4. Transitions & Opacity

- Rutten: 2.3, 2.4, 2.5
- Line transitions
- Einstein coefficients & relations
- Continuous Opacity

Sources of Opacity

- Bound-bound transitions
- Bound-free transitions
- Free-free transitions (Bremstrahlung)
- Scattering: electrons, molecules, dust,...

Calculate total opacity from

$$\rho \, \kappa(\nu) = \sum_{i} n_i \, \sigma_i(\nu)$$

where n_i is the number density of absorbers/scatteres, and σ_i is the cross section of the process.

Bound-Bound Line Transitions

Bound-bound transitions between upper u and lower l levels of an atom, ion, or molecule may occur as

Radiative Excitation Spontaneous Radiative De-excitation Induced Radiative De-excitation Collisional Excitation Collisional De-excitation

We use the *Einstein Coefficients* to describe these processes,

$$A_{ul}, B_{ul}, B_{lu}, C_{ul}, C_{lu}$$



Spontaneous De-excitation



Transition probability for spontaneous de-excitation from state u to state l per second per particle in state u

With no collisions or other transitions, the mean lifetime of particles in state *u* is $\Delta t = 1/A_{ul}$ seconds. The corresponding spread in energy is (Heisenberg) $\Delta E = h/(2 \pi \Delta t)$ or $\Delta v = \gamma^{rad}/2 \pi$ with $\gamma^{rad} = 1/\Delta t$ the *radiative damping constant*. This "natural" broadening process defines an emission probability distribution $\psi(v - v_0)$ around line center, v_0 , given by the area-normalized *Lorentz profile*:

$$\psi(\nu - \nu_0) = \frac{\gamma^{\text{rad}} / 4\pi^2}{(\nu - \nu_0)^2 + (\gamma^{\text{rad}} / 4\pi)^2}$$

The A_{ul} coefficient is a summation over the profile, describing the transition probability for the whole line.

We'll discuss the emission profile shape and other broadening mechanisms in more detail later. Other mechanisms are usually much more important than radiative damping. For a static atmosphere and assuming each deexcitation is independent of the preceding processes that put the atom in state u, i.e., *complete redistribution*, we get

$$\Psi(\nu - \nu_0) = \frac{H(a, \nu)}{\sqrt{\pi} \Delta \nu_D}$$

with Doppler width:

$$\Delta v_D \equiv \frac{v_0}{c} \sqrt{\frac{2kT}{m}}$$

Where *m* is the particle mass and H(a,v) is the Voigt function. It is Gaussian at line centre due to Doppler shifts from Maxwellian motions (*Doppler core*) and has extended wings caused by collisions perturbations (*Damping wings*).

The emission profile is more complex when frequency redistribution is incomplete (*partial redistribution*), which happens if the emitted photon is correlated with the photon that excited the atom in a scattering up-down sequence. Coherent scattering (no v change) is the other extreme.

Radiative Excitation



 $B_{lu} \,\overline{J}_{\nu_0}^{\varphi} \equiv \begin{array}{l} \text{Number of radiative excitations from state } l \text{ to state } u \\ \text{per second per particle in state } l \end{array}$

With the index v_0 defining a specific spectral line whose extinction profile $\varphi(v - v_0)$ is used in weighting the angle-averaged exciting radiation field over the spectral extent of the line

$$\overline{J}_{\nu_0}^{\varphi} \equiv \int_0^{\infty} J_{\nu} \varphi(\nu - \nu_0) \,\mathrm{d}\nu; \quad \int_0^{\infty} \varphi(\nu - \nu_0) \,\mathrm{d}\nu = 1$$

A more general expression which also holds when $\varphi(v - v_0)$ is anisotropic due to systematic Doppler shifts is:

$$\bar{J}_{\nu_0}^{\varphi} \equiv \frac{1}{4\pi} \int_0^{\infty} \int_{-1}^{+1} I_{\nu} \varphi(\nu - \nu_0) \, \mathrm{d}\mu \, \mathrm{d}\nu$$

Induced De-excitation

 $B_{ul} \overline{J}_{\nu_0}^{\chi} =$ Number of induced radiative de-excitations from state *u* to state *l* per second per particle in state *u*

similarly to B_{lu} , with frequency averaging:

$$\overline{J}_{\nu_0}^{\chi} \equiv \frac{1}{4\pi} \int_0^{\infty} \int_{-1}^{+1} I_{\nu} \chi(\nu - \nu_0) \, \mathrm{d}\mu \, \mathrm{d}\nu = \int_0^{\infty} J_{\nu} \chi(\nu - \nu_0) \, \mathrm{d}\nu$$

in which $\chi(v - v_0)$ is the area-normalized profile shape for induced emission.

Collisional Excitation / De-excitation



Number of collisional excitations from state l to state u per second per particle in state l



Number of collisional de-excitations from state u to state l per second per particle in state u

Electron collisions (usually most important) causing transitions from state i to state j have \square

$$n_i C_{ij} = n_i N_e \int_{v_0}^{\infty} \sigma_{ij}(\mathbf{v}) \mathbf{v} f(\mathbf{v}) d\mathbf{v}$$

With N_e the electron density, $\sigma_{ij}(v)$ the electron cross section, f(v) the area-normalized velocity distribution (usually Maxwellian) with mean value $\int vf(v)dv$, and v_0 the threshold velocity $mv_0^2/2 = hv_0$. σ_{ij} is a material property of each transition independent of external state parameters except velocity v. Similar to bb cross section, A_{ul} , B_{ul} , B_{lu}

Einstein Relations

The Einstein coefficients coupled by the Einstein relations:

$$\frac{B_{lu}}{B_{ul}} = \frac{g_u}{g_l}; \quad \frac{A_{ul}}{B_{ul}} = \frac{2h\nu^3}{c^2}$$
$$\frac{C_{lu}}{C_{ul}} = \frac{g_u}{g_l} e^{E_{lu}/kT}$$

g = statistical weight or degeneracy: g = 2J + 1

Formal Coefficients

The monochromatic line extinction coefficient per m³ is

$$\alpha_{v}^{l} = \frac{hv}{4\pi} \left[n_{l} B_{lu} \varphi(v - v_{0}) - n_{u} B_{ul} \chi(v - v_{0}) \right]$$
$$= \frac{hv}{4\pi} n_{l} B_{lu} \varphi(v - v_{0}) \left[1 - \frac{n_{u} g_{l} \chi(v - v_{0})}{n_{l} g_{u} \varphi(v - v_{0})} \right]$$

Where the [...] term corrects for induced emission, taken into account as negative extinction. The total line extinction coefficient is

$$\boldsymbol{\alpha}_{\nu_0}^{l} \equiv \int_{0}^{\infty} \boldsymbol{\alpha}_{\nu}^{l} \,\mathrm{d}\,\boldsymbol{\nu} \approx \frac{h\,\boldsymbol{\nu}_0}{4\pi} \big[n_l B_{lu} - n_u B_{ul} \big]$$

Using $\int hv \phi(v - v_0) dv \sim hv_0 \int \phi(v - v_0) dv = hv_0$ since lines are narrow. Throughout these notes, v_0 denotes summation or averaging over the line profile.

The monochromatic line extinction coefficient per particle is, without correction for induced emission

$$\sigma_{\nu}^{l} = \frac{h\nu}{4\pi} n_{l} B_{lu} \varphi(\nu - \nu_{0})$$

The total line extinction coefficient per particle is

$$\sigma_{\nu_0}^l = \int_0^\infty \sigma_{\nu}^l \,\mathrm{d}\nu \approx \frac{h\nu_0}{4\pi} B_{lu} = \frac{\pi e^2}{m_e c} f_{lu}$$

The latter is an ensemble-averaged extinction coefficient, given per particle, but averaged over the distribution specified by $\varphi(v - v_0)$. The parameter f_{lu} is the classical dimensionless *oscillator strength*. This was originally introduced to correct harmonic-oscillator line strength predictions for unknown quantum mechanical effects. Resonance lines such as Ly α have $f_{lu} \sim 1$.

The monochromatic line emission coefficient expressed in Einstein coefficients is, without induced emission:

$$j_{\nu}^{l} = \frac{h\nu}{4\pi} n_{u} A_{ul} \psi(\nu - \nu_{0})$$

The line source function is

$$S_{\nu}^{l} \equiv j_{\nu}^{l} / \alpha_{\nu}^{l} = \frac{n_{u} A_{ul} \psi(\nu - \nu_{0})}{n_{l} B_{lu} \varphi(\nu - \nu_{0}) - n_{u} B_{ul} \chi(\nu - \nu_{0})}$$

or using the Einstein relations

	$\underline{A_{ul}} \underline{\psi}$	2	
S^{l} –	$B_{ul} \varphi$	$2hv^{\circ}$	ψ/φ
$S_v =$	$\underline{n_l} \underline{B_{lu}} \underline{\chi}$	c^2	$g_u n_l \underline{\chi}$
	$n_u B_{ul} \phi$		$g_l n_u \varphi$

For complete redistribution the profile shapes are equal, $\phi = \phi = \chi$, so the line source function simplifies to:

$$S_{\nu_0}^{l} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{2h\nu_0^3}{c^2} \frac{1}{\frac{g_u n_l}{g_l n_u} - 1}$$

We'll see that this simplifies to $S_v = B_v$ when the population ratio n_l / n_u obeys the Boltzmann distribution for LTE.

Continuum Transitions

Bound-free:

For bound-free transitions the extinction cross section for hydrogen and hydrogen-like transitions is given by *Kramer's* formula:

$$\sigma_{\nu}^{\rm bf} = 2.815 \times 10^{33} \frac{Z^4}{n^5 \nu^3} g_{\rm bf} \quad \text{for } \nu \ge \nu_0$$

With *n* the principal quantum number of level *i* from which the atom or ion is ionized. *Z* the ion charge and g_{bf} the *Gaunt factor*, a quantum mechanical correction of order 1. The cross section decays as $1/v^3$ above the threshold ("edge") frequency v_0 and is zero below it.



Free-free:

Free-free transitions have $S_v = B_v$ when the Maxwell velocity distribution holds, "*thermal Bremsstrahlung*." The volume extinction coefficient is:

$$\alpha_{\nu}^{\rm bf} \approx 3.7 \times 10^8 N_{\rm e} N_{\rm ion} \frac{Z^2}{T^{\frac{1}{2}} v^3} (1 - e^{-h\nu/kT}) g_{\rm ff}$$

with Z the ion charge, $N_{\rm e}$, $N_{\rm ion}$ the electron and ion densities, $g_{\rm ff}$ the appropriate Gaunt correction factor

Scattering

Electron (Thomson) Scattering:

Thomson scattering of photons by free electrons has a frequency independent cross-section for low energy photons:

$$\sigma_{\nu}^{\mathrm{T}} \equiv \sigma^{\mathrm{T}} = \frac{8\pi}{3} r_{\mathrm{e}}^{3} = 6.65 \times 10^{-29} \mathrm{m}^{2}$$

The corresponding volume extinction coefficient is $\alpha^{T} = \sigma^{T} N_{e}$, with N_{e} the electron density. For high energy photons we have *Compton scattering*. For high energy electrons we have *inverse-Compton scattering*, which are frequency dependent. Thomson scattering is the major source of continuous extinction in the atmospheres of hot stars where hydrogen is ionized.

Rayleigh Scattering:

The cross-section for Rayleigh scattering of photons with $v \ll v_0$ by bound electrons with binding energy $h v_0$ is:

$$\boldsymbol{\sigma}_{\boldsymbol{v}}^{\mathrm{R}} \approx f_{lu}\boldsymbol{\sigma}^{\mathrm{T}} \left(\frac{\boldsymbol{v}}{\boldsymbol{v}_{0}}\right)^{4}$$

where the oscillator strength flu and frequency n0 characterize the major bound-bound "resonance transition" of the bound electron. For example the Ly α transition in neutral hydrogen of a weighted sum over all Lyman lines. The ν^4 (1/ λ^4) dependence makes the sky blue and sunsets red.

Redistribution in angle or Scattering Phase Functions: Thomson and Rayleigh scattering are coherent: the photon gets re-directed, but keeps the same v. The re-direction has the phase function ~ $1 + \cos^2\theta$. This is the angular shape that the scattered photons have.