Basics of Radiative Transfer with Applications to CO and H_2O

Radiative Transfer Principles

We concentrate on line radiation, i.e., a radiation field that interacts with the quantum states that electrons in an atom or molecule can enjoy (see David Flower's lectures). Our goal is to determine how line radiation is influenced as it traverses a medium rather than vacuum, i.e., it sees an atomic or molecular (radiation field dependent) opacity.

The equation of radiative transfer for the specific intensity I_ν (erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}) at frequency ν along a path with coordinate s reads:

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu$$

or

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

with optical depth $\tau_\nu = \int_0^s \alpha_\nu ds$, absorption coefficient α_ν (cm^{-1}), source function $S_\nu = j_\nu/\alpha_\nu$, emission coefficient j_ν (erg s^{-1} cm^{-3} Hz^{-1} sr^{-1}), and formal solution

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu) d\tau'_\nu \approx I_\nu(0)e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu}),$$

where the *approximation* in the second part of the equation follows if one assumes that the source function is constant along the considered path. We have used the redefinition, $\eta \equiv I_\nu e^{\tau_\nu}$ and $\xi \equiv S_\nu e^{\tau_\nu}$ (why?), to rewrite the equation of radiative transfer as $d\eta/d\tau_\nu = \xi$.

The formal solution, valid along any path, is the sum of two terms: The initial intensity diminished by absorption plus the integrated source diminished by absorption. Note that $I_\nu \to S_\nu$ for $\tau_\nu \to \infty$ (relaxation) and that the mean free path of a photon is approximately $1/\alpha_\nu$ since $\int_0^\infty \tau_\nu e^{-\tau_\nu} d\tau_\nu = 1$.

For two levels (i the lower and j the upper) one has, with Planck's constant h, the line profile function $\phi(\nu)$ and indices ordered by energy, that

$$j_\nu = \frac{h\nu}{4\pi} n_j A_{ji} \phi(\nu)$$

and

$$\alpha_\nu = \frac{h\nu}{4\pi}\phi(\nu)(n_i B_{ij} - n_j B_{ji}),$$

with the level populations n_i, the well known Einstein B coefficients $B_{ji} = 2h\nu^3/c^2 A_{ji}$, and the assumption that the frequency distribution of emitted radiation during spontaneous decay is the same as that of absorption, $\phi_{abs} = \phi_{em} = \phi$. Note that the level indices (i and j) are suppressed, i.e., $\phi = \phi_{ji}$. The same holds for α_ν, j_ν, S, I_ν and J (defined below). The latter condition is called complete redistribution of the lines, and it means that the quantum states of atoms and molecules have sufficient time to be re-arranged along the line profile. For levels $i, j; j > i$ one then has that

$$S_{ji} = \frac{n_j A_{ji}}{n_i B_{ij} - n_j B_{ji}}.$$

That is, the source function is independent of frequency (angle).

In any case, one needs to have a priori knowledge of the level populations which themselves depend on the average integrated (over frequency and solid angle Ω) intensity

$$J = \frac{1}{4\pi}\int I_\nu \phi(\nu) d\nu d\Omega$$

through the equations of statistical equilibrium

$$\Sigma_{j>l}[n_j A_{jl} + (n_j B_{jl} - n_l B_{lj})J] - \Sigma_{j<l}[n_l A_{lj} + (n_l B_{lj} - n_j B_{jl})J] + \Sigma_j[n_j C_{jl} - n_l C_{lj}] = 0,$$

which give, for any level l, the balance between all processes that populate and de-populate that particular level. One of the statistical equilibrium equations can be replaced by the conservation equation $\Sigma_k n_k = n_{\rm mol}$, for the total density $n_{\rm mol}$ of the species of interst. Additional radiative transitions, parameterized through P in $J \rightarrow J + P$, are caused by the presence of radiating dust grains and the cosmic microwave background at (effective) black body radiation temperatures of 10-100 K and 2.735 K, respectively.

Only when the ambient density is above the critical density, $n_{\rm cr} = A/C$ with C the (temperature- dependent) total collisional de-excitation coefficient to all lower levels, does one obtain a Boltzmann[1] distribution for the levels. Of course, very large line optical depths will als drive the level populations towards local thermodynamic equilibrium (why?).

[1] $n_i/n_j = g_i/g_j e^{h\nu/kT}$, $i < j$ and statistical weights g.

Since the optical depth depends on the frequency, the presence of a large-scale velocity field can impact the contribution of α_ν along the path $s - s'$. That is, in the line profile there can be an implicit dependence on the solid angle Ω through its argument $\delta\nu(\Omega) = \nu(1 - \Omega \cdot \mathbf{v}/c) - \nu_{ji}$ for a velocity vector $\mathbf{v}$ projected along the line of sight.

We can now rewrite the equation of radiative transfer to

$$\frac{dI_\nu}{ds} = -\frac{h\nu}{4\pi}(n_i B_{ij} - n_j B_{ji})\phi(\nu) I_\nu + \frac{h\nu}{4\pi} n_j A_{ji} \phi(\nu),$$

with a source function

$$S_\nu = 2h\nu^3/c^2 (\frac{g_j n_i}{g_i n_j})^{-1},$$

known as a generalized Kirchhoff's law. If matter is in thermal equilibrium (but not necessarily in equilibrium with the radiation field), then the level populations will follow a Boltzmann distribution (local thermodynamic equilibrium or LTE) and $S_\nu = B_\nu(T)$, with B the black body function. Of course, black body radiation results for the emerging intensity when the optical depth is large (why?). In general, the ISM is characterized by non-thermal level populations. Note that levels may even be inverted (lasers/masers) with $n_i/g_i < n_j/g_j$, for appropriate densities and radiation fields. In the latter case exponential amplification of the intensity occurs (why?).

In the end, we have a set of coupled integro-differential equations, which are generally difficult to solve. Note that special care has to taken in the shape of line profile $\phi(\nu)$, i.e., the frequency distribution over which photons are emitted by ambient atoms and molecules in their restframe. Typically a Doppler (Maxwellian) distribution

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-(\nu - \nu_{ji})^2/\Delta\nu_D^2},$$

with $\Delta\nu_D = \Delta V \nu_{ji}/c$, is appropriate if an effective (thermal) line width $\Delta V = (2kT/m_{\rm mol})^{1/2}$ can be defined, at temperature T and molecular mass $m_{\rm mol}$. Contributions from microscopic turbulent motions, ξ^2 (in m^2/s^2) through $\Delta V^2 + \xi^2$ can be added. Of course, $\int \phi(\nu) d\nu = 1$.

Sometimes the width of an atomic level is set by the Heisenberg uncertainty principle, $\Delta E \Delta t \sim \hbar$. For the total spontaneous decay rate γ of an upper (u) level quantum state n, one has $\gamma_u = \Sigma_{l<n} A_{nl}$ and a Lorentz

(natural) profile

$$\phi(\nu) = \frac{\gamma_u/4\pi^2}{(\nu - \nu_{ji})^2 + (\gamma_u/4\pi)^2}.$$

If the lower (l) level is not the ground state then $\gamma_u \to \gamma = \gamma_u + \gamma_l$. Also, if the Lorentz profile is collisionally broadened at a frequency ν_c, then $\gamma \to \Gamma = \gamma + 2\nu_c$, assuming the phase changes in the emitted radiation are completely random.

In some cases the convolution of a Lorentz (dominating the line wings) and Doppler (dominating the line core) profile is appropriate, i.e.,

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} H(a, u),$$

with $u = (\nu - \nu_{ji})/\Delta\nu_D$, $a = \Gamma/4\pi\Delta\nu_D$ and the Voigt function

$$\frac{a}{\pi}\int_{-\infty}^{+\infty} \frac{e^{-y^2}dy}{a^2 + (u - y)^2}.$$

Radiative Transfer Techniques

In general, it is difficult to obtain analytical solutions to the general problem of line radiative transfer with multiple coupled (e.g. water) levels. Therefore, one needs to resort to approximations and/or numerical techniques. Before discussing a number of these, one should realize that the main consideration is always: How can I approximate a fundamentally global problem with local solutions?

We will first consider the escape probability, $\beta(\tau)$, where τ is assumed to be averaged over the line profile. The fraction β gives the chance that a photon escapes along a column of gas that has an optical depth τ. Different expressions exist for β depending on the geometry at hand;
slab:

$$\beta(\tau) = [1 - e^{-3\tau}]/3\tau,$$

sphere:

$$\beta(\tau) = [1 - e^{-\tau}]/\tau.$$

Note the effect of geometry for the pre-factor of the optical depth. Also, β is the chance for escape, $e^{-\tau}$, averaged over de column $0 - \tau$

$$< e^{-\tau} >= \frac{1}{\tau} \int_0^\tau e^{-t} dt.$$

Escape probabilities are a local approximation, although τ contains global information, because a photon is either absorbed locally or escapes the medium. Cases where β is an excellent approximation are: large velocity gradients (LVG approximation), because a photon is shifted out off the line profile as it travels a short distance, or constant excitation conditions, since the average over the column $0 - \tau$ does not diminish our knowledge of the excitation conditions. Of course, only the frequency integral of the specific intensity is computed, not the line profile. For the latter, ray-tracing may be used provided the level populations are not affected strongly by global transfer effects.

Monte Carlo techniques are based on the principle that one can represent the radiation field with a discrete number of photon packages that travel through a numerical grid along different directions and with steps that are typically smaller than the frequency-dependent mean free path. Each grid-point contains information on abundance and level populations (as well as gas density and temperature) and allow one to compute the radiative interactions when a photon package visits the grid point. Clearly, this allow for

a great deal of flexibility, but one quickly runs into two related problems: statistics and speed. In order accurately represent the radiation field and its impact on the level populations, a large number, N, of photon packages are required while the typical noise level scales as $1/N^{1/2}$. Also, when the optical depth is large, photon packages need to be followed for a very long time (many mean free paths) as they diffuse out of the computational grid. Fortunately, computing power and memory is still increasing according to Morse's law and CPU time has become less of an issue.

One can speed up Monte Carlo methods by the so-called ALI (accelerated lambda iteration) scheme. In this, one uses the fact that the calculation required to find the angle-averaged intensity

$$J_\nu = \frac{1}{4\pi} \int I_\nu(\Omega) d\Omega,$$

can be written through a linear operator Λ as

$$J_\nu = \Lambda[S_\nu].$$

Clever approximations of Λ can then be found to speed things up, where one wishes to be able to invert Λ with ease and then correct through iteration on the level populations and radiation field. Therefore, if optical depths are prohibitively large and photons get 'trapped', one may write, for a cosine of direction $\mu = cos\theta$

$$I_{\mu\nu} = \Lambda^*_{\mu\nu}[S_{\mu\nu} + (\Lambda_{\mu\nu} - \Lambda^*_{\mu\nu})[S'_{\mu\nu}],$$

with Λ and Λ^* the exact and approximate operators, respectively, and S' the source function from the previous iteration. This intensity is inserted into the equations of statistical equilibrium and solved for the updated source function S. Note that no error is introduced by the above equation if the iterative procedure converges to $S_{\mu\nu} = S'_{\mu\nu}$. The central issue is of course the choice of the approximate operator. Often a very good approximation for the matrix $\Lambda^*_{\mu\nu}$ is the diagonal part of $\Lambda_{\mu\nu}$, i.e., an approximation where the equations of statistical equilibrium remain completely *local*. Of course, more complicated band (e.g. tridiagonal or 'nearest neighbor') approximations can be envisaged. One should note that S' as well as Λ and Λ^* are constructed from the level populations of the previous iteration. The level populations of the current iteration that one seeks enter only through S. Therefore, the

statistical equilibrium equations are expressed in terms of known quantities and the desired current n_i.

Finally, one can numerically integrate the equation of radiative transfer, as one iterates on the level populations, along different rays on a numerical grid. For this approach one may use the methods of short and long characteristics. Short implies that one follows a beam of radiation though a grid point, while long considers trajectories that run though multiple grid point to the upstream edge of the grid (see the figures).

In general, the CPU time that is required to perform a radiative transfer calculation scales with the number of frequency point (N_ν), the number of directions (N_Ω), the number of grid points ($n_x \times n_y \times n_z$) and the number of integrations steps required to get the intensity in a particular grid point (N_s). Therefore,

$$t_{\rm CPU} \propto N_s \times N_\nu \times N_\Omega \times n_x \times n_y \times n_z.$$

As discussed above, the best chance to speed things up lies in N_s. The short characteristics method basically requires one step unlike the long characteristics method. The escape probability is an intrinsically local description, but requires the total optical depth along a ray. Of course, one can truncate the integration along any direction once $\tau > M$, for some large number M. Similarly, the photon packages involved in the Monte Carlo method have intrinsic weights m_ν and one may delete those packages with $m_\nu < M_\nu$. Equivalently, one may choose to sample first the statistical distribution of traversed optical depths $e^{-\tau_\nu}$ for any photon package and then compute the actual distances travelled with the level populations from the previous iteration. This way, an effective region of interaction can be determined and the computational grid partitioned accordingly.

Models for CO and H_2O

We will concentrate on the S140 molecuar cloud, a sphere, which has been observed by SWAS (the submillimetre wave astronomy satellite). S140 is a PDR (photo-dissociation region) where photon processes dominate the thermal and chemical balance of the gas. S140 is also a site of star formation, with several embedded sources.

We will apply our knowledge to the observed and model spectra, in order to understand the physical characteristics of this source. The spectra show us, e.g., the following effects: optically thin versus optically thick emission, self-absorption (line trapping), and the impact of excitation energy and systemic velocity field.

Exercises

Do the "why's" in the main text, when not yet discussed during the lectures.

Literature

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