

Class 4 Notes: Radiation-matter interaction

Now that we have completed our review of the structure of atoms and molecules and developed a basic machinery to talk about how those atoms and molecules emit and absorb photons, we are in a position to discuss the statistical properties of radiation-matter interaction. We will first derive some general results that extend our Einstein coefficient framework, and then write down the equation of radiative transfer and solve it in some simple cases.

I. Relations between Einstein coefficients

Our first goal in this lecture is to derive relationships between the Einstein coefficients. The three Einstein coefficients are not independent of one another. We can see this using the same trick as we did for collisions of material particles: considering detailed balance for a system in LTE. In LTE, both the matter and the radiation field must follow the Boltzmann distribution (or its slightly modified form for bosons in the case of the photons). For the matter this implies

$$n_u = \frac{g_u}{g_\ell} e^{-h\nu/kT} n_\ell, \quad (1)$$

and for the radiation

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

where $B_\nu(T)$ is the Planck function. Clearly this is independent of direction, so $J_\nu = I_\nu$. If we approximate ϕ_ν as a δ function, so that we ignore the variation in I_ν over it, then we have

$$\bar{J} = \int J_\nu \delta(\nu) d\nu = \frac{2h\nu_{ul}^3}{c^2} \frac{1}{e^{h\nu_{ul}/kT} - 1}. \quad (3)$$

In LTE, we require that the rate of change of n_u and n_ℓ be zero, and substituting in for I_ν and n_u using LTE, we have

$$\begin{aligned} 0 &= \left(\frac{dn_u}{dt} \right)_{\text{abs.}} + \left(\frac{dn_u}{dt} \right)_{\text{stim. emiss.}} + \left(\frac{dn_u}{dt} \right)_{\text{spon. emiss.}} \\ &= n_\ell B_{\ell u} \frac{2h\nu_{ul}^3}{c^2} \left[\frac{1}{e^{h\nu_{ul}/kT} - 1} \right] - n_\ell \frac{g_u}{g_\ell} e^{-h\nu_{ul}/kT} \left(A_{ul} + B_{u\ell} \frac{2h\nu_{ul}^3}{c^2} \left[\frac{1}{e^{h\nu_{ul}/kT} - 1} \right] \right) \end{aligned} \quad (4)$$

This equation is required to hold independent of T . For $h\nu_{ul}/kT \ll 1$, the exponentials approach 1, so the terms in square brackets are very large, and we can ignore the A_{ul} term in comparison. This immediately shows us that

$$B_{\ell u} = \frac{g_u}{g_\ell} B_{u\ell}. \quad (6)$$

Similarly, for $h\nu/kT \gg 1$, the terms in square brackets become very small, so we can drop the $B_{u\ell}$ term in comparison to the $A_{u\ell}$ one. Doing so and solving, we find

$$B_{u\ell} = \frac{c^2}{2h\nu_{u\ell}^3} A_{u\ell}. \quad (7)$$

Thus the value of $A_{u\ell}$ and the degeneracies and energies of the two levels fully determines all the Einstein coefficients.

For convenience we sometimes define the dimensionless directionally-averaged photon occupation number:

$$\langle n_\gamma \rangle = \frac{c^2}{2h\nu_{u\ell}^3} J_\nu, \quad (8)$$

where the brackets indicate that we are dealing with a quantity that has been averaged over directions. This quantity has the virtue that it allows us to express the emission and absorption rates very simply:

$$\left(\frac{dn_\ell}{dt} \right)_{\text{spon. emiss.}} = n_u A_{u\ell} \quad \left(\frac{dn_\ell}{dt} \right)_{\text{stim. emiss.}} = n_u \langle n_\gamma \rangle A_{u\ell} \quad \left(\frac{dn_u}{dt} \right)_{\text{abs.}} = \frac{g_u}{g_\ell} n_\ell \langle n_\gamma \rangle A_{u\ell}. \quad (9)$$

This definition makes clear that stimulated emission is unimportant when the photon occupation number is $\ll 1$, and dominant when it is $\gg 1$.

II. Cross sections and line profiles

It is often convenient to recast the absorption process in terms of a cross section, using something like the collision formalism we developed earlier in the class. Since each photon has an energy $h\nu$, the number of photons per unit time with frequencies from ν to $\nu+d\nu$ passing a given point is $J_\nu/h\nu$. Thus, following our example of writing reaction rates as number density times number density times cross section times velocity, we define the cross section $\sigma_{\ell u}(\nu)$ by

$$\left(\frac{dn_u}{dt} \right)_{\text{abs.}} = n_\ell \int \sigma_{\ell u}(\nu) \frac{4\pi J_\nu}{h\nu} d\nu \approx n_\ell J_\nu(\nu_{u\ell}) \frac{4\pi}{h\nu_{u\ell}} \int \sigma_{\ell u}(\nu) d\nu. \quad (10)$$

Here we are integrating over all photons energies or frequencies, and the factor of 4π is inserted because we are integrating over all directions as well. In the second step, we have assumed that $\sigma_{\ell u}(\nu)$ is very narrowly peaked around the frequency $\nu = (E_u - E_\ell)/h$, so that $J_\nu/h\nu$ is nearly constant over the range where $\sigma_{\ell u}(\nu)$ has any appreciable value, and we can take it out of the integral. This is almost always the case, unless the radiation field varies extremely rapidly with frequency.

If we now equate our formula for $(dn_u/dt)_{\text{abs}}$ in terms of $\sigma_{\ell u}$ with our formula with that in terms of the Einstein coefficients, and do a little re-arranging, we obtain

$$\int \sigma_{\ell u}(\nu) d\nu = \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{u\ell}^2} A_{u\ell}, \quad (11)$$

where $\nu_{ul} = (E_u - E_\ell)/h$ is the frequency corresponding to the exact energy difference between the levels. We therefore define the line profile function ϕ_ν by

$$\sigma_{\ell u}(\nu) = \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{ul}^2} A_{ul} \phi_\nu, \quad \int \phi_\nu d\nu = 1. \quad (12)$$

The function ϕ_ν contains all the information about how $\sigma_{\ell u}$ depends on frequency. Thus we see that the line profile function we introduced earlier is just a representation of how the microphysical absorption cross section depends on frequency.

Similarly, considering stimulated emission gives

$$n_u J_\nu(\nu_{ul}) \frac{4\pi}{h\nu} \int \sigma_{ul}(\nu) d\nu = \left(\frac{dn_\ell}{dt} \right)_{\text{stim. emiss.}}, \quad (13)$$

so we can write

$$\sigma_{ul}(\nu) = \frac{c^2}{8\pi\nu_{ul}^2} A_{ul} \phi_\nu = \frac{g_\ell}{g_u} \sigma_{\ell u}(\nu) \quad (14)$$

Note that we are implicitly assuming that the line profile function ϕ_ν is the same for absorption and stimulated emission. To see that this must be true, simply note that, in LTE, the rates of stimulated plus spontaneous emission must balance the rate of spontaneous emission at every frequency, and that this must be true independent of the temperature, which of course changes the functional form of ϕ_ν . This is only possible if all three rates have the same frequency dependence.

A. Natural broadening

One might think that $\sigma_{\ell u}(\nu)$ should be an infinitely sharp δ function; after all, how can a photon whose energy does not precisely match the energy difference between the two levels be absorbed? However, that ignores the uncertainty principle: one cannot precisely determine the photon energy or the exact velocity of the emitting particle. It also ignores the fact that, even in the absence of quantum uncertainty, for a population of particles at finite temperature there will be a range of velocities, and thus the Doppler effect will allow emission and absorption of a range of frequencies.

First let's consider the intrinsic quantum effect, which is called natural broadening. The exact line profile this produces can be computed quantum mechanically (a full treatment is given in Rybicki & Lightman), but to good approximation we can write it in a form that resembles the strength of response of a system to driving near a resonance, which varies as the square of the difference between the driving and resonant frequencies. This is the Lorentz profile:

$$\phi_\nu \approx \frac{4\gamma_{ul}}{16\pi^2(\nu - \nu_{ul})^2 + \gamma_{ul}^2}. \quad (15)$$

Here γ_{ul} has units of frequency. The full width at half max of this profile is

$$(\Delta\nu)_{\text{FWHM}} = \frac{\gamma_{ul}}{2\pi}. \quad (16)$$

What is the quantity γ_{ul} ? We can estimate this from the uncertainty principle. The lifetimes of the upper and lower states are

$$\tau_u = \left(\sum_{j < u} A_{uj} \right)^{-1} \quad \tau_\ell = \left(\sum_{j < \ell} A_{\ell j} \right)^{-1}. \quad (17)$$

The uncertainty principle states that $\Delta E \Delta t \geq \hbar$, or equivalently in terms of photon frequency $\Delta \nu \Delta t \geq 1/2\pi$. Since $\Delta t \sim \tau_u$ for the upper level, it follows that $\Delta \nu \sim 1/\tau_u = \sum_{j < u} A_{uj}$, and similarly for the lower one. In fact, a precise calculation gives

$$\gamma_{ul} = \sum_{j < u} A_{uj} + \sum_{j < \ell} A_{\ell j}. \quad (18)$$

Thus we can compute the natural linewidth from the Einstein A 's.

It is sometimes convenient to think of this width in terms of velocity: what Doppler shift would be required to produce the same shift in frequency? This is just (for non-relativistic motion)

$$(\Delta v)_{\text{FWHM}} = c \frac{(\Delta \nu)_{\text{FWHM}}}{\nu_{ul}} = \frac{\lambda_{ul} \gamma_{ul}}{2\pi}, \quad (19)$$

where $\lambda_{ul} = c/\nu_{ul}$. Typical linewidths for allowed UV and optical transitions are $\sim 0.01 \text{ km s}^{-1}$, while for X-ray transitions they can reach $\sim 10 \text{ km s}^{-1}$. The most prominent example is Lyman α , which has $(\Delta v)_{\text{FWHM}} = 0.0121 \text{ km s}^{-1}$.

B. Doppler broadening and the Voigt profile

The second main source of line broadening in the context of the ISM is Doppler broadening. The effect is simply that the gas has a non-zero velocity dispersion, so there are a range of atom velocities, each producing a different Doppler shifted frequency of emission or absorption. In fact, except for X-ray lines, it is almost always the case that the Doppler width is much greater than the natural width we have just computed – since gas is usually moving around much faster than $\sim 0.01 \text{ km s}^{-1}$.

For gas with a Maxwellian velocity distribution, the fraction f_v of particles with velocity between v and $v + dv$ is

$$f_v = \frac{1}{\sqrt{2\pi\sigma_v^2}} e^{-(v-v_0)^2/2\sigma_v^2}, \quad (20)$$

where v_0 is the mean velocity and $\sigma_v = \sqrt{kT/m}$ is the velocity dispersion. For convenience we sometimes use the broadening parameter $b = \sqrt{2}\sigma_v$ in place of σ_v . Since the Doppler shift is simply $\nu_{ul}v/c$, the corresponding line profile is

$$\phi_\nu = \frac{1}{\sqrt{2\pi\sigma_\nu^2}} e^{-(\nu-\nu_0)^2/2\sigma_\nu^2}, \quad (21)$$

where $\sigma_\nu = (\sigma_v/c)\nu_{ul}$ and $\nu_0 = \nu_{ul}(1 - v_0/c)$.

In reality, both Doppler broadening and natural broadening operate at the same time. Every particle at a given velocity emits a line that is naturally broadened. As a result, the true line profile is a convolution of the Doppler and Lorentz profiles:

$$\phi_\nu = \frac{1}{\sqrt{2\pi}\sigma_v^2} \int_{-\infty}^{\infty} e^{-v^2/2\sigma_v^2} \frac{4\gamma_{ul}}{16\pi^2(\nu - (1 - v/c)\nu_{ul})^2 + \gamma_{ul}^2} dv, \quad (22)$$

This is known as the Voigt profile. Note the factor of $(1 - v/c)$ in the denominator of the Lorentz profile function, representing the Doppler shift of a particular particle. For simplicity we have dropped the v_0 , since we can always choose to shift our rest frame to one in which the gas is at rest.

The integral cannot be evaluated analytically in general, but we can approximate it for the most common case $\gamma_{ul} \ll (\sigma_v/c)\nu_{ul}$, i.e. where the Doppler width is much greater than the natural width. In this case the Lorentz profile is much more sharply peaked than the Doppler profile near $v = 0$, so for small velocities we can approximate it by a δ function, i.e.

$$\frac{4\gamma_{ul}}{16\pi^2[\nu - (1 - v/c)\nu_{ul}]^2 + \gamma_{ul}^2} \approx \delta(v - c[1 - \nu/\nu_{ul}]) \quad (23)$$

In this case the integral is trivial, and reduces to simply the Doppler profile we derived earlier.

However, note that the Doppler profile falls off as $(\nu - \nu_{ul})^{-2}$ for frequencies far away from ν_{ul} , whereas the Maxwellian profile falls off as e^{-v^2} , which is much faster. For frequencies far from ν_{ul} , this means that we can instead think of the $e^{-v^2/2\sigma_v^2}$ term as a $\delta(v)$. In this case the integral is again trivial, and reduces to the Lorentz profile.

Thus we see that the shape of the Voigt profile is simply a “core” that looks like a Doppler profile, but with broad “wings” that fall off as $(\nu - \nu_{ul})^{-2}$, rather than $e^{-(\nu - \nu_{ul})^2/2\sigma_v^2}$, as a pure Doppler profile would. We can roughly estimate the velocity for which the transition between these two shapes occurs by solving for the velocity / frequency at which the two line profiles are equal. This is given by

$$\frac{4\gamma_{ul}}{16\pi^2(v/c)^2\nu_{ul}^2 + \gamma_{ul}^2} = \frac{1}{\sqrt{2\pi}\sigma_v^2} e^{-v^2/2\sigma_v^2}, \quad (24)$$

where in the Lorentz profile we have written the difference in frequency $\nu - \nu_{ul}$ as $(v/c)\nu_{ul}$. For convenience we define the Doppler broadening parameter

$$b = \sqrt{2}\sigma_v, \quad (25)$$

and if we let $z = v/b$, then the velocity of the core / wings transition is given implicitly by

$$e^{z^2} = \frac{4\pi^{3/2}b}{\gamma_{ul}\lambda_{ul}} z^2 + \frac{\gamma_{ul}}{4\pi b}. \quad (26)$$

Since $b \gg \gamma_{ul}$ for almost all astrophysical applications, we can generally drop the last term. This still leaves a transcendental equation that cannot be solved analytically, but the solution is reasonably well approximated by

$$z^2 \approx 10.31 + \ln \left[\frac{7618 \text{ cm s}^{-1}}{\gamma_{ul} \lambda_{ul}} b_6 \right], \quad (27)$$

where we have normalized to the value of $\gamma_{ul} \lambda_{ul}$ for Lyman α , and $b_6 = b/10 \text{ km s}^{-1}$. Since the logarithmic term generally isn't large (unless we're dealing with gas at X-ray temperatures, we see that the damping wings dominate the profile for $|z| \gtrsim 3.2$, i.e. for velocities of more than about 4.5 times the velocity dispersion.

III. Radiative transfer

We are now in a position to discuss the propagation of a beam of radiation through a material medium, and the interactions that take place as the photons move through the matter.

A. The transfer equation

Consider a beam of radiation of intensity I_ν (where we've dropped the argument list for conciseness) entering a slab of material of thickness ds . On the far side of the slab, the intensity that emerges is $I_\nu + dI_\nu$. The equation of radiative transfer states that

$$dI_\nu = -I_\nu \kappa_\nu ds + j_\nu ds, \quad (28)$$

where j_ν is the emissivity of the material (with units of power per unit volume per unit frequency per unit solid angle), and κ_ν is the attenuation coefficient (with units of 1/length).

Suppose now that the dominant emission and absorption processes are line emission and absorption by atoms and molecules. We can write the emissivity and attenuation coefficient in terms of the theory we have developed for these processes. For simplicity, let us continue to consider a single species with upper and lower states u and ℓ , and number densities n_u and n_ℓ for particles in that state.

For emission, recall that the rate of spontaneous decays per unit volume from state u is $n_u A_{u\ell}$ integrated over all frequencies. The rate at a specific frequency ν is $n_u A_{u\ell} \phi_\nu$. Each emission produces a photon of energy $h\nu$. Thus the power radiated per unit volume is $n_u A_{u\ell} h\nu$. In the frame comoving with the emitting particles, the emission is isotropic, and thus is evenly directed over 4π sr. Thus the emissivity is

$$j_\nu = \frac{1}{4\pi} n_u A_{u\ell} h\nu \phi_\nu. \quad (29)$$

If the material is moving this should be corrected for both Doppler shifting and beaming, although the latter is usually unimportant for non-relativistic flows.

For attenuation, we must compute the net rate of absorption, i.e. absorption minus stimulated emission. We can also do this in terms of the Einstein coefficients. The rate at which stimulated emission produces new photons of frequency ν traveling in direction \mathbf{n} is $n_u B_{u\ell}(I_\nu/4\pi)\phi_\nu$ photons per unit time per unit frequency. Each photon carries energy $h\nu$. Similarly, the rate at which absorption removes photons from the beam is $n_\ell B_{\ell u}(I_\nu/4\pi)\phi_\nu$. Thus the net absorption minus emission rate is

$$\kappa_\nu = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \phi_\nu - \frac{h\nu}{4\pi} n_u B_{u\ell} \phi_\nu. \quad (30)$$

Note that this has the right units: 1/length. The I_ν is not included because of the way κ_ν is defined. Recalling the relationship between the B coefficients from last class, we can rewrite this as

$$\kappa_\nu = n_\ell \frac{h\nu}{4\pi} B_{\ell u} \left(1 - \frac{g_\ell n_u}{g_u n_\ell} \right) \phi_\nu. \quad (31)$$

The combination that appears inside the parentheses has a specific name. In LTE, Boltzmann's law tells us that

$$n_u = \frac{g_u}{g_\ell} n_\ell e^{-E_{u\ell}/kT} \quad \implies \quad \frac{g_\ell n_u}{g_u n_\ell} = e^{-E_{u\ell}/kT}. \quad (32)$$

We therefore define the excitation temperature of two levels by

$$e^{-E_{u\ell}/kT_{\text{exc}}} = \frac{g_\ell n_u}{g_u n_\ell}. \quad (33)$$

Clearly in LTE we have $T_{\text{exc}} = T$, but out of LTE this need not hold. With this definition, the attenuation coefficient becomes

$$\kappa_\nu = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \left(1 - e^{-E_{u\ell}/kT_{\text{exc}}} \right) \phi_\nu. \quad (34)$$

B. Integrating the transfer equation: formal solution and uniform media

It is often convenient to make a change of variables in the transfer equation by letting

$$d\tau_\nu = \kappa_\nu ds, \quad (35)$$

which turns the transfer equation into

$$dI_\nu - I_\nu d\tau_\nu + S_\nu d\tau_\nu, \quad (36)$$

where

$$S_\nu = \frac{j_\nu}{\kappa_\nu}. \quad (37)$$

The equation can be solved formally by isolating the I_ν :

$$dI_\nu + I_\nu d\tau_\nu = S_\nu d\tau_\nu. \quad (38)$$

If we then multiply by e^{τ_ν} on both sides, we can integrate the equation:

$$e^{\tau_\nu} (dI_\nu + I_\nu d\tau_\nu) = e^{\tau_\nu} S_\nu d\tau_\nu \quad (39)$$

$$d(e^{\tau_\nu} I_\nu) = e^{\tau_\nu} S_\nu d\tau_\nu \quad (40)$$

$$e^{\tau_\nu} I_\nu(\tau_\nu) - I_\nu(0) = \int_0^{\tau_\nu} e^{\tau'} S_\nu d\tau' \quad (41)$$

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu-\tau')} S_\nu d\tau' \quad (42)$$

It's worth pausing to understand the physical meaning of this equation. Formally, it tells us the intensity along some particular ray. On this ray we have marked some starting point and labelled it optical depth 0, and we want to compute the intensity I_ν at some optical depth τ_ν further along the ray. This has two parts. The first is the intensity at the starting point, decreased by a factor of $e^{-\tau_\nu}$. It is the radiation entering the slab and being attenuated by it. The second term is an integral over the radiation that is added by emission within the slab, but also attenuated by it – radiation from the back of the slab is attenuated by more than the radiation from the front.

The physical meaning of this equation is perhaps easiest to understand by considering some special cases. Consider an infinite slab of matter in LTE at temperature T . The energy levels must therefore have an excitation temperature $T_{\text{exc}} = T$, and the radiation field must be equal to the Planck function $I_\nu = B_\nu(T)$. Since the intensity does not change anywhere, it follows that

$$dI_\nu = 0 = B_\nu d\tau_\nu + S_\nu d\tau_\nu \implies S_\nu = \frac{j_\nu}{\kappa_\nu} = B_\nu(T). \quad (43)$$

This is another example of the trick we've been using for several classes: we have deduced this equality from LTE considerations, which ultimately come from nothing more than counting arguments. However, note that $S_\nu = j_\nu/\kappa_\nu$ is a function only of local properties of the matter, and thus must hold locally at every point. This is known as Kirchoff's Law: for matter in LTE, the emissivity and attenuation coefficients are related by

$$\frac{j_\nu}{\kappa_\nu} = B_\nu(T). \quad (44)$$

If we substitute this into the formal solution to the transfer equation, we have

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu-\tau')} B_\nu(T_{\text{exc}}) d\tau'. \quad (45)$$

Note that T_{exc} can be a function of position, since Kirchoff's law applies locally. However, if the temperature inside the slab is constant, the $B_\nu(T_{\text{exc}})$ comes out of the integral, and we can evaluate it trivially:

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\text{exc}})(1 - e^{-\tau_\nu}). \quad (46)$$

The physical meaning of this becomes clear if we consider how the equation behaves in the limit of large and small τ_ν . For small τ_ν , the $e^{-\tau_\nu}$ factor is unity, so the first term is $I_\nu(0)$, and the second is zero. Thus the radiation is the same as what it was on the far side of the slab. On the other hand, for large τ_ν the first term goes to zero and the second one dominates. This says that the radiation field simply approaches the Planck function for temperature $T = T_{\text{exc}}$. Thus as the radiation passes through the matter, it becomes thermalized.

C. Masers

An interesting phenomenon is possible when matter is out of LTE in a specific way. Under some conditions collisions or radiative processes can lead to a population inversion, meaning that $n_u/g_u > n_\ell/g_\ell$. In other words, there are more particles in the upper state than one would expect for a Boltzmann distribution at any temperature. Formally, in fact, in this case the excitation temperature $T_{\text{exc}} < 0$.

Consider what happens as radiation moves through matter in which a population inversion exists. We cannot use the form of the transfer equation that applies in LTE, since of course the gas cannot be in LTE if a population inversion exists. Instead, recall that we showed earlier that

$$\kappa_\nu = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \left(1 - \frac{g_\ell}{g_u} \frac{n_u}{n_\ell} \right) = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \left(1 - e^{-E_{u\ell}/kT_{\text{exc}}} \right). \quad (47)$$

If a population inversion exists, then the term in parenthesis is negative, and the attenuation coefficient is positive. For simplicity, let us consider matter of negligible emissivity and constant, negative excitation temperature. In this case the transfer equation becomes

$$dI_\nu = -I_\nu d\tau_\nu \quad \implies \quad I_\nu = I_\nu(0)e^{-\tau_\nu} \quad (48)$$

but with the twist that $d\tau_\nu = -\kappa_\nu ds$ is negative as one proceeds along the ray, so the total optical depth is negative as well. This means that the intensity increases rather than decreases exponentially as radiation propagates through the matter.

This is known as a maser or laser (microwave or light amplified by stimulated emission of radiation) because the physical origin of the effect is that stimulated emission adds new photons to the beam faster than absorptions remove them. In some astrophysical situation the $e^{-\tau_\nu}$ factor can be very large, and as a result the intensity can be huge. For some astrophysical sources the brightness temperature exceeds 10^{11} K.