Lecture 5
Rate Equations & Temperature Correction

Where are we?

- Know how to solve RTE given $T, \chi_\nu, \eta_\nu \rightarrow J_\nu$
- We've skipped over how to get χ_ν, η_ν given n_i, n_e, T
- So now we look at how to get n_i, n_e given J_ν?

Rate Equations I

The change in the number density of species k in state i is

$$\frac{\partial n_{i,k}}{\partial t} = -\nabla \cdot (v n_{i,k}) + \sum_{j \neq i} P_{ji} n_{j,k} - P_{ij} n_{i,k}$$

where P_{ji} is the total transition rate from level j to level i. If we sum over all states i then

$$\frac{\partial N_k}{\partial t} = -\nabla \cdot (v N_k)$$

Now if we multiply by the mass of species k, m_k and $\sum_k$ we get the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (v \rho)$$

In steady state

$$\frac{\partial n_{i,k}}{\partial t} = 0$$

Rate Equations II

so

$$\sum_{j \neq i} P_{ji} n_{j,k} - P_{ij} n_{i,k} = \nabla \cdot (v n_{i,k})$$

so in the case of either a static flow or in the co-moving frame

$$\sum_{j \neq i} P_{ji} n_{j,k} - P_{ij} n_{i,k} = 0$$

The total transition rate P_{ji} contains both radiative and collisional terms which we now need to examine in detail.

Einstein Coefficients I

Total number of absorptions

$$n_i B_{ij} \phi_\nu I_\nu d\nu \frac{d\Omega}{4\pi} = n_i \frac{\alpha_{ij}}{h\nu} \phi_\nu I_\nu d\nu d\Omega$$

$$4\pi \frac{\alpha_{ij}}{h\nu} = B_{ij}$$

$$\alpha_{ij}(\nu) = \alpha_{ij} \phi_\nu$$

Absorption Rate

$$\begin{aligned} n_i R_{ij} &= \int\int n_i B_{ij} \phi_\nu I_\nu \, d\nu \, \frac{d\Omega}{4\pi} \\ &= n_i B_{ij} \int \phi_\nu J_\nu \, d\nu \\ &= n_i B_{ij} \bar{J}_{ij} \\ &= n_i \frac{\alpha_{ij}}{h\nu_{ij}} \bar{J}_{ij} \end{aligned}$$

Einstein Coefficients II

Thus we can just consider

$$\bar{J}_{ij} = \int \phi_\nu J_\nu \, d\nu$$

and move other quantities in and out of the integral because
$\phi_\nu \approx \delta -$ function
Stimulated Emissions

$$n_j B_{ji} \int \phi_\nu J_\nu \, d\nu = n_j B_{ji} \bar{J}_{ij}$$

$$g_j B_{ji} = g_i B_{ij}$$

$$\begin{aligned} n_j B_{ji} \int \phi_\nu J_\nu \, d\nu &= n_j \frac{g_i B_{ij}}{g_j} \bar{J}_{ij} \\ &= n_j \frac{4\pi}{h\nu_{ij}} \frac{g_i \alpha_{ij}}{g_j} \bar{J}_{ij} \end{aligned}$$

Einstein Coefficients III

$$\frac{g_i}{g_j} = \frac{n_i^*}{n_j^*} e^{-h\nu/(kT)}$$

Spontaneous Emissions

$$\begin{aligned} n_j A_{ji} \int \phi_\nu \, d\nu = n_j \frac{2h\nu^3}{c^2} B_{ji} &= n_j \frac{2h\nu^3}{c^2} \frac{g_i B_{ij}}{g_j} \\ &= = n_j \frac{2h\nu^3}{c^2} \frac{4\pi\alpha_{ij}}{h\nu} \frac{g_i}{g_j} \end{aligned}$$

Now the total downward rate is

$$\begin{aligned} n_j R'_{ji} &\equiv n_j \left(\frac{n_i}{n_j}\right)^* R_{ji} \\ &= n_j [A_{ji} + B_{ji} \bar{J}_{ij}] \\ &= n_j \frac{g_i}{g_j} \left[4\pi \int \frac{\alpha_{ij}(\nu)}{4\pi} [\frac{2h\nu^3}{c^2} + J_\nu] \, d\nu \right] \end{aligned}$$

Einstein Coefficients IV

Now using

$$\frac{g_i}{g_j} = \frac{n_i^*}{n_j^*} e^{-h\nu/(kT)}$$

$$n_j R'_{ji} = n_j \left(\frac{n_i}{n_j}\right)^* 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} e^{-h\nu/(kT)}$$

$$n_j R'_{ji} = n_j \left(\frac{n_i}{n_j}\right)^* 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} e^{-h\nu/(kT)} (\frac{2h\nu^3}{c^2} + J_\nu)\, d\nu$$

$$R_{ji} = 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} e^{-h\nu/(kT)} (\frac{2h\nu^3}{c^2} + J_\nu)\, d\nu$$

Bound Free Transitions

Let $\alpha_{i\kappa}(\nu)$ be the photoionization cross section at frequency ν

Then the rate per unit volume of photoionizations is

$$n_i R_{i\kappa} = 4\pi n_i \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} J_\nu\, d\nu$$

Einstein Coefficients V

In TE: the number of recombinations = number of photoionizations and $J_\nu = B_\nu$

Thus:

spontaneous recombinations + # stimulated recombinations = # photoionizations

hence

spontaneous recombinations = # photoionizations - # stimulated recombinations

$$\text{\# spontaneous recombinations} = \text{\# photoionizations}(1 - e^{-h\nu/(kT)})$$

Hence

$$(n_\kappa R_{\kappa i})^*_{\rm spon} = 4\pi n_i^* \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} B_\nu (1 - e^{-h\nu/(kT)})\, d\nu$$

$$B_\nu = \frac{2h\nu^3}{c^2}(e^{h\nu/(kT)} - 1)^{-1}$$

Einstein Coefficients VI

$$B_\nu = \frac{2h\nu^3}{c^2} \frac{e^{-h\nu/(kT)}}{(1 - e^{-h\nu/(kT)})}$$

but spontaneous recombinations are a *thermal* process, so they should in fact depend only on n_κ^*. Thus in NLTE

$$(n_\kappa R'_{\kappa i})_{\mathrm{spon}} \quad = 4\pi n_\kappa \left(\frac{n_i}{n_\kappa}\right)^* \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} B_\nu (1 - e^{-h\nu/(kT)})\, d\nu$$

$$(n_\kappa R'_{\kappa i})_{\mathrm{spon}} \quad = 4\pi n_\kappa \left(\frac{n_i}{n_\kappa}\right)^* \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} \frac{2h\nu^3}{c^2} e^{-h\nu/(kT)}\, d\nu$$

and

$$\left(\frac{n_i}{n_\kappa}\right)^* = n_e \Phi i\kappa(T)$$

so that the rate properly depends only on thermal quantities, n_κ, and n_e

Einstein Coefficients VII

Now we already showed that in TE the rate of stimulated recombinations is

$$(n_\kappa R'_{\kappa i})^*_{\rm stim} \quad = 4\pi n_i \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} B_\nu e^{-h\nu/(kT)}\, d\nu$$

That is simply
stimulated emission = absorption $e^{-h\nu/(kT)}$. So to get the NLTE value we simply have to replace $B_\nu \rightarrow J_\nu$ and $n^*_\kappa \rightarrow n_\kappa$ Thus,

$$(n_\kappa R'_{\kappa i})_{\rm stim} \quad = 4\pi n_\kappa \left(\frac{n_i}{n_\kappa}\right)^* n_i \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} J_\nu e^{-h\nu/(kT)}\, d\nu$$

Then the total recombination rate is:

$$n_\kappa((R'_{\kappa i})_{\rm stim} + (R'_{\kappa i})_{\rm spon})$$

$$= 4\pi n_\kappa \left(\frac{n_i}{n_\kappa}\right)^* n_i \int_{\nu_0}^{\infty} \frac{\alpha_{i\kappa}(\nu)}{h\nu} (J_\nu + \frac{2h\nu^3}{c^2}) e^{-h\nu/(kT)}\, d\nu$$

Einstein Coefficients VIII

Thus, following Mihalas we can systematize our notation by writing all upward rates whether bound or free as:

$$R_{lu} = 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{lu}(\nu)}{h\nu} J_\nu \, d\nu$$

and all downward rates whether bound or free as:

$$R_{ul} = 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ul}(\nu)}{h\nu} (J_\nu + \frac{2h\nu^3}{c^2}) e^{-h\nu/(kT)} \, d\nu$$

Then in LTE

$$R_{lu}^* = 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{lu}(\nu)}{h\nu} B_\nu \, d\nu$$

and

$$R_{ul}^* = 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ul}(\nu)}{h\nu} (B_\nu (1 - e^{-h\nu/(kT)}) + B_\nu e^{-h\nu/(kT)}) \, d\nu$$

so

$$R_{lu}^* = R_{ul}^*$$

Collisional Rates I

In neutral gases collisions with H atoms and molecules are very important but in ionized gases one needs to only worry about electron collisions because the flux of electrons is so much greater due to the fact that $m_e \sim m_H/2000$.
We will write the cross-section for producing the transition $(i \rightarrow j)$ as σ_{ij} where j may be a bound or free state.
Then the rate per unit volume of such transitions is:

$$n_i C_{ij} = n_i n_e \int_{v_0}^{\infty} \sigma_{ij}(v) f(v) v \, dv$$

where $1/2 m v_0^2 = E_0$ is the threshold energy for producing the transition.
Now by detailed balance

$$n_i^* C_{ij} = n_j^* C_{ji}$$

Collisional Rates II

$$n_j C_{ji} = n_j (\frac{n_i^*}{n_j^*}) C_{ij}$$

so we will work with only the C_{lu}
We can define q_{ij}

$$n_j C_{ji} = n_j (\frac{n_i^*}{n_j^*}) n_e q_{ij}(T)$$

$$C_{ij} = n_e q_{ij}(T)$$

It turns out that cross sections are usually given in units of the Bohr radius

$$\sigma_{ij} = \pi a_0^2 Q_{ij}$$

Then

$$q_{ij} = C_0 T^{1/2} \int_{u_0}^{\infty} Q_{ij}(ukT) u e^{-u} \, du$$

Collisional Rates III

$u = E/kT$, $u_0 = E_0/kT$

$$C_0 = \pi a_0^2 (\frac{8k}{m\pi})^{1/2} = 5.5 \times 10^{-11} \text{ (T in K)}$$

Then

$$q_{ij} = C_0 T^{1/2} e^{-E_0/kT} \Gamma_{ij}(T)$$

$$\Gamma_{ij} = \int_0^\infty Q_{ij}(E_0 + xkT)(x + u_0) e^{-x}\, dx$$

Rate Equaions

$$\sum_{j<i} n_j \left(R_{ji} + C_{ji}\right) \quad - n_i \left\{ \sum_{j<i} \left(\frac{n_j^*}{n_i^*}\right) \left(R_{ij} + C_{ji}\right) + \sum_{j>i} \left(R_{ij} + C_{ij}\right) \right\} + \sum_{j>i} n_j \left(\frac{n_i^*}{n_j^*}\right) \left(R_{ji} + C_{ij}\right) = 0. \tag{1}$$

Where

$$n_i^* \equiv \frac{g_i}{g_\kappa} n_\kappa \frac{2h^3 n_e}{(2\pi mkT)^{3/2}} e^{(\chi_i - \chi_\kappa)/(kT)}$$

A simple fixed point iteration scheme for the solution of the rate equations will converge much too slowly to be useful for most cases of practical interest. Therefore, we use an extension of the operator splitting idea for the solution of the rate equations.
We rewrite the rate equations in the form of an “operator equation.” This equation is then used to introduce an “approximate rate operator” in analogy to the approximate Λ-operator which can then be used to iteratively solve the rate and statistical equations by an operator splitting method, details of the approach are given in Hauschildt (1993).
We introduce first the “rate operator” $[R_{ij}]$ for upward transitions in analogy to the Λ-operator. $[R_{ij}]$ is defined so that

$$R_{ij} = [R_{ij}][n]. \tag{2}$$

Here, $[n]$ denotes the “population density operator”, which can be considered as the vector of the population densities of all levels at all points in the medium under consideration. The radiative rates are (linear) functions of the mean intensity J, which is given by

$J(\lambda) = \Lambda(\lambda)S(\lambda)$, where $S = \eta(\lambda)/\chi(\lambda)$ is the source function. Using the Λ-operator, we can write $[R_{ij}][n]$ as:

$$[R_{ij}][n] = \frac{4\pi}{hc} \int \alpha_{ij}(\lambda)\Lambda(\lambda)S(\lambda)\,\lambda d\lambda. \tag{3}$$

This can be brought into the form (see Hauschildt (1993) for details)

$$[R_{ij}][n] = \frac{4\pi}{hc} \left[\int_0^\infty \alpha_{ij}(\lambda)\Psi(\lambda)E(\lambda)\,\lambda d\lambda\right][n]. \tag{4}$$

The corresponding expression for the emission rate-operator $[R_{ji}]$ is given by

$$[R_{ji}][n] = \frac{4\pi}{hc} \int_0^\infty \alpha_{ji}(\lambda) \left\{\frac{2hc^2}{\lambda^5} + \Psi(\lambda)[E(\lambda)][n]\right\} \exp\left(-\frac{hc}{k\lambda T}\right)\,\lambda d\lambda \tag{5}$$

where we have used the definition

$$\Lambda(\lambda) = \Psi(\lambda)/\chi(\lambda), \tag{6}$$

and $[E(\lambda)]$ is a *linear* operator such that $[E(\lambda)][n]$ gives the emissivity $\eta()$.
Using the rate operator, we can write the rate equations in the form

$$\begin{aligned} \sum_{j<i} n_j \left([R_{ji}][n] + C_{ji}\right) \quad - \quad & n_i \left\{ \sum_{j<i} \left(\frac{n_j^*}{n_i^*}\right) \left([R_{ij}][n] + C_{ji}\right) \right. \\ + \quad & \left. \sum_{j>i} \left([R_{ij}][n] + C_{ij}\right) \right\} \\ & + \sum_{j>i} n_j \left(\frac{n_i^*}{n_j^*}\right) \left([R_{ji}][n] + C_{ij}\right) = 0. \end{aligned} \tag{7}$$

This form shows, explicitly, the non-linearity of the rate equations with respect to the population densities. Note that in addition, the rate equations are non-linear with respect to the electron density via the collisional rates. Furthermore, the charge conservation constraint

condition directly couples the electron densities and the population densities of all level of all atoms and ions with each other.
In analogy to the operator splitting method discusses above, we split the rate operator, by writing $[R_{ij}] = [R^*_{ij}] + ([R_{ij}] - [R^*_{ij}]) \equiv [R^*_{ij}] + [\Delta R_{ij}]$ (analog for the downward radiative rates), where $[R^*_{ij}]$ is the "approximate rate-operator". We then rewrite the rate R_{ij} as

$$R_{ij} = [R^*_{ij}][n_{\rm new}] + [\Delta R_{ij}][n_{\rm old}] \tag{8}$$

and analogously for the downward radiative rates. In Eq. 8, $[n_{\rm old}]$ denotes the current (old) population densities, whereas $[n_{\rm new}]$ are the updated (new) population densities to be calculated. The $[R^*_{ij}]$ and $[R^*_{ji}]$ are linear functions of the population density operator $[n_k]$ of any level k, due to the linearity of η and the usage of the Ψ-operator instead of the Λ-operator.

If we insert Eq. 8 into Eq. 1, we obtain the following system for the new population densities:

$$
\begin{aligned}
&\sum_{j<i} n_{j,\mathrm{new}}[R^*_{ji}][n_{\mathrm{new}}] - n_{i,\mathrm{new}} \left\{ \sum_{j<i} \left(\frac{n^*_j}{n^*_i}\right) [R^*_{ij}][n_{\mathrm{new}}] + \sum_{j>i} [R^*_{ij}][n_{\mathrm{new}}] \right\} \\
&\quad + \sum_{j>i} n_{j,\mathrm{new}} \left(\frac{n^*_i}{n^*_j}\right) [R^*_{ji}][n_{\mathrm{new}}] + \sum_{j<i} n_{j,\mathrm{new}} \left([\Delta R_{ji}][n_{\mathrm{old}}] + C_{ji}\right) \qquad (9) \\
&\quad - n_{i,\mathrm{new}} \left\{ \sum_{j<i} \left(\frac{n^*_j}{n^*_i}\right) \left([\Delta R_{ij}][n_{\mathrm{old}}] + C_{ji}\right) + \sum_{j>i} \left([\Delta R_{ij}][n_{\mathrm{old}}] + C_{ij}\right) \right\} \\
&\quad + \sum_{j>i} n_{j,\mathrm{new}} \left(\frac{n^*_i}{n^*_j}\right) \left([\Delta R_{ji}][n_{\mathrm{old}}] + C_{ij}\right) = 0.
\end{aligned}
$$

Due to its construction, the $[R^*_{ij}]$-operator contains information about the influence of a particular level on *all* radiative transitions. Therefore, we are able to treat the complete multi-level non-LTE radiative transfer problem including active continua and overlapping lines. The $[E(\lambda)]$-operator, at the same time, gives us information about the strength of the coupling of a radiative transition to all levels that are considered. This information may be used to include or neglect certain couplings *dynamically* during the iterative solution of Eq. 9. Furthermore, we have not yet specified either a method for the formal solution of the radiative transfer equation or a method for the construction of the approximate Λ-operator (and, correspondingly, the $[R^*_{ij}]$-operator). We proceed by considering rapidly expanding spherically symmetric media and use the tri-diagonal ALO given by Hauschildt Hauschildt (1992). However, any method for the formal solution of the radiative transfer equation and the construction of the ALO may be used, including multi-dimensional and/or time dependent methods.

In the outermost level of the nested iteration scheme we also iterate for the temperature structure of the atmosphere using a generalization of the Unsöld-Lucy temperature correction scheme to spherical geometry and NLTE model calculations. This has proven to work very well even in extreme NLTE cases such as nova and supernova atmospheres. The temperature correction procedure also requires virtually no memory and CPU time overheads. The Unsöld-Lucy correction scheme (see Mihalas Mihalas (1970) for a discussion of this and other temperature correction schemes), uses the global constraint equation of energy conservation to find corrections to the temperature that will fulfill energy conservation better than the previous temperatures. We have found it to be more stable than a Newton-Raphson linearization scheme and it allows us to separate the temperature corrections from the statistical equations discussed above.

To derive the Unsöld-Lucy correction, one uses the fact that the *ratios* of the wavelength averaged absorption and extinction coefficients

$$\kappa_P = \left(\int_0^\infty \kappa_\lambda B_\lambda \, d\lambda\right) / B \qquad (10)$$

$$\kappa_J = \left(\int_0^\infty \kappa_\lambda J_\lambda \, d\lambda\right) / J \qquad (11)$$

$$\chi_J = \left(\int_0^\infty \chi_\lambda F_\lambda \, d\lambda\right) / F \qquad (12)$$

$$(13)$$

(where B, J, F denote the wavelength integrated Planck function, mean intensity and radiation flux, respectively) depend much less on values of the independent variables than do the averages themselves. Dropping terms of order (v/c), one can then use the angular moments of the SSRTE to show that in order to obtain radiation equilibrium B should be corrected by an amount

$$\begin{aligned}\delta B(r) &= \frac{1}{\kappa_P}\big\{\kappa_J J - \kappa_P B + \dot{S}/(4\pi)\big\} \\ &\quad -\frac{\kappa_J}{\kappa_P}\big\{2(H(\tau=0) - H_0(\tau=0)) \\ &\quad -\frac{1}{fqr^2}\int_r^R q\, r'^2\, \chi_F\, (H(r') - H_0(r'))\, dr'\big\},\end{aligned} \tag{14}$$

where $H \equiv F/4\pi$, $H_0(\tau)$ is the value of the target luminosity at that particular depth point (variable due to the velocity terms in the SSRTE and non-mechanical energy sources, the total *observed* luminosity $H_0(0)$ is an input parameter), Here, q is the "sphericity factor" given by

$$q = \frac{1}{r^2} \exp(\int_{r_{\rm core}}^{r} \frac{3f-1}{r'f}\,dr'),$$

where $r_{\rm core}$ is the inner radius of the atmosphere, R is the total radius, $f(\tau) = K(\tau)/J(\tau)$ is the "Eddington factor", and $K = \int \mu^2 I\, d\mu$ is the second angular moment of the mean intensity. $\dot{S}$ describes all additional sources of energy such as mechanical energy supplied by winds or non-thermal ionization due to γ–ray deposition.
Key to the derivation above is:

$$\frac{d(r^2H')}{dr} + r^2\frac{\dot{S}'}{4\pi} = r^2(\kappa_P B' - \kappa_J J') = 0$$

The first term in Eq. 14 corresponds simply to a Λ iteration term and will thus provide too small temperature corrections in the *inner* parts of the atmosphere (but work fine in the outer, optically thin parts). The second term of Eq. 14, however, is the dominant term in the inner parts of the atmosphere. It provides a very good approximation to the temperature corrections ΔT deep inside the atmosphere. Following Unsöld (1968), we found that it is sometimes better to modify this general scheme by, e.g., excluding the contributions of extremely strong lines to the opacity averages used in the ΔT calculations because they tend to dominate the average opacity but do not contribute as much to the total error in the energy conservation constraint.

But target value of $H'(r)$ is an observer's frame quantity. And we have co-moving frame values. We have to find out how $H'(r)$ varies. Can't do it exactly, but we can keep the moment equations to first order in v/c and use the Eddington ratios:

$$f = H/J \qquad g = K/J$$

Then we can derive an equation for J (and $H = fJ$).

$$(f+\beta)\frac{\partial(r^2 J)}{\partial r} = \frac{r^2 \dot{S}}{4\pi\gamma} - r^2 J\left\{\frac{\partial f}{\partial r} + \frac{\beta}{r}(1-g) + \gamma\frac{\partial\beta}{\partial r}(1+g+2\beta f)\right\}$$

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