Chapter 6

The LTE Extinction Coefficient

In this chapter, we will assume both LTE and coherent and isotropic scattering. With these assumptions, we can write the radiation transfer equation in terms of the local density, temperature, composition, and mean intensity. This is an enormous simplification.

In general, to solve an atmosphere, we need both the extinction coefficient χ and the source function S_ν. With these, we can integrate the formal solution.

Under the assumption of LTE, all properties of matter are properties of the local temperature, density, and composition. This includes the extinction coefficient χ and its components the absorption coefficient α and the scattering coefficient σ. However, under the assumptions of both LTE and coherent and isotropic scattering, equation 3.9 gives

$$S_\nu = \frac{\alpha B_\nu + \sigma J_\nu}{\alpha + \sigma}. \qquad (6.1)$$

Thus, we see that the source function also depends only on the local properties of the matter, through $B_\nu(T)$, α, and σ, and the local mean intensity J_ν.

The solution for a static atmosphere in LTE and with coherent and isotropic scattering thus has two parts. The first is the determination of α and σ for given properties of matter. The second is the determination of the temperature and density in a manner that satisfies the equation of transfer of radiation, thermal (often radiative) equilibrium, and mechanical (often hydrostatic) equilibrium. These two parts are coupled (since radiation determines the properties of the material and the properties of the material determine radiation), and so the solutions is typically iterative.

In this chapter, we will address the determination of α and σ for a given temperature, density, and composition. We will defer solution of the global problem for a subsequent chapter.

The Extinction Coefficient in Microscopic Terms

To proceed, we need to relate the macroscopic extinction coefficient, with its absorption and scattering components, to the microscopic properties of the material.

Consider Figure 6.1, which shows the volume dV formed by sweeping an area dA centered on $\boldsymbol{r}$ thought a length ds parallel
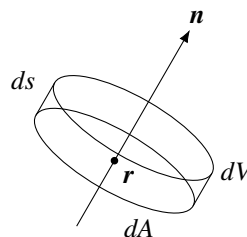

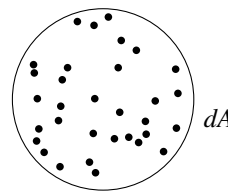Figure 6.1: The geometry of the definition of cross-section

Figure 6.2: The cross-section interpreted classically.

to $\boldsymbol{n}$ which is perpendicular to dA. Consider dV is filled with a single type of particle with number density n. If these particles can interact with radiation, there is a probability that a photon that enters dV in the direction n will be absorbed or scattered. We define the cross-sections for absorption a^a and scattering a^s such that the probability of absorption or scattering of a photon is given by $na^a\,ds$ and $na^s\,ds$. (It is conventional to use σ to denote the cross-section, but here we will use a to avoid confusion with the scattering coefficient σ.)

Naively, we can interpret the cross-section as the area around a particle within which the probability of interaction is 1 and outside of which the probability is 0. This is illustrated in Figure 6.2. Under this interpretation, the total area in dV for interactions is the number of particles in dV is the total number of particles ndV multiplied by the cross-section per particle a. Thus, the probabilidad of an interaction is $ndVa/dA = nads$. This discussion helps motivate the definition of a, but we must remember that quantum mechanics teaches us that the interaction is probabilistic, not deterministic like this.

If we have many types of particles, the total probability of

absorption or scattering is given by $(\sum_i n_i a_i^a)ds$ and $(\sum_i n_i a_i^s)ds$, in which the index i extends over all types of particles.

We saw in Problem 2.1 that the probability density function for the absorption of a photon is an exponential distribution in the optical depth τ with a mean of 1. Thus, the probability $P(< d\tau)$ that a photon is extinguished between $\tau = 0$ and $\tau = d\tau$ is

$$P(< d\tau) = 1 - \exp^{-d\tau} \tag{6.2}$$
$$= 1 - (1 - d\tau) \tag{6.3}$$
$$= d\tau, \tag{6.4}$$

in which we have expanded for small $d\tau$. Now, since

$$d\tau = \chi ds \tag{6.5}$$
$$= (\alpha + \sigma)ds, \tag{6.6}$$

by comparison to our definition of the cross-section, we can identify absorption and scattering coefficients as

$$\alpha = \sum_i n_i a_i^a(v) \tag{6.7}$$

and

$$\sigma = \sum_i n_i a_i^s(v), \tag{6.8}$$

in which n_i is the number density of particles of type i and $a_i^a(v)$ and a_i^s are the absorption or scattering cross-section per particle at frequency v.

Thus, we can divide the problem of determining the opacity into two subproblems: determining the number densities n_i and determining the cross-sections a_i.

Distributions and Densities

The assumption of LTE is that matter has the same state as it would in thermodynamic equilibrium at the same density and temperature, and we can use this to determine the number densities n_i of particles.

For matter in thermodynamic equilibrium and hence also for matter in LTE, Boltzmann's relation requires that probability P of finding a system in a given state satisfies

$$P \propto g e^{-E/kT}, \tag{6.9}$$

where g is the degeneracy and E is the energy of the state (Reif 1965, pp. 201–203). The constant of proportionality can be found from the normalization condition that $\sum P = 1$. From Boltzmann's relation and a knowledge of the degeneracies g and energies E of all states, we can derive the distributions of velocities, excitation, and ionization for matter in thermal equilibrium and, hence, in LTE.

We will typically apply the continuum approximation, that the scale of the macroscopic system is sufficiently large that the density of particles in a given state n is proportional to the probability P of finding the system in that state. Thus, for two states a and b, the relative densities are given by

$$\frac{n_a}{n_b} = \frac{P_a}{P_b}. \tag{6.10}$$

Velocity Distribution

The probability dP that a particle of mass m has a velocity between v and $v + dv$ is given in terms of the probability distribution function $f(v)$ by

$$dP \equiv f(v)dv. \tag{6.11}$$

In thermodynamic equilibrium we can use the Boltzmann relation, which gives us

$$f(v)dv \propto g(v)dv \, e^{-E(v)/kT}. \tag{6.12}$$

If the mass of the particle is m, then the energy $E(v)$ is just the kinetic energy $\frac{1}{2}mv^2$. The factor $g(v)dv$ is the number of states between v and $v+dv$. Thinking back to basic quantum mechanics, and in particular to the the particle in a box, the density of states in position-momentum phase space is $2/h^3$, where the 2 comes from the two spin states of the particle (which we assume to be a spin-1/2 fermion) and the h^3 from the packing of wave functions. The volume of phase space per particle is the product of volume of position space per particle, the inverse of the density n, and to the volume of momentum space corresponding to speeds between v and $v + dv$, which in turn is proportional to $4\pi p^2 dp = 4\pi m^3 v^2 dv$. So,

$$g(v)dv = \frac{8\pi m^3 v^2}{nh^3} dv, \tag{6.13}$$

and

$$f(v) \propto v^2 e^{-\frac{1}{2}mv^2/kT}. \tag{6.14}$$

Applying the normalization condition that $\int_0^\infty dv \, f(v) = 1$, we obtain the constant of proportionality and in full we have

$$f(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{1}{2}mv^2/kT}. \tag{6.15}$$

This is the Maxwell distribution for particle velocities.

We can integrate the energy and the momenum flux of each particle over the distribution to obtain the energy density $\frac{3}{2}nkT$ (assuming ideal particles with no internal degrees of freedom) and the pressure nkT. The mean kinetic energy per particle $\frac{1}{2}m\langle v^2 \rangle$ is $\frac{3}{2}kT$. Thus, the RMS speed is

$$\langle v^2 \rangle^{1/2} = \left(\frac{3kT}{m}\right)^{1/2}. \tag{6.16}$$

That is, the RMS speed is proportional to the square root of the temperature and inversely proportional to the square root of the mass. Cooler and more massive particles have lower RMS speeds; this will be important when we consider the Doppler broadening of lines.

Excitation Distribution

In thermodynamic equilibrium, and hence in LTE, the relative probability that an atom will be found in an excitation state i is given directly by the Boltzmann relation. By excitation state we mean an arrangement of a fixed number of electrons forming a bound state of the atom. The density of atoms in an given excitation state is directly proportional to the probability that an individual atom will be found in that state. If we denote by n_{ijk} the density of atoms in excited state i of ionization state j of species k, the population of a state i relative to the ground state is

$$\frac{n_{ijk}}{n_{0jk}} = \frac{P_{ijk}}{P_{0jk}} = \frac{g_{ijk}}{g_{0jk}} e^{-E_{ijk}/kT}, \tag{6.17}$$

where E_{ijk} is the energy of the excited state above the ground state and g_{ijk} is the degeneracy of a given state. This can obviously be extended to give the relative populations of two excited states.

We can sum over all states to obtain the total density n_{jk} of atoms of ionization state j of species k, obtaining

$$n_{jk} \equiv \sum_i n_{ijk} \tag{6.18}$$

$$= n_{0jk} \sum_i \frac{n_{ijk}}{n_{0jk}} \tag{6.19}$$

$$= \frac{n_{0jk}}{g_{0jk}} \sum_i g_{ijk} e^{-E_{ijk}/kT}. \tag{6.20}$$

We can write this more concisely as

$$n_{jk} = \frac{n_{0jk}}{g_{0jk}} U_{jk}, \tag{6.21}$$

where the partition function U_{jk} is defined by

$$U_{jk} \equiv \sum_i g_{ijk} e^{-E_{ijk}/kT} \tag{6.22}$$

and the sum extends over all bound states. From this, the population of the ground state is

$$n_{0jk} = \left(\frac{n_{jk}}{U_{jk}} \right) g_{0jk}, \tag{6.23}$$

and, generalizing, the population of the excitation state i is

$$n_{ijk} = \left(\frac{n_{jk}}{U_{jk}} \right) g_{ijk} e^{-E_{ijk}/kT}. \tag{6.24}$$

This is a particularly useful for calculations, as it gives the population of each state i as a function of its degeneracy, the temperature, and the density of all atoms in the ionization state.

Disconcertingly, the partition function for an isolated atom is divergent, as an isolated atom has an infinite number of bound states and a upper-bound for E_{ijk} is χ_{jk}, the ionization potential of ionization state j of species k. However, in real systems this is not a problem, since the higher bound states are increasingly spatially

extended and so at some point in a real system the interaction of the electron with the enviroment will cause these states to cease to be bound. For example, in an ionized gas, the presence of free electrons causes the outermost states of an atom to be unbound. If the density of free electrons is n_e, the potential of a nucleus of charge Z will be sheilded beyond the Debye length L_D. This leads effectively to the ionization potential being reduced by

$$\Delta\chi \approx \frac{Ze^2}{L_D}, \tag{6.25}$$

$$\approx 3 \times 10^{-8} \, Z n_e^{1/2} T^{-1/2} \text{ eV}, \tag{6.26}$$

when n_e and T are measured in cm^{-3} and K. For typical values of, say, $n_e = 10^{14}$ cm^{-3} and $T = 10^4$ K, this lowering is only 3×10^{-3} eV, and so it will not significantly change the ionization structure or the position of ionization edges. However, it is enough to give only a finite number of bound states. To see this, consider the outer wave functions of atoms, which can be approximated by hydrogenic wave functions with an effective nuclear charge of Z. In this case, the excited state with principal quantum number n lies $13.6Z^2/n^2$ eV below the continuum. Equating this with the energy by which the ionization potential is lowered by the free electrons, we see that the last bound state has principal quantum number $n_{\max}$ given by

$$n_{\max} \approx 2 \times 10^4 \, Z^{1/2} n_e^{-1/4} T^{1/4}. \tag{6.27}$$

At $n_e = 10^{14}$ cm^{-3} and $T = 10^4$ K, we have

$$n_{\max} \approx 60 Z^{1/2}. \tag{6.28}$$

However, this is enough that the sum in the partition function for an atom in a stellar atmosphere should only extend over some tens or hundreds of states, rather than over an infinite number of states, and the partition function should be finite. On the other hand, it is sufficiently high that the inner wave functions, which result in transitions at high frequencies, in the ultraviolet, optical, and infrared, are not significantly perturbed.

Although the partition for an isolated atom is a function of temperature only, the partition function for an atom in an atmosphere is a function of both the temperature and the electron density, because of the direct dependence on T of the Boltzmann factors and the indirect dependence on both T and n_e of the number of bound states. However, the later dependence is weak enough that it is usually ignored, and the number of bound states is calculated for characteristic values of, say, $n_e = 10^{14}$ cm^{-3} and $T = 10^4$ K. The dependence of partition functions on T is relatively smooth, so polynomial approximates are more commonly used.

Ionization Distribution

We can calculate the populations of different ions of the same species in thermodynamic equilibrium, and hence LTE, by applying the Boltzmann relation and taking into account the continuous states available to a free electron. Consider one discrete state

formed by the ground state of a neutral atom and another state formed by the ground state of the corresponding singly-ionized ion and an electron. The probability that the atom is in the ground state and neutral is P_{00k} and the probability that the atom is in the ground state and ionized and the electron has speed between v and $v + dv$ is $P_{01k} f(v) dv$, where $f(v)$ is the Maxwell distribution. The ionized atom and the electron are independent, hence their probabilities and degeneracies are multiplicative. Applying the Boltzmann relation we have

$$\frac{P_{01k} f(v) dv}{P_{00k}} = \frac{g_{01k} g(v) dv}{g_{00k}} e^{-(\chi_{0k} + \frac{1}{2} m_e v^2)/kT}. \qquad (6.29)$$

In this, χ_{0k} is the ionization potential of the ground state of the neutral atom. Using the degeneracy of free electron states $g(v) = 8\pi m_e^3 v^2 / n_e h^3$, obtained in our derivation of the Maxwell distribution, and dividing by $f(v)$, we obtain

$$\frac{n_{01k}}{n_{00k}} = \frac{P_{01k}}{P_{00k}} = \frac{2}{n_e} \left(\frac{2\pi kT m_e}{h^2}\right)^{3/2} \frac{g_{01k}}{g_{00k}} e^{-\chi_{0k}/kT}. \qquad (6.30)$$

We've not made any explicit reference to the lack of charge on the atom, so we can generalize this equation to any two subsequent stages of ionization j and $j + 1$, obtaining

$$\frac{n_{0,j+1,k}}{n_{0,j,k}} = \frac{2}{n_e} \left(\frac{2\pi kT m_e}{h^2}\right)^{3/2} \frac{g_{0,j+1,k}}{g_{0,j,k}} e^{-\chi_{jk}/kT}. \qquad (6.31)$$

This gives the ionization balance between the ground states of two subsequent ionization stages. If we use $n_{0jk} = n_{jk} g_{0jk} / U_{jk}$, then we can write the ionization balance between all states of two subsequent ionization stages as

$$\frac{n_{j+1,k}}{n_{j,k}} = \frac{2}{n_e} \left(\frac{2\pi kT m_e}{h^2}\right)^{3/2} \frac{U_{j+1,k}}{U_{j,k}} e^{-\chi_{jk}/kT}. \qquad (6.32)$$

This is the Saha equation. It can be applied to atoms, ion, and electrons to give the ionization state.

We might think that we need to take into account the density of momentum states available to the the atom and ion in the same way as we take into account the density of states of the electron. However, since both have the same mass, if we include these, we discover that they cancel.

The Saha equation obviously states that the degree of ionization increases with the temperature and decrease with the density of electrons. However, we can gain a better quantitative feeling for this by defining $n_S(T) \equiv 2(2\pi kT m_e/h^2)^{3/2}$ and writing the Saha equation as

$$\frac{n_{j+1,k}}{n_{j,k}} = \frac{n_S}{n_e} \frac{U_{j+1,k}}{U_{j,k}} e^{-\chi_{jk}/kT}. \qquad (6.33)$$

The ratio of the partition function is of order unity, so we have parity between the two ionization states when

$$kT \approx \frac{\chi}{\ln(n_S/n_e)}. \qquad (6.34)$$

At 10^4 K, $n_S \approx 5 \times 10^{21}$ cm^{-3}, which is orders of magnitude larger than the electron densities of 10^{14} cm^{-3} that are typical of stellar atmospheres. This implies that atoms become substantially ionized when $kT \sim \chi/20$ rather than when $kT \sim \chi$ as might be naively expected. For example, hydrogen begins to be substantially ionized around $\chi/20k \approx 8,000$ K rather than around $\chi/k \approx 150,000$ K. Consider how different O stars would be if their atmospheres consisted largely of neutral hydrogen!

Electron Density

In order to solve for the ionization equilibrium using the Saha equation, we need to electron density, which is in turn *determined* by the ionization equilibrium. Once again, we have a coupled problem.

We consider the gas as consisting of free electrons, bound electrons, and nuclei. The density of nuclei n_n is

$$n_n = \frac{\rho}{\mu_n m_H}. \qquad (6.35)$$

If we define the number fraction of nuclei of type k as $x_k \equiv n_k/n_n$, the mean molecular mass per nuclei μ_n is given by

$$\mu_n m_H \equiv \sum_k x_k m_k. \qquad (6.36)$$

Thus, for a given composition (set of x_k) and density, the density of nuclei is known. We can determine the free electron density from the requirement that the gas be neutral,

$$n_e = \sum_k \sum_j j n_{jk}. \qquad (6.37)$$

Here we take $j = 0$ for neutral atoms, $j = 1$ for singly-ionized ions, and so on. We can define the ionization fraction of each ionization stage $f_{jk} \equiv n_{jk}/n_k$ and write

$$n_e = \sum_k \sum_j j n_k f_{jk} \qquad (6.38)$$

$$= n_n \sum_k \sum_j j x_k f_{jk}. \qquad (6.39)$$

We now need an expression for f_{jk}, and in LTE we obtain this from the Saha equation for the ionization balance between all states of two subsequent ionization stages,

$$\frac{n_{j+1,k}}{n_{j,k}} = \frac{n_S}{n_e} \frac{U_{j+1,k}}{U_{j,k}} e^{-\chi_{jk}/kT} \qquad (6.40)$$

$$= \frac{\tilde{n}_{j,k}}{n_e}, \qquad (6.41)$$

where $\tilde{n}_{j,k}(T) \equiv n_S(T)(U_{j+1,k}/U_{j,k}) e^{-\chi_{jk}/kT}$. Now we can write

$$\frac{n_{j+1,k}}{n_{0,k}} = \prod_{j' \leq j} \frac{n_{j'+1,k}}{n_{j',k}} = \prod_{j' \leq j} \frac{\tilde{n}_{j',k}}{n_e}, \qquad (6.42)$$

and summing over all ionization states we can obtain the total density n_k of all ions of species k,

$$\frac{n_k}{n_{0k}} \equiv \sum_j \frac{n_{jk}}{n_{0k}} = \sum_j \prod_{j'<j} \frac{\tilde{n}_{j'k}}{n_e}. \tag{6.43}$$

We can combine the previous two equations to obtain the fraction f_{jk} of atoms in ionization state j relative to all atoms of that species as

$$f_{jk} \equiv \frac{n_{jk}}{n_k} = \frac{\prod_{j'<j} \frac{\tilde{n}_{j'k}}{n_e}}{\sum_{j'} \prod_{j''<j'} \frac{\tilde{n}_{j''k}}{n_e}}. \tag{6.44}$$

We can now expand Equation (6.39) as

$$n_e = n_n \sum_k \sum_j j x_k f_{jk} \tag{6.45}$$

$$= n_n \sum_k \sum_j \left(j x_k \frac{\prod_{j'<j} \frac{\tilde{n}_{j'k}}{n_e}}{\sum_{j'} \prod_{j''<j'} \frac{\tilde{n}_{j''k}}{n_e}} \right). \tag{6.46}$$

Since n_n and T are known, this is an implicit equation for n_e. It can be rearranged as a polynomial in n_e, whose order is the number of stages of ionization present (i.e., quadratic for neutral and single-ionized species, cubic for neutral, singly-ionized, and doubly-ionized species, and so on). Except in special cases, the order will be sufficiently high that cannot solve for n_e directly but instead we must solve for n_e iteratively, using standard algorithms such the Newton-Raphson method (Press et al. 1992, chapter 10).

Application to Hydrogen

The electron density in a pure hydrogen gas can be solved analytically if we consider only neutral and singly-ionized hydrogen and ignore H^- and all molecules. In this case, $x_1 = 1$, $n_n = n_{01} + n_{11} = n_1$, so Equation (6.46) becomes

$$n_e = n_1 \frac{\frac{\tilde{n}_{01}}{n_e}}{1 + \frac{\tilde{n}_{01}}{n_e}}, \tag{6.47}$$

which can be rearranged to give the quadratic equation

$$n_e^2 + \tilde{n}_{01} n_e - \tilde{n}_{01} n_1 = 0. \tag{6.48}$$

We anticipated a quadratic equation, because we have two stages of ionization present. This equation can also be obtained by considering conservation of nuclei,

$$n_{01} + n_{11} = n_1, \tag{6.49}$$

conservation of electrons combined with the requirement that the gas be electrically neutral,

$$n_e + n_{01} = n_1, \tag{6.50}$$

and the Saha equation for the ionization of neutral hydrogen,

$$\frac{n_{11}}{n_{01}} = \frac{\tilde{n}_{01}}{n_e}. \tag{6.51}$$

If these three equations are solved simultaneously for n_e in terms of n_1 and $\tilde{n}_{01}$, one obtains the same quadratic equation.

The quadratic equation can be solved exactly to give

$$n_e = \frac{\tilde{n}_{01}}{2} \left[\left(1 + \frac{4n_1}{\tilde{n}_{01}} \right)^{1/2} - 1 \right]. \tag{6.52}$$

In the limit of low density or high temperature (i.e., low n_1 or high $\tilde{n}_{01}$), we have $n_1 \ll \tilde{n}_{01}$ and so $n_e \approx n_1$, which corresponds to a gas that is almost completely ionized. In the limit of high density or low temperature, we have $n_1 \gg \tilde{n}_{01}$ we have $n_e \approx \tilde{n}_{01}/2$, which corresponds to a gas that is almost completely neutral. These limits correspond to our expectations based on the behavior of the Saha equation with temperature and density.

Radiative Processes

Bound-Bound Transitions

Bound-bound transitions arise between two bound states, each of which has a more-or-less well-defined energy and as such give rise to lines. Bound-bound transitions occur as spontaneous emissions from an upper state to a lower state, absorptions from a lower state to an upper state, and stimulated emissions from an upper state to a lower state.

Einstein Coefficients

At the atomic level we have spontaneous emission, stimulated emission, and absorption. The processes of spontaneous emission and absorption are straightforward and can be represented by

$$X_u \rightleftharpoons X_l + \gamma, \tag{6.53}$$

with X_u representing the upper level and X_l the lower level. Stimulated emission is not so obvious. It occurs when a photon "stimulates" a particle in the upper state to decay to the lower state and emit a photon. It can be represented by

$$X_u + \gamma \rightarrow X_l + 2\gamma. \tag{6.54}$$

In his work on black body radiation, Einstein was forced to postulate stimulated emission to give the correct form of the Planck function. Later it was shown to arise naturally from the statistics of massless bosones particles like the photon, as the probablity of emission into a state is proportional to 1 plus the number of bosons in that state (Dirac 1958, sections 61 and 62). The part proportional to 1 corresponds to spontaneous emission and part proportional to the number of bosons corresponds to stimulated emission. The photon created by stimulated emission has the same direction, frequency, and polarization as the stimulating photon.

The Einstein coefficients A_{ul}, B_{ul}, and B_{lu} quantify the strength of a line in terms of spontaneous emission, stimulated emission, and absorption. The coefficients are defined in terms of the probability per unit time of a transition:

1. The probability of a spontaneous emission per unit time per unit solid angle per unit frequency for an atom in the upper state is

$$\frac{1}{4\pi} A_{ul}\psi. \tag{6.55}$$

   The function $\psi(\nu)$ is the emission profile and is normalized by

$$\int_0^\infty d\nu\, \psi \equiv 1. \tag{6.56}$$

2. The probability of a stimulated emission per unit time per unit solid angle per unit frequency for an atom in the upper state is

$$\frac{1}{4\pi} B_{ul}\psi I_\nu. \tag{6.57}$$

3. The probability of an absorption per unit time per unit solid angle per unit frequency for an atom in the lower state is

$$\frac{1}{4\pi} B_{lu}\phi I_\nu. \tag{6.58}$$

   The function $\phi(\nu)$ is the absorption profile and is normalized by

$$\int_0^\infty d\nu\, \phi \equiv 1. \tag{6.59}$$

Other definitions of the Einstein coefficients have the probabilities being the product of the coefficients and the energy density u_ν, which leads to B_{ul} and B_{lu} differing by a factor of $c/4\pi$ from those defined here.

In the definition of the Einstein coefficients, we have carefully distinguished between the emission profile ψ and the absorption profile ϕ. In thermodynamic equilibrium, the principal of detailed balance requires that emissions and absorptions at each frequency exactly balance, and so the emission profile ψ and absorption profile ϕ must be equal. More generally, when we have complete redistribution (that is, no correlation between the frequencies of the absorbed or emitted photons) or when the specific intensity is constant over the line, the absorption and emission profiles will be equal. Complete redistribuition is a good approximation for lines in which the Doppler core dominates, and in these cases we can assume that the profiles are identical.

However, when we have partial redistribution (that is, correlations between the frequencies of the absorbed and emitted photons) coupled with changes of the specific intensity over the line, the absorption and emission profiles can be different. By their very nature, lines are places where the specific intensity can vary dramatically, so we need to be wary of partial redistribution. It can occur in strong lines that are dominated by their wings. In a strong line, a photon is absorbed and then rapidly re-emitted; in the wing of the line, the frequency of the emitted photon is strongly correlated with the frequency of the absorbed photon. Roughly, then, the emission profile will be the product of the absorption profile and the mean intensity. If the mean intensity varies significantly over the line, for example, being small in the core and large in the wings, the emission profile can be very different from the absorption profile. Nevertheless, dealing with the difference between the absorption and emission profiles creates significant additional complexity, and for this reason we'll often assume that the two are equal even when this is cannot be justified on physical grounds.

The Einstein coefficients are related by the Einstein Relations, which we can derive by considering the behaviour of a population of atoms in thermodynamic equilibrium. In thermodynamic equilibrium we have detailed balance, and so the rate of upward radiative transitions at a given frequency and in a given direction must be exactly balanced by the rate of downward transitions at the same frequency and in the same direction. The rate of a transition from one state to a second is simply the number of atoms in the first state multiplied by the probability per unit time of a transition to the second state. Thus, if the density of atoms in the upper states is n_u and the density of atoms in the lower state is n_u, then we must have

$$n_u(A_{ul} + B_{ul}I_\nu)\psi = n_l B_{lu}\phi I_\nu. \tag{6.60}$$

Furthermore, detailed balance requires that the emission and absorption profiles be equal and we also have $I_\nu = B_\nu$, and so

$$n_u(A_{ul} + B_{ul}B_\nu) = n_l B_{lu}B_\nu. \tag{6.61}$$

We can rearrange this to obtain

$$B_\nu = \frac{A_{ul}/B_{ul}}{(n_l/n_u)(B_{lu}/B_{ul}) - 1}. \tag{6.62}$$

Since in thermodynamic equlibrium the level populations are given by a Boltzman distribution, $n_l/n_u = (g_l/g_u)e^{E/kT}$, where $E = h\nu$ is the energy difference between the levels, we have

$$B_\nu = \frac{A_{ul}/B_{ul}}{(g_l/g_u)(B_{lu}/B_{ul})e^{h\nu/kT} - 1}. \tag{6.63}$$

On the righthand side, the only variables are ν and T; all other quantities are constants or properties of the atom that are independent of temperature or frequency. Thus, in order for this equation to hold at all temperatures, we must have

$$g_u B_{ul} = g_l B_{lu} \tag{6.64}$$

and

$$A_{ul} = \frac{2h\nu^3}{c^2} B_{ul}. \tag{6.65}$$

These equations are known as the Einstein relations. They show that a line has a unique intrinsic strength – which we can choose to measure by any one of the three Einstein coefficients. The intrinsic strength of a line is ultimately derived from the dipole matrix element between the two states.

The Line Emission and Absorption Coefficients

We can define the contribution of a single line to the emission coefficient $j_\nu(\nu)$ to be $j_\nu^{\mathrm{L}}(\nu)$ and the contribution of a single line to the absorption coefficient $\alpha(\nu)$ to be α^{L}.

The Einstein coefficients give the probability of a transition per unit time per atom. If we multiply them by the density of atoms in the initial state, n_u or n_l, and by the energy of the transition, $h\nu$, we obtain the rate of exchange of energy between the radiation field and matter per unit volume per unit solid angle per unit frequency. Depending on the direction of the exchange, these are just the absorption and emission coefficients. Thus, we have

$$j_\nu^{\mathrm{L}} = \frac{h\nu}{4\pi} A_{ul} n_u \psi \qquad (6.66)$$

and

$$\alpha^{\mathrm{L}} = \frac{h\nu}{4\pi}(B_{lu} n_l \phi - B_{ul} n_u \psi). \qquad (6.67)$$

Note that we consider stimulated emission to be a negative absorption. This is mathematically convenient, as it ensures that the emission remains independent of direct dependence on the specific intensity and the processes that depend directly on the specific intensity are gathered in the absorption coefficient. Physically, the photon created by stimulated emission has the same direction, frequency, and polarization as the stimulating photon and so stimulated emission can be thought of a photon passing an atom and the result being two photons rather than none, the result for absorption.

There is one difference, however, betweeen absorption and stimulated emission. The probability for stimulated emission is proportional to the emission profile ψ whereas probability of absorption is proportional to the absorption profile ϕ. In general, these need not be equal – for example, the absorbing and emitting atoms might have different velocity distributions – and so in general stimulated emission does not correspond exactly to negative absorption. Nevertheless, we commonly assume that the difference between the profiles is not important. In this case, stimulated emission can be treated exactly as a negative absorption.

We can write the contribution of a single line to the emission coefficient $j_\nu(\nu)$ and the absorption coefficient α as

$$j_\nu^{\mathrm{L}}(\nu) \equiv j^{\mathrm{L}} \psi(\nu) \qquad (6.68)$$

and

$$\alpha^{\mathrm{L}}(\nu) \equiv \alpha^{\mathrm{L}} \phi(\nu). \qquad (6.69)$$

Here we have ignored the difference between the profiles for absorption and stimulated emission. Because of the normalization of ψ and ϕ, we have

$$j^{\mathrm{L}} = \int_0^\infty d\nu \, j_\nu^{\mathrm{L}}(\nu) \qquad (6.70)$$

and

$$\alpha^{\mathrm{L}} = \int_0^\infty d\nu \, \alpha^{\mathrm{L}}(\nu), \qquad (6.71)$$

and so j^{L} and α are known as the integrated line emission and aborption coefficients. We can now see that j^{L} and α characterize the strength of a line, whereas ψ and ϕ characterize its shape. In terms of the Einstein coefficients, the intergrated coefficients are given by

$$j^{\mathrm{L}} = \frac{h\nu}{4\pi} A_{ul} n_u \qquad (6.72)$$

and

$$\alpha^{\mathrm{L}} = \frac{h\nu}{4\pi}(B_{lu} n_l - B_{ul} n_u). \qquad (6.73)$$

We can use the Einstein relation that $g_l B_{lu} = g_u B_{ul}$ to write the integrated emission coefficient as

$$\alpha^{\mathrm{L}} = \frac{h\nu}{4\pi} B_{lu} n_l \left(1 - \frac{g_l n_u}{g_u n_l}\right). \qquad (6.74)$$

This has the form of the coefficient for true absorption multiplied by a correction factor that accounts for stimulated emission. If $n_u/n_l > g_u/g_l$ we have a *population inversion* and the absorption coefficient becomes negative. In this case, stimulated emission more than compensates for absorption, and as light passes through the medium it will be amplified by stimulated emission, producing a laser or maser (Light or Microwaves Amplified by the Stimulated Emission of Radiation). This can be seen from the solution to the equation of radiative transfer: when the extinction coefficient is positive, the optical depth also is positive, the $e^{-\tau}$ factor is less than 1 and diminishes incoming light; when the extinction coefficient is negative, when the optical depth is also negative, the $e^{-\tau}$ factor is greater than 1 and amplifies incoming light. Masers are often seen in the dense circumstellar environments of young and old stars.

In LTE the populations of the upper and lower states have a Boltzmann distribution, then $n_u/n_l = g_u/g_l e^{-h\nu/kT}$, and we have

$$\alpha^{\mathrm{L}} = \frac{h\nu}{4\pi} B_{lu} n_l (1 - e^{-h\nu/kT}). \qquad (6.75)$$

The correction factor is thus always positive; we cannot have a maser when the populations are given by a Boltzmann distribution. To create a maser, we need non-LTE conditions. Figure 6.3 compares the LTE correction factor for stimulated emission $1 - e^{-h\nu/kT}$ at 10^4 K against the Planck function. It also shows
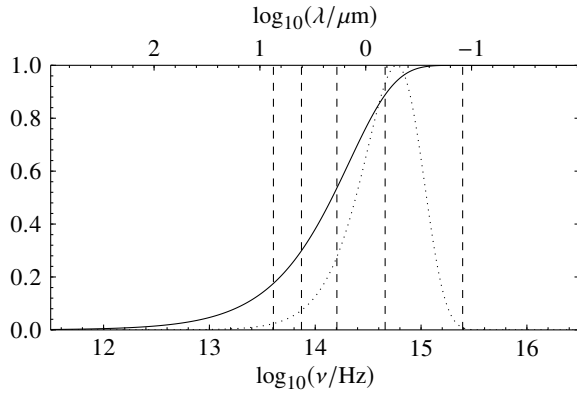
Figure 6.3: The LTE correction factor for stimulated emission $1 - e^{-h\nu/kT}$ at 10^4 K (solid line) compared to a scaled version of the Planck function (dotted line). Also shown (dashed, right to left) are the frequencies of Lyα, Hα, Paα, Brα, and Pfα.

the positions of Lyα ($n = 2 \to 1$, 1216 Å), Hα ($n = 3 \to 2$, 6563 Å), Paα ($n = 4 \to 3$, 1.875 μm), Brα ($n = 5 \to 4$, 4.051 μm), and Pfα ($n = 6 \to 5$, 7.458 μm). It shows that the correction for stimulated emission is negligible in the Wien tail (e.g., for Lyα), small but nonetheless not negligible close the peak of the Planck function (e.g., for Hα), and large in the Rayleigh-Jeans tail (e.g., for Paα, Brα, and Pfα).

In the Rayleigh-Jeans tail we have $1 - e^{-h\nu/kT} \approx h\nu/kT$, which is small; stimulated emission almost exactly balances absorption. The increasing importance of stimulated emission means that only a small over population of the upper level relative to its LTE value is sufficient to cause the line to mase. For example, in H II regions the levels of hydrogen have non-LTE populations and recombination lines such as H72α ($n = 73 \to 72$), which has a correction factor of only 8.2×10^{-5} at 10^4 K, are observed to mase because even a slight departure of LTE is enough to cause a population inversion.

Permitted and Forbidden Transitions

In astrophysics we distinguish between permitted and forbidden transitions. The lines observed in stellar atmospheres are almost exclusively permitted lines. Permitted transitions arise from electric dipole transitions and have a high probability, with A_{ul} typically being of order unity, whereas forbidden transitions arise from electric quadrupole or magnetic dipole transitions and have lower probabilities, with A_{ul} typically being 10^{-3} or less. The rules on the changes in quantum number that produce permitted rather than forbidden transitions are known as selection rules.

Forbidden lines are rarely seen in absorption because they are so weak; recall that α^L is directly proportional to B_{lu}, which in turn is directly proportional to A_{ul}. Thus, forbidden absorption lines will be many orders of magnitude weaker than permitted absorption lines, and are only detectable in spectral with excellent signal-to-noise ratios.

Stellar emission lines most often arise in the chromosphere and winds. Permitted lines are again typically the strongest. The probability of a forbidden transition is relatively low, so an atom has to spend a relatively long time (typically A_{lu}^{-1} or longer than 1000 s) in an excited state before it can emit by a forbidden transition. In this time, at the relatively high densities in the photosphere, chromosphere, and even the wind, the atom is likely to undergo a collision, which can de-excite it without emitting a photon. We say that at these high densities the lines are *collisionally quenched*.

Oscillator Strengths

Absorption lines can be modelled classically as the interaction of photons with oscillating electrons. The result is adequate in some aspects, but its major failing of the model is that it predicts that all lines have the same strength. This is because it attributes only one characteristic – energy difference – to a transition. However, quantum mechanics shows us that an equally important characteristic is the dipole element.

An ad hoc solution to this problem is to attribute an *oscillator strength* to each line, and to arbitrarily modify the model line strengths by multiplying them by this factor. The oscillator strengths are determined by requiring that the modified model line strengths match the the true line strengths, determined from quantum mechanical calculation, laboratory experiment, or astrophysical observation. The classical absorption oscillator strength f_{lu} is defined in terms of Einstein coefficient B_{lu} by

$$B_{lu} = \frac{4\pi^2 e^2}{h\nu m_e c} f_{lu}. \tag{6.76}$$

An equivalent emission oscillator strength f_{ul} can be defined in terms of B_{ul}. Oscilator strengths are always given in the combination gf, the degeneracy of the originating state multiplied by the oscilator strength for the transition, as the Einstein relation that $g_u B_{ul} = g_l B_{lu}$ implies that $g_u f_{ul} = g_l f_{lu}$. The oscilator strength has no direct physical meaning beyond quantifying the relative strengths of lines; it is simply the empirical correction factor we have to apply to an incorrect theory in order to obtain the correct result. Nonetheless, for reasons of precedent, line strengths are still often given in terms of the oscillator strengths.

From the definition of the oscilator strength, we can see that the integrated absorption coefficient is given by

$$\alpha^L = n_l f_{lu} \left(\frac{\pi e^2}{m_e c} \right) \left(1 - \frac{g_l n_u}{g_u n_l} \right), \tag{6.77}$$

in which the last factor is the correction for stimulated emission, and the integrated emission coefficient is given by

$$j^L = \left(\frac{2h\nu^3}{c^2} \right) n_u f_{ul} \left(\frac{\pi e^2}{m_e c} \right). \tag{6.78}$$

Determination of Oscillator Strengths

[*Quantum mechanical calculations. Exact for H and H-F for others. R-L p.$\tilde{2}$76 say why we need good wave functions. Coulomb*

approximation? Laboratory measurements. Observations. Sum rules. Give table of oscillator strengths for some common lines.]

Bound-Free and Free-Bound Transitions

[*The stuff in Osterbrock on heavy-element ionization and dielectronic recombination is good.*]

Bound-free radiative transitions correspond to photoionizations and free-bound radiative transitions to recombinations. They can be represented by

$$X^+ + e^- \rightleftharpoons X + \gamma. \tag{6.79}$$

As with bound-bound transitions, there is a stimulated recombination process which can be represented by

$$X^+ + e^- + \gamma \rightarrow X + 2\gamma. \tag{6.80}$$
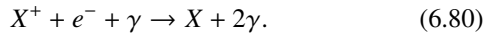
Rate of photoionizations per unit volume per unit frequency per unit solid angle is

$$\frac{1}{h\nu} a_{bf}(1 - e^{-h\nu/kT}) I_\nu n_n \tag{6.81}$$

[*The second part is stimulated recombination. I'm not sure why it has exactly this form.*]

Rate of radiative recombinations per unit volume per unit velocity is

$$n_i n_e a_{fb}(v) f(v) v \tag{6.82}$$

Milne Relations

In TE and using detailed balance, we have

$$\frac{a_{bf}}{a_{fb}} = \frac{n_i n_e}{n_n} \frac{h\nu f(v)v}{4\pi(1 - e^{-h\nu/kT})B_\nu} \frac{dv}{d\nu} \tag{6.83}$$

$$= \frac{n_i n_e}{n_n} e^{h\nu/kT} \frac{f(v)vc^2}{8\pi\nu^2} \frac{dv}{d\nu} \tag{6.84}$$

and $h\nu = mv^2/2 + \chi$, so $hd\nu = mvdv$, so

$$\frac{a_{bf}}{a_{fb}} = \frac{n_i n_e}{n_n} e^{h\nu/kT} \frac{f(v)hc^2}{8\pi m_e v^2}. \tag{6.85}$$

But Maxwell says

$$f(v) = 4\pi \left(\frac{m_e}{2\pi kT}\right)^{3/2} v^2 e^{-mv^2/2kT} \tag{6.86}$$

and Saha says

$$\frac{n_i n_e}{n_n} = 2 \left(\frac{2\pi m_e kT}{h^2}\right)^{3/2} \frac{g_i}{g_n} e^{-\chi/kT} \tag{6.87}$$

Thus,

$$\frac{a_{bf}}{a_{fb}} = \frac{m_e^2 c^2 v^2}{\nu^2 h^2} \frac{g_i}{g_n} e^{(h\nu - mv^2/2 - \chi)/kT} \tag{6.88}$$

and since $h\nu = mv^2/2 - \chi$,

$$\frac{a_{bf}}{a_{fb}} = \frac{g_i}{g_n} \frac{m_e^2 c^2 v^2}{\nu^2 h^2}. \tag{6.89}$$

Emission and Absorption Coefficients

As above,

$$\alpha^{bf} = n_n a_{bf}(1 - e^{-h\nu/kT}) \tag{6.90}$$

and

$$j_\nu^{bf} = \frac{h\nu}{4\pi} n_i n_e a_{fb}(v) f(v) v dv/d\nu \tag{6.91}$$

Determination

Determination again proceeds mainly from QM using similar methods to those for BB transitions. Having obtained a_{bf}, we can use the Milne relation to obtain a_{bf}.

For hydrogen-like transition, ionization from a state with a given n has

$$a_{bf} = \left(\frac{64\pi n}{3\sqrt{3}Z^2}\right) \alpha a_0^2 (\nu_n/\nu)^3 g_{bf}(\nu, n, l, Z) \tag{6.92}$$

where $\alpha \equiv e^2/\hbar c$, $a_0 = \hbar^2/me^2$, $h\nu_n = \chi_n$ and the Gaunt factor g is close to 1 near the edge and decreases with increasing ν.

Free-Free Transitions

$$\alpha^{ff} = \frac{4e^4}{3mhc} \left(\frac{2\pi}{3km}\right)^{1/2} T^{-1/2} Z^2 n_e n_i \nu^{-3}(1 - e^{-h\nu/kT}) \bar{g}_{ff} \tag{6.93}$$

$$j_\nu^{ff} = B_\nu \alpha^{ff}. \tag{6.94}$$

Electron Scattering

The cross-section for scattering is constant at non-relativistic wavelength and each electron contributes a cross-section of

$$a_T = \frac{8\pi e^4}{3m_e^2 c^4} = 6.652 \times 10^{-25} \text{ cm}^2, \tag{6.95}$$

so the scattering coefficient is given in terms of the free electron density n_e by

$$\sigma = n_e a_T. \tag{6.96}$$

At relativistic energies ($\lambda < 1$Å or $h\nu > 10$keV), the cross-section is smaller and is given by the Klein-Nishina formula.

Electron scattering is only strictly coherent in the rest frame of the electron, and electrons can impart a small change in energy either because of their thermal motions (leading to a broadening of the frequencies of scattered photons) or their bulk motion (leading to a systematic shift in the frequencies of scattered photons). In stellar photospheres, the electrons are relatively cool. The cool electrons will lead to relatively small broadening of the frequencies of the scattered photons, and will be insignificant if

the spectrum is smooth. Thus, when considering the continuum, a good approximation is to ignore the incoherence. However, if we have relativistic electrons or if electron scattering becomes important at the frequency of a line, as it can in winds, we cannot ignore the incoherence.

The phase function is not isotropic, but neverthess we often assume it is.

$$\sigma = n_e a_{\mathrm{T}} \qquad (6.97)$$

$$j_\nu = n_e a_{\mathrm{T}} J_\nu = \sigma J_\nu \qquad (6.98)$$

Notes and Further Reading

Partition Functions

Mihalas (1978, §5-1 and §9-4), Shu (1991, p. 62–63), Shu (1992, p. 8–10), andHummer & Mihalas (1988) discuss the lowering of the ionization potential in the presence of neighbors. Gray (1992, appendix D) gives polynomial approximations for the partition functions of atoms and ions in atmospheres.