Non-LTE line formation with coherent scattering and the Mg II h&k lines

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Radiative transfer with Non-Local Thermodynamic Equilibrium (Non-LTE), the role of scattering.

The role of coherent scattering: Partial frequency ReDistribution (PRD).

The Mg II h&k lines.

Diagnostics of the Mg II h&k lines.
\[ \Delta E = h\nu = \frac{hc}{\lambda} \]
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Termdiagram and Transitions in Hydrogen

$$\Delta E = h\nu = \frac{hc}{\lambda}$$
Radiative bound–bound transitions

\[ \Delta E = E_2 - E_1 = h\nu = hc/\lambda \]

absorption

Spontaneous emission

Stimulated emission
Collisional bound–bound transitions

Collisional bound - bound

$E_2 - E_1 = E_b - E_a$

collisional excitation

collisional de-excitation
Radiative bound–free transitions

\[ E_e = h\nu - (E_{cont} - E_1) \]

- Radiative ionization
- Radiative recombination
- Stimulated radiative recombination

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Collisional bound–free transitions

\[ E_a - (E_b + E_c) = (E_{\text{cont}} - E_1) \]

Collisional ionization

Collisional recombination

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Non-LTE Radiative Transfer with PRD
Specific intensity $I_\nu$ is the **radiative** energy that flows, at the location $\vec{r}$, per second, per wavelength interval, and per solid angle, in the direction $\vec{l}$ through the surface area $dA'$ perpendicular to $\vec{l}$. Intensity is **conserved** with distance in the absence of emission and absorption or scattering processes.

**Specific Intensity:**

$$dE_\lambda^{\text{rad}} \equiv I_\lambda(\vec{r}, \vec{l}, t) \, dt \, dA' \, d\lambda \, d\Omega = I_\lambda(\vec{r}, \vec{l}, t) \, dt \, \cos \theta \, dA \, d\lambda \, d\Omega$$

**Units:** $\text{J s}^{-1} \, \text{m}^{-2} \, \text{nm}^{-1} \, \text{ster}^{-1}$
Angle-averaged Mean intensity:

\[ J_\nu(\vec{r}, t) \equiv \frac{1}{4\pi} \int I_\lambda d\Omega = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi I_\lambda \sin \theta \, d\theta \, d\varphi \]

Units: \( J \, s^{-1} \, m^{-2} \, \text{nm}^{-1} \, \text{ster}^{-1} \)

Unlike the Specific Intensity the Angle-averaged Mean Intensity is not conserved with distance.
**Absorption** $\alpha \lambda$:

$$I_\lambda(s + ds) = I_\lambda(s) + dI_\lambda = I_\lambda - \alpha \lambda l_\lambda ds$$

**Units:** $m^{-1}$
Basic Radiative Transfer: Emission

Emission $j_\lambda$:

$$I_\lambda(s + ds) = I_\lambda(s) + dl_\lambda = I_\lambda + j_\lambda(s)ds$$

Units: J m$^{-3}$ s$^{-1}$ nm$^{-1}$ ster$^{-1}$
Source function:

\[ S_\lambda \equiv \frac{j_\lambda}{\alpha_\lambda} \]

Units: J s\(^{-1}\) m\(^{-2}\) nm\(^{-1}\) ster\(^{-1}\)

For multiple processes active at the same wavelength:

\[ S_{\lambda}^{\text{tot}} = \frac{\sum j_\lambda}{\sum \alpha_\lambda} \]

\[ S_{\lambda}^{\text{tot}} = \frac{j_\lambda^c + j_\lambda^l}{\alpha_\lambda^c + \alpha_\lambda^l} = \frac{S_\lambda^c + \eta_\lambda S_\lambda^l}{1 + \eta_\lambda}, \quad \eta_\lambda \equiv \frac{\alpha_\lambda^l}{\alpha_\lambda^c} \]
Transport along a ray:

\[ dl_\lambda(s) = l_\lambda(s + ds) - l_\lambda(s) = j_\lambda(s)ds - \alpha_\lambda(s)l_\lambda(s)ds \quad (1) \]

\[ \frac{dl_\lambda}{ds} = j_\lambda - \alpha_\lambda l_\lambda \]

\[ \frac{dl_\lambda}{\alpha_\lambda ds} = \frac{dl_\lambda}{d\tau_\lambda} = S_\lambda - l_\lambda \]

Optical length and thickness:

\[ d\tau_\lambda \equiv \alpha_\lambda(s)ds \quad (2) \]

\[ \tau_\lambda(D) = \int_0^D \alpha_\lambda(s)ds \]
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
Scattering

Identity of photon is conserved, only its direction is changed.
No exchange with the local thermal pool.
Basic Radiative Transfer: Scattering

Absorption:

\[ dI_\nu \equiv -\sigma_\nu I_\nu ds \]

Emission:

\[ dI_\nu = \sigma J_\nu ds; \quad \text{(isotropic scattering)} \]

Scattering source function:

\[ S_\nu = \frac{\sigma_\nu J_\nu}{\sigma_\nu} = J_\nu \]

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).
Total emission and absorption coefficients:

\[ \eta_\nu = \alpha_\nu B_\nu + \sigma_\nu J_\nu \]
\[ \chi_\nu = \alpha_\nu + \sigma_\nu \]

Total source function:

\[ S_\nu \equiv \frac{\eta_\nu}{\chi_\nu} = \frac{\sigma_\nu}{\alpha_\nu + \sigma_\nu} J_\nu + \frac{\alpha_\nu}{\alpha_\nu + \sigma_\nu} B_\nu; \]
\[ \epsilon_\nu \equiv \frac{\alpha_\nu}{\alpha_\nu + \sigma_\nu} \]

\[ = (1 - \epsilon_\nu) J_\nu + \epsilon_\nu B_\nu \]
\[ = (1 - \epsilon_\nu) \Lambda_\nu [S_\nu] + \epsilon_\nu B_\nu \]
Operator equation for source function:

\[ S_\nu = (1 - \epsilon_\nu)\Lambda_\nu \left[ S_\nu \right] + \epsilon_\nu B_\nu \]

Simple iterative solution:

\[ S^{(0)}_\nu = B_\nu \]
\[ S^{(n)}_\nu = (1 - \epsilon_\nu)\Lambda_\nu \left[ S^{(n-1)}_\nu \right] + \epsilon_\nu B_\nu \]
Lamda Iteration: $\epsilon = 0.5$

\[ B_{\text{Planck}} \]

\[ S^{(0)} \quad S^{(1)} \quad S^{(10)} \]

\[ \epsilon = 5.0E-01 \]
Lamda Iteration: $\epsilon = 0.1$

\[ S(0) = 1.0 \times 10^{-6} \]

\[ S(1) = 1.0 \times 10^{-4} \]

\[ S(100) = 1.0 \times 10^{-2} \]

\[ B_{\text{Planck}} \]

Optical depth $\tau$

\[ \epsilon = 1.0 \times 10^{-1} \]

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Lamda Iteration: $\epsilon = 0.01$

Planck $S(0)$

$S(1)$

$S(100)$

$\tau$

$0.1$

$1.0$

$\epsilon = 1.0E-02$

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Lamda Iteration: $\epsilon = 0.001$

\[ \begin{align*}
\tau & = 0.1 \\
S^{(0)} & = 1.0 \\
S^{(1)} & = 0.1 \\
S^{(100)} & = 1.0 \times 10^{-3} \\
\end{align*} \]

$B_{\text{Planck}}$

$\epsilon = 1.0 \times 10^{-3}$

optical depth $\tau$
Lamda Iteration: $\epsilon = 0.001$, 3000 Iterations

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Non-LTE Radiative Transfer with PRD

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

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 \( \Lambda \) operator were just a multiplication, i.e., if it were a local operator. Use the local part of the operator, i.e., its diagonal \( \Lambda^* \) (see Olson, Auer & Buchler, 1986, JQSRT 35, 431).
Split off the diagonal part:

\[ J_k = \Lambda_\nu [S_\nu]_k \equiv \Lambda_k^* S_k + (\Delta J)_k \quad \rightarrow \quad \Delta J_k = \Lambda [S]_k - \Lambda_k^* S_k \]

\[ S_k = (1 - \epsilon_k) \{ \Lambda_k^* S_k + \Delta J_k \} + \epsilon_k B_k \]

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 Lambda Iteration: $\epsilon = 0.0001$

Source function

Optical depth

$N_{\text{iter}} = 142$

$\epsilon = 1.0 \times 10^{-04}$
Accelerated Lambda Iteration: $\epsilon = 0.0001$
with convergence extrapolation

K.C. Ng 1974, J. Chem. Phys. 61, 2680
Absorption and emission coefficients for bound-bound transitions

Spontaneous emission $j \to i$:

$$j_{\nu}^{\text{spont}} = n_j (A_{ji} h \nu_{ij}/4\pi) \phi_{\nu}$$

Stimulated emission $j \to i$:

$$j_{\nu}^{\text{stim}} = n_j (B_{ji} h \nu_{ij}/4\pi) \phi_{\nu} I_{\nu}, \quad A_{ji} = (2h\nu^3/c^2) B_{ji}$$

Absorption $i \to j$:

$$\alpha_{\nu} = n_i (B_{ij} h \nu_{ij}/4\pi) \phi_{\nu}, \quad g_i B_{ij} = g_j B_{ji}$$
Transfer equation:

\[
\frac{dl_\nu}{ds} = j_\nu^{\text{spont}} + j_\nu^{\text{stim}} - \alpha_\nu l_\nu \\
= n_j (A_{ji} h\nu_{ij}/4\pi) \phi_\nu - h\nu_{ij}/4\pi \phi_\nu (n_i B_{ij} - n_j B_{ji}) l_\nu
\]

Source function:

\[
S_\nu = \frac{j_\nu}{\alpha_\nu} = \frac{n_j A_{ji}}{n_i B_{ij} - n_j B_{ji}} \\
= \frac{2 h\nu_{ij}^3}{c^2} \frac{n_j}{g_j/g_i n_i - n_j} = (1 - \epsilon) \overline{J} + \epsilon B_\nu; \\
\epsilon \equiv \frac{C_{ji}}{C_{ji} + A_{ji} + B_{ji} \overline{J}}
\]
Radiative rates

Radiative excitation

\[ R_{ij} = B_{ij} \frac{h \nu}{4\pi} \int d\Omega \int \frac{d\nu}{h \nu} I_\nu \phi_\nu \]

\[ = B_{ij} \overline{J} \]

\[ \overline{J} \equiv \frac{1}{4\pi} \int d\Omega \int d\nu I_\nu \phi_\nu \]

Radiative de-excitation

\[ R_{ij} = A_{ji} + B_{ji} \frac{h \nu}{4\pi} \int d\Omega \int \frac{d\nu}{h \nu} I_\nu \phi_\nu \]

\[ = A_{ji} + B_{ji} \overline{J} \]
Basic Equation: Statistical Equilibrium

Consider an atom (or molecule) with levels \( i = 0, \ldots, N - 1 \).

**Statistical equilibrium for level i:**

\[
\frac{dn_i}{dt} = \sum_{j=0}^{N-1} n_j (Cji + Rji) - \sum_{j=0}^{N-1} n_i (Cij + Rij)
\]

**Stationary state:**

\[
\sum_{j=0}^{N-1} n_j (Cji + Rji[n]) = \sum_{j=0}^{N-1} n_i (Cij + Rij[n])
\]

The set of equations for all levels forms a generally non-linear, and non-local, set of equations for the population numbers \( n_i \).
When density is high and collisions are frequent enough, population numbers are determined by local conditions, and given by the Saha-Boltzmann relations at the kinetic temperature of the gas.

The radiation field is then given by the Planck function.

As densities drop with height, collisions become less frequent, and radiative transitions become relatively more important.

Populations are now determined by non-local conditions, namely the radiation field that comes from different places in the atmosphere.

Need to find a global solution, not only in space, but also in wavelength.
The Redistribution Function $R_{ij}$


The laboratory frame redistribution function:

$$R_{ij}(\nu, \mathbf{n}; \nu', \mathbf{n}') d\nu d\nu' \frac{d\Omega}{4\pi} \frac{d\Omega'}{4\pi}$$

Describes the conditional probability that, when a photon in line $(i, j)$ and solid angle $d\Omega'$ around direction $\mathbf{n}'$ and frequency range $(\nu', \nu' + d\nu')$ is scattered by that line, it will be emitted into angle $d\Omega$ around direction $\mathbf{n}$ and frequency range $(\nu, \nu + d\nu)$.

Complete frequency in the laboratory frame:

$$R_{ij}(\nu, \mathbf{n}; \nu', \mathbf{n}') = \phi_{ij}(\nu, \mathbf{n}) \phi_{ij}(\nu', \mathbf{n}')$$
The Redistribution Function $R_{ij}$ (2)

**Normalization:**

$$\iint \frac{d\Omega}{4\pi} \frac{d\Omega'}{4\pi} \iiint d\nu' d\nu \ R_{ij}(\nu, n; \nu', n') \equiv 1.$$  

$$\iint \frac{d\Omega'}{4\pi} \int d\nu' \ R_{ij}(\nu, n; \nu', n') \equiv \phi_{ij}(\nu, n)$$

**Coherency fraction:**

$$R_{ij} = \gamma R_{ij}^V + (1 - \gamma) R_{ij}^{III}$$

$$\gamma = \frac{P_j}{P_j + Q_E}$$
Partial Frequency Redistribution in the emission profile

\[
\psi_{ij}^{\text{PRD}}(\nu) = \phi_{ij}(\nu) \left\{ 1 + \gamma \frac{n_i B_{ij}}{n_j P_j} \int \left[ \frac{R_{iji}(\nu, \nu')}{\phi_{ij}(\nu)} - \phi_{ij}(\nu') \right] J(\nu') d\nu' \right\}
\]
Partial Frequency Redistribution in the emission profile

\[ \psi_{ij}^{\text{PRD}}(\nu) = \phi_{ij}(\nu) \left\{ 1 + \gamma \frac{n_i B_{ij}}{n_j P_j} \int \left[ \frac{R_{ijji}(\nu, \nu')}{\phi_{ij}(\nu)} - \phi_{ij}(\nu') \right] J(\nu') d\nu' \right\} \]
Partial Frequency Redistribution in the emission profile

\[ \psi_{ij}^{\text{PRD}}(\nu) = \phi_{ij}(\nu) \left\{ 1 + \gamma \frac{n_i B_{ij}}{n_j P_j} \int \left[ \frac{R_{iji}^{\text{II}}(\nu, \nu')}{\phi_{ij}(\nu)} - \phi_{ij}(\nu') \right] J(\nu') d\nu' \right\} \]

- Complete redistribution in core
- Coherent scattering in the wings
- Decoupling of wing source function
PRD in the Mg II h and k lines

![Graph showing intensity vs. wavelength for Mg II h and k lines.](image-url)
PRD in the Mg II h and k lines

![Graph showing intensity vs wavelength with CRD and PRD curves.]

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PRD in the Mg II h and k lines

Wavelength [nm]

Intensity $[\text{J m}^{-2} \text{s}^{-1} \text{Hz}^{-1} \text{sr}^{-1}]$

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Non-LTE Radiative Transfer with PRD
PRD in the Mg II h and k lines

Intensity \( [J m^{-2} s^{-1} Hz^{-1} sr^{-1}] \)

Wavelength \([\text{nm}]\)

279.0
279.5
280.0
280.5
281.0

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Non-LTE Radiative Transfer with PRD
The Mg II h&k lines

![Graph showing the intensity of various elements across different wavelengths.](image-url)
The Mg II Termdiaagram

Energy [eV]

MG III GROUND TERM

MG II 2P6 3S
MG II 2P6 3P
MG II 2P6 4S MG II 2P6 3D
MG II 2P6 4P
MG II 2P6 5S
MG II 2P6 4D
MG II 2P6 4I

2SE 2PO 2DE 2FO
The h&k lines are in emission on the whole disk

HRTS 9, Morrill et al., 2001
The Mg $\text{II}$ h&k lines, limb spectra

![Graph showing Mg II h&k lines with counts and wavelength axes.](image-url)
Non-LTE modeling of the Mg II h&k lines with PRD in state-of-the-art Radiation Magneto-HydroDynamic (Rad-MHD) simulations of the solar atmosphere:

- **The formation of IRIS diagnostics. I. quintessential model atom of Mg II and general formation properties of the Mg II h&k lines,**

- **The formation of IRIS diagnostics. II. The formation of the Mg II h&k lines in the solar atmosphere,**

- **The formation of IRIS diagnostics. III. Near-ultraviolet spectra and images,**
Identification of line components

\[ I \left[ 10^{-10} \text{ J s}^{-1} \text{ m}^2 \text{ Hz}^{-1} \text{ sr}^{-1} \right] \]

- \( k_{2v} \)
- \( k_3 \)
- \( k_{2r} \)
Formation heights of central reversals and correlation with velocity

(a) -0.39
(b) -0.35
(c) 0.99
(b) 0.98
Correlation of peak intensities with temperature
Correlation of velocity with peak separation and position

- **Mg II k**
  - (a) 0.61
  - Comparison of max(Δv) vs. peak separation [km s\(^{-1}\)]

- **Mg II h**
  - (b) 0.54
  - Comparison of max(Δv) vs. peak separation [km s\(^{-1}\)]

- **c)** 0.67
  - Comparison of \(v_z\) at average \(\tau=1\) [km s\(^{-1}\)] vs. average Doppler shift [km s\(^{-1}\)]

- **d)** 0.64
  - Comparison of \(v_z\) at average \(\tau=1\) [km s\(^{-1}\)] vs. average Doppler shift [km s\(^{-1}\)]
Comparison of simulations with observations

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Conclusions

- The Mg II h&k lines provide unique information about the top layers of the chromosphere, just below the transition region.
Conclusions

- The Mg $\text{II}$ $h$&$k$ lines provide unique information about the top layers of the chromosphere, just below the transition region.
- In particular the wavelength position of the $h_3$ and $k_3$ reversals is a good indicator of velocity, and the peak heights $h_2$, $k_2$ are reasonable indicators of temperature.
The Mg II h&k lines provide unique information about the top layers of the chromosphere, just below the transition region.

In particular the wavelength position of the h₃ and k₃ reversals is a good indicator of velocity, and the peak heights h₂, k₂ are reasonable indicators of temperature.

The lines can be fairly well described by modeling in state-of-the-art 3-D Rad-MHD modeling, but peak separation is still underestimated.
The Mg II h&k lines provide unique information about the top layers of the chromosphere, just below the transition region. In particular the wavelength position of the h₃ and k₃ reversals is a good indicator of velocity, and the peak heights h₂, k₂ are reasonable indicators of temperature. The lines can be fairly well described by modeling in state-of-the-art 3-D Rad-MHD modeling, but peak separation is still underestimated. Modeling these lines does require Non-LTE with PRD, but this is very well possible.
Planck function:

\[ B_\lambda(T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1} \]
Maxwellian Velocity Distribution

Maxwellian:

\[ f(v) \, dv = \frac{m^2}{\pi kT} \frac{3}{2} \exp\left(-\frac{mv^2}{2kT}\right) \frac{4}{\pi v^2} \, dv \]

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Maxwellian Velocity Distribution

Maxwellian:

\[ f(v)dv = \left( \frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right) 4\pi v^2 dv \]
Saha–Boltzmann statistics

**Boltzmann distribution for excitation:**

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

**Saha distribution for ionization:**

\[
\left[ \frac{n_{r+1,1}}{n_{r,1}} \right]_{\text{LTE}} = \frac{1}{N_e} \frac{2g_{r+1,1}}{g_{r,1}} e^{-\Delta \chi_r/kT}
\]
Mean intensity as operator working on $S$:

\[
J_\nu = \frac{1}{4\pi} \int I_\nu(\tau, \vec{l}) \, d\Omega \\
= \frac{1}{4\pi} \int d\Omega \int_{\tau_\nu}^{\infty} S_\nu(t, \vec{l}) e^{-(t-\tau_\nu)} \, dt \\
= \Lambda_\nu [S_\nu]
\]
Voigt Functions

\[ \phi(\nu - \nu_0) = \frac{H(a, \nu)}{\sqrt{\pi} \Delta \nu_D} \]

\[ \Delta \nu_D \equiv \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}} \]

\[ a = \frac{\Gamma}{4\pi \Delta \nu_D} \]