Radiative Transfer under conditions of Non-Local Thermodynamic Equilibrium

Han Uitenbroek National Solar Observatory/Sacramento Peak Sunspot, USA



Hale COLLAGE, Boulder, Feb 11, 2016

Han Uitenbroek/NSO Non-LTE Radiative Transfer

Today's lecture will introduce the principle of non-Local Thermodynamic Equilibrium (non-LTE), where the radiation field is (partially) decoupled from local conditions and is able to communicate thermodynamic conditions of one part of the plasma to a totally different part. Scattering.

Rationale for doing Radiative Transfer

- In general we cannot visit the astronomical objects we are interested in, and thus cannot take in-situ measurements
- Instead, to determine the object's properties, we have to rely on the information carried to us by the electromagnetic radiation emitted and/or reflected by the object.
- Multi-wavelength (spectroscopic) observations and analysis are the only available means to determine the physical conditions of astronomical objects.
- To analyze spectroscopic data meaningfully we need to understand how physical information is encoded (Radiative Transfer) in the radiation that we oberve.
- We need to understand how the radiative signal is modified as it travels to our instruments and is detected with them.

• **Rutten:** Radiative Transfer in Stellar Atmospheres (http://esoads.eso.org/abs/2003rtsa.book.....R)

- **Rutten:** Radiative Transfer in Stellar Atmospheres (http://esoads.eso.org/abs/2003rtsa.book.....R)
- Hubeny & Mihalas: Theory of Stellar Atmospheres: An Introduction to Astrophysical Non-equilibrium Quantitative Spectroscopic Analysis









Courtesy: Mats Carlsson, UIO, Norway

Han Uitenbroek/NSO Non-LTE Radiative Transfer

The dynamic and Inhomogeneous Solar Atmosphere

Courtesy: Yukio Katsukawa, NAOJ, Japan

Han Uitenbroek/NSO Non-LTE Radiative Transfer

The best tool: Analysis of Spectral Lines





Spatially Resolved Spectral Lines



Basic Radiative Transfer: Absorption

Absorption α_{λ} :

$$I_{\lambda}(s + \mathrm{d}s) = I_{\lambda}(s) + \mathrm{d}I_{\lambda} = I_{\lambda} - \alpha_{\lambda}I_{\lambda}\mathrm{d}s$$

Units: m⁻¹



Emission η_{λ} :



Source function:

$$S_{\lambda} \equiv \eta_{\lambda} / \alpha_{\lambda}$$

Units: $J s^{-1} m^{-2} nm^{-1} ster^{-1}$

For multiple proceses active at the same wavelength:

$$\begin{split} S_{\lambda}^{\text{tot}} &= \sum \eta_{\lambda} / \sum \alpha_{\lambda} \\ S_{\lambda}^{\text{tot}} &= \frac{\eta_{\lambda}^{c} + \eta_{\lambda}'}{\alpha_{\lambda}^{c} + \alpha_{\lambda}'} = \frac{S_{\lambda}^{c} + r_{\lambda}S_{\lambda}'}{1 + r_{\lambda}}, \quad r_{\lambda} \equiv \alpha_{\lambda}' / \alpha_{\lambda}^{c} \end{split}$$

Transport along a ray:

$$dI_{\lambda}(s) = I_{\lambda}(s + ds) - I_{\lambda}(s) = \eta_{\lambda}(s)ds - \alpha_{\lambda}(s)I_{\lambda}(s)ds \quad (1)$$
$$\frac{dI_{\lambda}}{ds} = \eta_{\lambda} - \alpha_{\lambda}I_{\lambda}$$
$$\frac{dI_{\lambda}}{\alpha_{\lambda}ds} = \frac{dI_{\lambda}}{d\tau_{\lambda}} = S_{\lambda} - I_{\lambda}$$

Optical length and thickness:

$$d\tau_{\lambda} \equiv \alpha_{\lambda}(s) ds$$
(2)
$$\tau_{\lambda}(D) = \int_{0}^{D} \alpha_{\lambda}(s) ds$$

Basic Radiative Transfer: Plane-Parallel

Optical path:

$$\mathrm{d}\tau_{\mu\lambda} = \alpha_{\lambda}\mathrm{d}\boldsymbol{s} \equiv -\alpha_{\lambda}\frac{\mathrm{d}\boldsymbol{z}}{\mu}$$

Standard plane parallel transport equation:

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

Basic Radiative Transfer: Eddington-Barbier

Emergent intensity at the surface:

$$I_{\lambda}^{+}(au_{\lambda}=0,\mu)=\int_{0}^{\infty}S_{\lambda}(t)e^{-t/\mu}\mathrm{d}t/\mu$$

Substitute power series:

$$S_{\lambda}(\tau_{\lambda}) = \sum_{n=0}^{N} a_n \tau_{\lambda}^n \qquad (\text{using}: \int_0^{\infty} e^{-t} t^n dt = !n)$$
$$J_{\lambda}^+(\tau_{\lambda} = 0, \mu) = a_0 + a_1 \mu + 2a_2 \mu^2 + \ldots + n! a_N \mu^N$$

Eddington–Barbier relation:

$$I_{\lambda}^{+}(au_{\lambda}=0,\mu)pprox \mathcal{S}_{\lambda}(au_{\lambda}=\mu)$$

Eddington-Barbier approximation



Basic Radiative Transfer: Limb Darkening



Local Thermodynamic Equilibrium (LTE)



- Radiation field is given by Planck function
- Velocities are given by Maxwellian distribution
- Ionization and excitation are given by Saha–Boltzmann statistics



- Identity of photon is concerved, only its direction is changed
- No exchange with the local thermal pool

Absorption:

$$\mathrm{d}I_{\nu} \equiv -\sigma_{\nu}I_{\nu}\mathrm{d}s$$

Emission:

$$\mathrm{d}I_{\nu} = \sigma J_{\nu}\mathrm{d}s;$$
 (isotropic scattering)

Scatering source function:

$$S_{\nu} = \sigma_{\nu} J_{\nu} / \sigma_{\nu} = J_{\nu}$$

In the case of pure scattering the source function is solely determined by the radiation field and, therefore, completely decoupled from local conditions in the atmosphere, resulting in possible departures from Local Thermodynamic Equilibrium (LTE).

Radiative Transfer with Absorption and Scattering

Total emission and absorption coefficients:

$$\eta_{\nu} = \alpha_{\nu} B_{\nu} + \sigma_{\nu} J_{\nu}$$
$$\chi_{\nu} = \alpha_{\nu} + \sigma_{\nu}$$

Total source function:

$$S_{\nu} \equiv \frac{\eta_{\nu}}{\chi_{\nu}}$$

= $\frac{\sigma_{\nu}}{\alpha_{\nu} + \sigma_{\nu}} J_{\nu} + \frac{\alpha_{\nu}}{\alpha_{\nu} + \sigma_{\nu}} B_{\nu}; \qquad \epsilon_{\nu} \equiv \frac{\alpha_{\nu}}{\alpha_{\nu} + \sigma_{\nu}}$
= $(1 - \epsilon_{\nu}) J_{\nu} + \epsilon_{\nu} B_{\nu}$
= $(1 - \epsilon_{\nu}) \Lambda_{\nu} [S_{\nu}] + \epsilon_{\nu} B_{\nu}$

Operator equation for source function:

$$S_{\nu} = (1 - \epsilon_{\nu}) \Lambda_{\nu} [S_{\nu}] + \epsilon_{\nu} B_{\nu}$$

Simple iterative solution:

$$egin{aligned} S^{(0)}_
u &= B_
u\ S^{(n)}_
u &= (1-\epsilon_
u) \Lambda_
u \left[S^{(n-1)}_
u
ight] + \epsilon_
u B_
u \end{aligned}$$

Lamda Iteration: $\epsilon = 0.5$





Lamda Iteration: $\epsilon = 0.01$



Lamda Iteration: $\epsilon = 0.001$





Lamda Iteration: $\epsilon = 0.001$, 3000 Iterations



L. Auer, in "Numerical Radiative Transfer", 1987, ed. W. Kalkofen, p. 101

$$S_{\nu} = (1 - \epsilon_{\nu}) \Lambda_{\nu} [S_{\nu}] + \epsilon_{\nu} B_{\nu}$$

For one wavelength, this is a matrix equation in depth points:

$$S_k = (1 - \epsilon_k) \Lambda_{\nu} [S_{\nu}]_k + \epsilon_k B_k$$

We could solve this equation easily if the Λ operator where just a multiplication, i.e., if it where a local operator. Use the local part of the operator, i.e., its diagonal Λ^* (see Olson, Auer & Buchler, 1986, JQSRT 35, 431).

Split off the diagonal part:

$$J_{k} = \Lambda_{\nu} [S_{\nu}]_{k} \equiv \Lambda_{k}^{*} S_{k} + (\Delta J)_{k} \rightarrow \Delta J_{k} = \Lambda [S]_{k} - \Lambda_{k}^{*} S_{k}$$
$$S_{k} = (1 - \epsilon_{k}) \{\Lambda_{k}^{*} S_{k} + \Delta J_{k}\} + \epsilon_{k} B_{k}$$

New iterative scheme:

$$\Delta J^{(n)} = \Lambda^{(n)} \left[S^{(n)} \right] - \Lambda^* S^{(n)}$$
$$S_k^{(n+1)} = \frac{(1 - \epsilon_k) \Delta J_k^{(n)} + \epsilon_k B_k}{1 - (1 - \epsilon_k) \Lambda_k^*}$$

We can invert the diagonal part now directly and only have to lambda iterate the weaker off-diagonal contributions.

Accelerated Lamda Iteration: $\epsilon = 0.0001$



K.C. Ng 1974, J. Chem. Phys. 61, 2680

Let x⁽ⁿ⁾k be a sequence of iterative solutions of xk, with n at least Norder + 2.

K.C. Ng 1974, J. Chem. Phys. 61, 2680

- Let x⁽ⁿ⁾_k be a sequence of iterative solutions of x_k, with n at least N_{order} + 2.
- The acceleration process to be described will provide a new estimate $\tilde{x_k}$ of the solution written as the linear combination of the current solution x_k^0 and N_{order} previous solutions $x_k^i, i = 1, \ldots, N_{\text{order}}$, where N_{order} is the order of the acceleration process:

$$\tilde{x_k} = \left(1 - \sum_{i=0}^{N_{\text{order}}-1} \alpha_i\right) x_k^0 + \sum_{i=0}^{N_{\text{order}}-1} \alpha_i x_k^{(i+1)}$$

Convergence Acceleration

 The coefficients α_i defining the acceleration procedure are found by suitably minimizing the residual

$$r^{2} = \sum_{k=0}^{N-1} w_{k} \left(\tilde{x_{k}} - \tilde{x_{k}}' \right)^{2}$$

Convergence Acceleration

 The coefficients α_i defining the acceleration procedure are found by suitably minimizing the residual

$$r^{2} = \sum_{k=0}^{N-1} w_{k} \left(\tilde{x_{k}} - \tilde{x_{k}}' \right)^{2}$$

between successive accelerated estimates.

• Minimization in the least squares sense requires:

$$\frac{\partial r^2}{\partial \vec{\alpha}} = \frac{\partial}{\partial \vec{\alpha}} \left[\sum_{k=0}^{N-1} w_k \left(\tilde{x}_k - \tilde{x}_k' \right)^2 \right] = 0$$

• The minimization condition for the residual r^2 provides a linear set of equations for the coefficients α_i in terms of the privious N_{order} iterative solutions.

- The minimization condition for the residual r^2 provides a linear set of equations for the coefficients α_i in terms of the privious N_{order} iterative solutions.
- The solution to the linear set can then be used to construct an extrapolated new estimate x_k.

- The minimization condition for the residual r^2 provides a linear set of equations for the coefficients α_i in terms of the privious N_{order} iterative solutions.
- The solution to the linear set can then be used to construct an extrapolated new estimate x_k.
- Resulting convergence is sped up considerably.

Accelerated Lamda Iteration: $\epsilon = 0.0001$ with convergence extrapolation



Han Uitenbroek/NSO Non-LTE Radiative Transfer

• The process of scattering, i.e. the absorption and subsequent emission of a (nearly) identical photon, without exchange with the thermal pool, decouples the radiation field from local conditions.

- The process of scattering, i.e. the absorption and subsequent emission of a (nearly) identical photon, without exchange with the thermal pool, decouples the radiation field from local conditions.
- Solution of the radiative transfer becomes a non-linear, non-local problem that has to be solved iteratively

- The process of scattering, i.e. the absorption and subsequent emission of a (nearly) identical photon, without exchange with the thermal pool, decouples the radiation field from local conditions.
- Solution of the radiative transfer becomes a non-linear, non-local problem that has to be solved iteratively
- However, efficient techniques for this solution exist, in particular ones using a local approximate operator.

Next lecture we will talk about practical (numerical) solutions to the transfer equation.

Molecular Oxygen in the Earth Atmosphere





Planck Function



Planck function:

$$B_{\lambda}(T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$

Han Uitenbroek/NSO Non-LTE Radiative Transfer



Maxwellian Velocity Distribution



Maxwellian:

$$f(\mathbf{v})\mathrm{d}\mathbf{v} = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp(-mv^2/2kT) 4\pi v^2 \mathrm{d}\mathbf{v}$$

Han Uitenbroek/NSO Non-LTE Radiative Transfer

Boltzmann distribution for excitation:

$$\left[\frac{n_j}{n_i}\right]_{\rm LTE} = \frac{g_j}{g_i} e^{-\Delta E_{ji}/kT}$$

Saha distribution for ionization:

$$\left[\frac{n_{r+1,1}}{n_{r,1}}\right]_{\rm LTE} = \frac{1}{N_{\rm e}} \frac{2g_{r+1,1}}{g_{r,1}} e^{-\Delta \chi_r/kT}$$

Angle-averaged Mean intensity:

$$J_{\nu}(\vec{r},t) \equiv \frac{1}{4\pi} \int I_{\lambda} d\Omega = \frac{1}{4\pi} \int_{0}^{2\pi} \int_{0}^{\pi} I_{\lambda} \sin \theta \, \mathrm{d}\theta \, \mathrm{d}\varphi$$

Units: J s⁻¹ m⁻² nm⁻¹ ster⁻¹

Unlike the Specific Intensity the Angle-averaged Mean Intensity is not conserved with distance

Mean intensity as operator working on S:

$$\begin{split} J_{\nu} &= \frac{1}{4\pi} \int I_{\nu}(\tau, \vec{I}) \,\mathrm{d}\Omega \\ &= \frac{1}{4\pi} \int \mathrm{d}\Omega \int_{\tau_{\nu}}^{\infty} S_{\nu}(t, \vec{I}) \, e^{-(t - \tau_{\nu})} \,\mathrm{d}t \\ &= \Lambda_{\nu} \left[S_{\nu} \right] \end{split}$$