontaneous}} = A_{ul}\,[\mathrm{s}^{-1}]$$

Einstein coefficient of spontaneous emission is a radiative rate.

The new ones are:

$$R_{ul}^{\text{stimulated}} = B_{ul}\bar{J}$$

$$R_{ul}^{\text{absorption}} = B_{lu}\bar{J}$$

Rate equations

So what is going on now? There are also collisional rates: C_{ul} and C_{lu}.

$$C_{ij} \propto n_e T^{\alpha}$$

where α depends on the atom, exact level configuration, etc.

Collision and radiative rates both contribute to the so called **statistical equilibrium:**

$$\frac{dn_i}{dt} = \sum n_j(R_{ji} + C_{ji}) - n_i(R_{ij} + C_{ij}) = 0$$

Very simple case - prominence

No stimulated emission, no collisions.

$$n_u A_{ul} = n_l B_{lu} \overline{J}$$

$$\eta \propto \overline{J} \times \phi(\lambda)$$

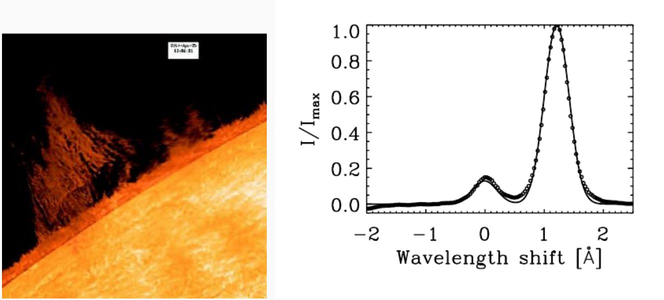


Figure 5: Prominence observed by HINODE (Heinzel 2008), and He 10830 line profile from Asensio Ramos et al (2010).

NLTE in spectral lines

$$\frac{dn_i}{dt} = \sum n_j(R_{ji} + C_{ji}) - n_i(R_{ij} + C_{ij}) = 0$$

Replaces both Saha and Boltzmann equations. Rates can also be between a bound and unbound state.

Solution yields all n_i. We need n_i to calculate the opacity and emissivity.

Which determine the intensity.

That goes into scattering integral that goes in the SE equation.

That yields n_i. See where are we going?

Solving the problem

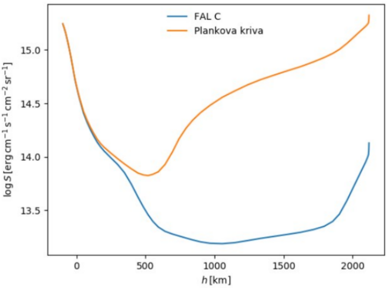
You can use the Λ iteration again.

It converges very slowly. There are many ways to make it faster, many of those also give physical insight. A lot of great papers and books from 70s, 80s and 90s:

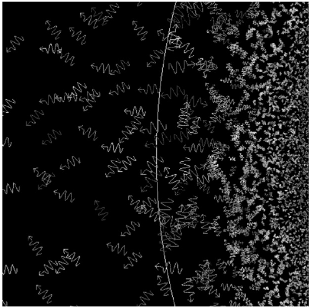
- Cannon (1985), Scharmer (1981), Rybicki & Hummer (1991)
- Mihalas (book, from 1978), but also papers from 1970-1978
- Uitenbroek (2001), Carlsson & Scharmer (1985)
- Auer, Avrett, Athay, Ayres, Atanackovic, Faurobert, Heinzel, Hubeny, Kalkofen, Kneer, Fabiani-Bendicho, Olson, Paletou, Rutten, Steiner, Trujillo-Bueno (sorry to whoever I forgot).

NLTE effects

Photons “leak”, the mean intensity, and the excitation, drop, and so does the emission (source function).



D. Vukadinovic, Master thesis,
University of Belgrade (2018)



Credits: Mats Carlsson, poster
for THE Oslo summer school

NLTE effects

In the Sun, it usually means that lines turn to absorption.

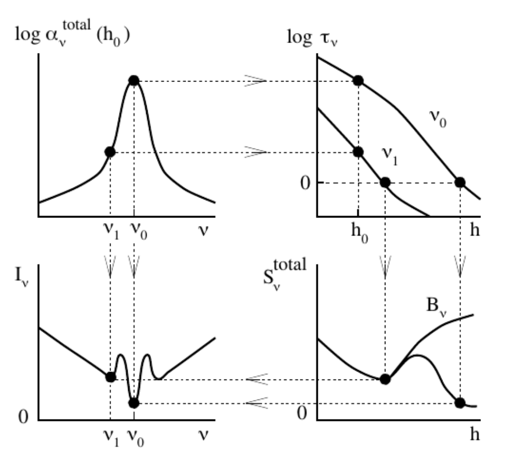
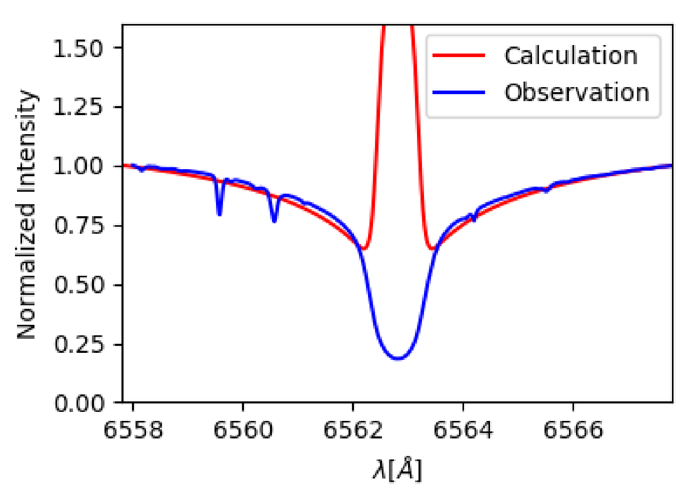


Figure 6: Example from page 20 of Rob Rutten's book.

Hα from previous lecture



Hα from previous lecture

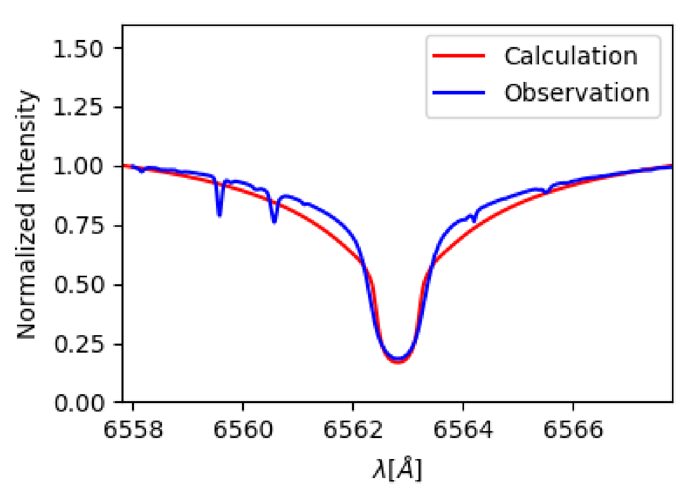


Figure 7: Far from perfect but much better

Some concluding remarks

- Continuum weak lines and strong line wings - LTE.
- Strong line cores - NLTE.
- UV continuum also in NLTE.
- Examine source function for Mg I b line from the hands on. It exhibits strong NLTE effects. Replace it with LTE one (one from continuum), to see how the line would look in LTE.
- That was it. Next week we move to polarization.