V. RADIATION-MATTER INTERACTIONS

Now that we have reviewed the quantum mechanical structures of atoms and molecules, we are in a position to develop a theory of how those levels interact with photons. We will first develop a description of the radiation field, and then a model for how radiation and matter couple.

Describing the Radiation Field

Let's begin with a discussion of how to describe the radiation field. The most common description is in terms of the specific intensity $I_\nu = I(\nu, \hat{n}, r, t)$, the amount of energy per unit time, unit area, unit frequency, and unit solid angle (in units of erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}). In LTE, the intensity is equal to the Planck function

$$I_\nu = B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1} \text{ (in LTE).}$$

Alternative descriptions of the radiation field include the photon occupation number

$$n_\gamma(\nu, \hat{n}, \hat{r}, t) = \frac{c^2}{2h\nu^3} I(\nu, \hat{n}, \hat{r}, t)$$

the brightness temperature

$$T_B(\nu, \hat{n}, \hat{r}, t) = \frac{h\nu/k}{\ln[1 + 2h\nu^3/c^2 I(\nu, \hat{n}, \hat{r}, t)]}$$

and the antenna temperature

$$T_A(\nu, \hat{n}, \hat{r}, t) = \frac{c^2}{2k\nu^2} I(\nu, \hat{n}, \hat{r}, t).$$

All of these are equivalent and each has a different physical interpretation. The *photon occupation number* is *dimensionless*, and measures the number of photons per polarization mode. *It is the natural quantum mechanical description of the radiation field, since in quantum mechanics the radiation field may be considered a harmonic oscillator*, and n_γ just corresponds to the quantum number describing its oscillation. The *brightness temperature* is the temperature of a blackbody that has an intensity equal to the given intensity. Finally, the *antenna temperature* is an approximate form of the brightness temperature, which has the virtue of being linear, and which is the same as the brightness temperature whenever $kT \gg h\nu$, i.e. in the *Rayleigh-Jeans limit* of the Planck function $B_\nu(T)$, which is usually the case at radio frequencies.

The intensity or its equivalents describe all there is to know about the radiation field *except polarization* (we could have two different intensities for two different polarizations, but for simplicity we'll neglect that). Often this is more information than we need, and instead we care only about certain *averages of the intensity*. One such commonly-used average is the *frequency-integrated intensity I*

$$I = \int I_\nu \, d\nu$$

This is the quantity that is relevant when we don't care about the frequency of the radiation, or if we are observing through *broadband filters*.

In some other circumstances we might not care about the direction $\hat{n}$, so we integrate over it. We define

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

as the *directionally-averaged intensity*. These averages are closely related to more familiar physical quantities. In particular, suppose that we are interested in the *specific energy density* in the radiation field, which is the energy per unit volume per unit frequency range. This is given by

$$u_\nu = \frac{1}{c} \int I(\nu, \hat{n}, \hat{r}, t) \, d\Omega = \frac{4\pi}{c} J_\nu.$$

To understand where this comes from intuitively, first note that we clearly want to average over directions, since we only want to know the *total energy density at a point*. To understand where the $1/c$ factor comes from, suppose that instead of photons we were describing some other particle traveling at half the speed of light. We are *holding the intensity fixed*, so that the same number of ergs per second of these particles pass a given point — they're just traveling half as fast. Clearly they must therefore be bunched up twice as closely as the photons, so the density will be twice as high. This is the effect that the $1/c$ captures.

Higher moments of *I* give the *radiation flux* (first moment), the *radiation pressure* (second moment), and so forth.

Einstein Coefficients

Important caution: in this section we introduce the *Einstein coefficients,* and there are two different conventions as to how the *Einstein B* coefficients are defined. Here we follow the convention that Rybicki & Lightman uses, in which they are defined relative to the *radiation intensity*. Draine uses a different convention, in which they are defined relative to the *radiation energy density*. Draine's definition of the *B* coefficients may be obtained by taking the ones we compute here and multiplying by a factor of *c*/4π. The Einstein *A* coefficient does not contain this ambiguity, and is the same in either convention.

Consider a particle of species *X* having *lower and upper energy levels* X_ℓ and X_u with energies E_ℓ and E_u. If a member of this species is in state ℓ, it can absorb a photon and transition to state *u*:
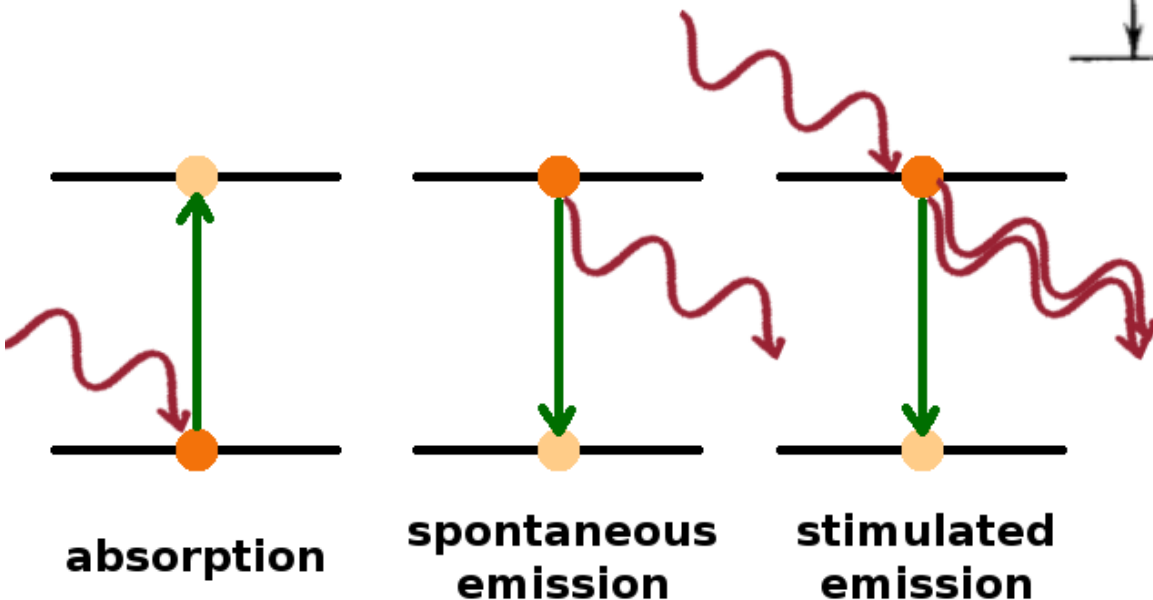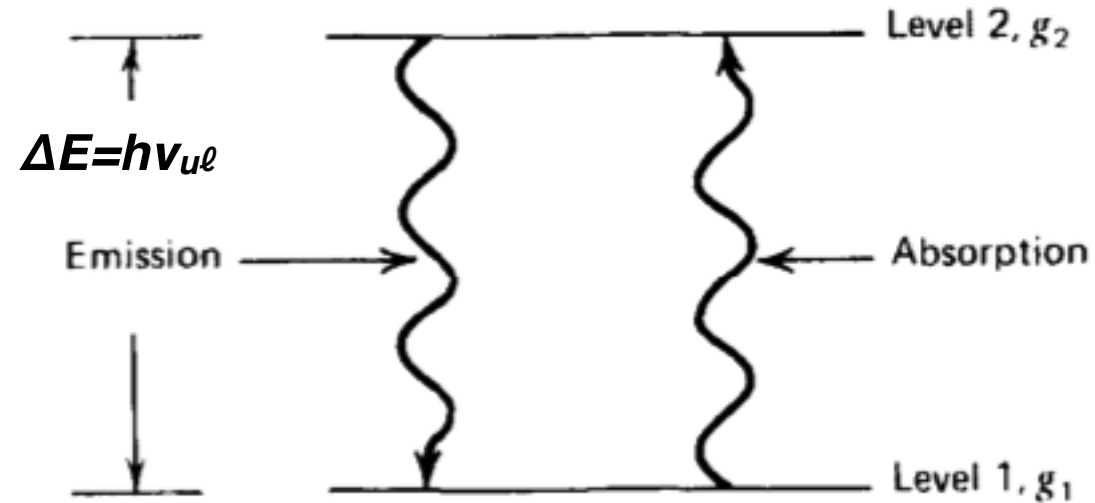
$$X_\ell + h\nu \rightarrow X_u, \qquad h\nu = E_u - E_\ell$$

Suppose we now have a population of members of species *X* in state X_ℓ with number density n_ℓ, and that this population interacts with a radiation field of intensity I_ν. Photons with frequencies *near* $h\nu = E_u - E_\ell$ can be absorbed. We define the *line profile function* ϕ_ν as giving the *relative probability* that a photon of frequency ν will be *absorbed*, and normalize so that

$$\int_0^\infty \phi_\nu \, d\nu = 1$$

For now we can think of **ϕ_ν** as closely approximating a δ-function at frequency *$h\nu_{u\ell}$= E_u - E_ℓ* and we will calculate its true form later.

Emission and absorption from a two level atom.

Level 2, g_2

$\Delta E = h\nu_{u\ell}$

Emission →

← Absorption

Level 1, g_1

absorption

spontaneous emission

stimulated emission

As with any other collisional process, the rate at which collisions between particles and photons produce transitions must be proportional to the *number density of target particles times the number density of photons in the beam.* Thus we write the *excitation rate* — the rate at which photons are absorbed — as

$$\left(\frac{dn_u}{dt}\right)_{\text{abs}} = -\left(\frac{dn_\ell}{dt}\right)_{\text{abs}} = n_\ell B_{\ell u} \bar{J}, \quad \text{where } \bar{J} = \int J_\nu \phi_\nu \, d\nu,$$

since the photon number density at frequencies where they can be absorbed is proportional to $\bar{J}$. Here $B_{\ell u}$ is the *rate coefficient for this absorption*, in units of cm^2 erg^{-1} s^{-1} ster .This type of <u>rate coefficient</u> has a special name: $B_{\ell u}$ is the *Einstein absorption coefficient for this transition.* It can be calculated quantum mechanically using a semi-classical approach; one treats the *radiation field classically*, and uses perturbation theory to compute the probability of the atom undergoing a change in state due to the perturbation. In practice these calculations are analytically tractable only for the very simplest atoms, and are numerically tractable only for slightly more complex ones. For most complex multi-electron atoms and molecules, however, the absorption rate must be measured in the lab.

In addition to *absorption*, two other types of transition are possible. First, a particle in the excited state can *spontaneously decay*, emitting a photon:

$$X_u \to X_\ell + h\nu$$

The rate at which this happens per unit volume simply depends on the number density of particles that can decay:

$$-\left(\frac{dn_u}{dt}\right)_{\text{spon emiss}} = \left(\frac{dn_\ell}{dt}\right)_{\text{spon emiss}} = n_u A_{u\ell}$$

where $A_{u\ell}$, which we introduced in the last class, is a *constant* with units of s^{-1}. It is called the *Einstein spontaneous emission coefficient*, or just the Einstein *A*-coefficient.

Finally, there is another emission process. Just as a time-varying electromagnetic field can induce a particle in state ℓ to transition to state u by perturbing it, the reverse is true: a particle in state u can be induced to transition to state ℓ

$$X_u + h\nu \rightarrow X_\ell + 2h\nu$$

The *extra photon* has the *same direction (and phase and polarization)* as the one that induced the emission *(i.e. emitted photon is coherent)*. This process is known as *stimulated emission*. The stimulated emission rate must have the same functional form as the absorption rate, since it is essentially the same process in reverse. Thus we write

$$-\left(\frac{dn_u}{dt}\right)_{\text{stim. emiss.}} = \left(\frac{dn_\ell}{dt}\right)_{\text{stim. emiss.}} = n_u B_{u\ell} \bar{J}$$

Here $B_{u\ell}$ has the same units as $B_{\ell u}$, and is called the Einstein *stimulated emission coefficient.*

Relations Between 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

$$n_u = \frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/kT} n_\ell \qquad (1)$$

and for the radiation

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

Clearly $B_\nu(T)$ is independent of direction, so $J_\nu = I_\nu$. If we approximate again ϕ_ν as a δ-function, so that we can ignore the variation of I_ν over the line profile, then we have

$$\bar{J} = \int J_\nu \delta(\nu - \nu_{u\ell})\, d\nu = \frac{2h\nu_{u\ell}^3}{c^2} \frac{1}{e^{h\nu_{u\ell}/kT} - 1} = B_{\nu_{u\ell}}(T)$$

In TE, we require that the rate of change of n_u and n_ℓ must be *zero* (i.e. number of transitions per unit time per unit volume *into a state* equals the number of transitions per unit time per unit volume *out of that state*):

$$0 = \left(\frac{dn_u}{dt}\right) = \left(\frac{dn_u}{dt}\right)_{\ell \to u} + \left(\frac{dn_u}{dt}\right)_{u \to \ell} = \left(\frac{dn_u}{dt}\right)_{\text{abs}} + \left(\frac{dn_u}{dt}\right)_{\text{stim emiss}} + \left(\frac{dn_u}{dt}\right)_{\text{spon emiss}}$$

$$= n_\ell B_{\ell u} \bar{J} - n_u B_{u\ell} \bar{J} - n_u A_{u\ell}$$

Solving for $\bar{J}$ gives
$$\bar{J} = \frac{n_u A_{u\ell}}{n_\ell B_{\ell u} - n_u B_{u\ell}} = \frac{A_{u\ell}/B_{u\ell}}{(n_\ell/n_u)(B_{\ell u}/B_{u\ell}) - 1}$$

In LTE, the ratio of n_u to n_ℓ is given by eq. (1), so

$$\bar{J} = \frac{A_{u\ell}/B_{u\ell}}{(g_\ell B_{\ell u}/g_u B_{u\ell})e^{h\nu_{u\ell}/kT} - 1} \qquad (3)$$

But in thermodynamic equilibrium we also know $J_\nu = B_\nu(T)$ and $\bar{J} = B_{\nu u\ell}(T)$. *For the expression above to be equal to the Planck function <u>for all temperatures</u>, one must have the following Einstein relations:*

$$\boxed{B_{u\ell} = \frac{c^2}{2h\nu_{u\ell}^3} A_{u\ell}} \qquad \boxed{B_{\ell u} = \frac{g_u}{g_\ell} B_{u\ell}}$$

Thus the value of $A_{u\ell}$ and the degeneracies and energies of the two levels fully determines all the Einstein coefficients. Note that Einstein's relations connect _atomic properties_ $B_{u\ell}$, $B_{\ell u}$, and $A_{u\ell}$, and have no reference to the temperature T. Thus they must hold whether or not the atoms are in _thermodynamic equilibrium_!

A Stroke of Genius: Einstein was led to include the process of _stimulated emission_ by the fact that _without it he could not get Planck's law_, but only _Wien's law_, which was known to be incorrect. Without _stimulated emission_, eq. (3) becomes

$$\bar{J} = \frac{n_u A_{u\ell}}{n_\ell B_{\ell u}} = \frac{g_u}{g_\ell} \frac{A_{u\ell}}{B_{\ell u}} e^{-h\nu_{u\ell}/kT}$$

This cannot equal the Planck function with $A_{u\ell}/B_{\ell u}$ independent of temperature. However, the choice

$$\frac{g_u}{g_\ell} \frac{A_{u\ell}}{B_{\ell u}} = \frac{2h\nu_{u\ell}^3}{c^2}$$

does yield $\bar{J} = B_{\nu u\ell}(T)$ _in the Wien limit,_ $h\nu_{u\ell} \gg kT$. Why does one obtain the Wien law when stimulated emission is neglected? Remember that the Wien law is the expression of the Planck spectrum when $h\nu \gg kT$. But in this limit level u is very sparsely populated relative to level ℓ, $n_u \ll n_\ell$. Then _stimulated emission is unimportant compared to absorption_, since these are proportional to n_u and n_ℓ, respectively.

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

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

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:

and

$$\left(\frac{dn_u}{dt}\right)_{\ell \to u} = \left(\frac{dn_u}{dt}\right)_{\text{abs}} = n_\ell \frac{g_u}{g_\ell} A_{u\ell} \langle n_\gamma \rangle$$

$$\left(\frac{dn_\ell}{dt}\right)_{u \to \ell} = \left(\frac{dn_\ell}{dt}\right)_{\text{spon emiss}} + \left(\frac{dn_\ell}{dt}\right)_{\text{stim emiss}} = n_u A_{u\ell}(1 + \langle n_\gamma \rangle)$$

This definition makes clear that <u>*stimulated emission is unimportant compared to spontaneous emission*</u> when the photon occupation number is $\ll 1$, and dominant when it is $\gg 1$.

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, where we wrote <u>*volumetric reaction rates*</u> as products of the <u>*number densities*</u> of the reactants times a *cross section* times a <u>*velocity*</u>.

The velocity is clearly the speed of light, and the number density of photons with frequencies from ν to $\nu+d\nu$ is $u_\nu/h\nu$, where u_ν is the energy density. Thus we define the cross section $\sigma_{\ell u}(\nu)$ by

$$\left(\frac{dn_u}{dt}\right)_{\ell\to u} = \left(\frac{dn_u}{dt}\right)_{\text{abs}} = n_\ell \int_0^\infty \sigma_{\ell u}(\nu)\frac{cu_\nu}{h\nu}\,d\nu = n_\ell \int_0^\infty \sigma_{\ell u}(\nu)\frac{4\pi J_\nu}{h\nu}\,d\nu$$

where the last equality uses $u_\nu = (4\pi J_\nu/c)$, and we must now integrate over all photon frequencies. Assuming, as previously, that $\sigma_{\ell u}$ is very sharply peaked around the frequency $\nu_{u\ell}=(E_u-E_\ell)/h$ (i.e. the *line profile ϕ_ν is sharply peaked*), so that $J_\nu/h\nu$ is nearly constant over the range where $\sigma_{\ell u}$ has any appreciable value, we can then take it out of the integral:

$$\left(\frac{dn_u}{dt}\right)_{\text{abs}} = n_\ell \frac{4\pi J_\nu(\nu_{u\ell})}{h\nu_{u\ell}} \int_0^\infty \sigma_{\ell u}(\nu)\,d\nu = n_\ell \frac{g_u}{g_\ell} A_{u\ell}\langle n_\gamma\rangle$$

With a little re-arranging we obtain

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

We can therefore define the *line profile function* ϕ_ν by

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

The function ϕ_ν contains all the information about how $\sigma_{\ell u}$ depends on frequency ⇨ 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

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

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

Note that we are implicitly assuming that the *line profile function 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 absorption at every frequency*, and that this must be true *independent of temperature*, which of course changes the frequency dependence of $J_\nu=B_\nu(T)$. This is only possible if all three rates have the same frequency dependence.

Natural Broadening

Now what about this line profile function ϕ_ν ? One might think that $\sigma_{\ell u}$ should be an *infinitely sharp 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 Chapter 10), 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_:

$$\phi_\nu \approx \frac{4\gamma_{u\ell}}{16\pi^2 (\nu - \nu_{u\ell})^2 + \gamma_{u\ell}^2}$$

where $\gamma_{u\ell}$ has units of frequency. The _full width at half maximum_ of this profile is

$$(\Delta\nu)_{\mathrm{FWHM}} = \frac{\gamma_{u\ell}}{2\pi}$$

What is the quantity $\gamma_{u\ell}$? Recall that the Einstein $A_{u\ell}$ coefficients provide the rate of spontaneous decay from an upper to a lower state. Thus the _lifetimes of the upper and lower states is just the inverse of the aggregate decay rate to all lower states_:

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

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

$$\gamma_{u\ell} = \sum_{j<u} A_{uj} + \sum_{j<\ell} A_{\ell j}$$

which we can intuitively think of as the *combined natural broadening of both the upper and lower states.* Thus we can compute the natural line width directly from the Einstein A coefficients.

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

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

Typical linewidths for allowed UV and optical transitions are ~ 0.01 km s^{-1}. The most prominent example is *hydrogen Lyα*, which has $(\Delta v)_{\text{FWHM}} = 0.0121$ km s^{-1}.

Doppler Broadening and Voigt Profile

The second main source of line broadening in the context of the ISM is *Doppler broadening*. An atom is in thermal motion, so that the *frequency of emission or absorption in its own frame corresponds to a different frequency for an observer*. Each atom has its own Doppler shift, so that the net effect is to spread the line out, but not to change its total strength. 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 0.01 km s⁻¹.

If the motions are entirely *thermal*, then the atoms/ions/molecules will follow a Maxwellian velocity distribution, and the fraction f_v of particles with velocity between v and $v+dv$ is then just a *Gaussian*

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

where v_0 is the mean bulk velocity and $\sigma v = \sqrt{kT/m}$ is the 1d velocity dispersion. Since both *Doppler broadening and natural broadening* operate at the same time, *every particle with a given velocity will emit or absorb a line that is naturally broadened.* As a result, the true line profile will be a convolution of the Doppler and Lorentz profiles:

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

This is known as the *Voigt profile*. Note that the factor of *(1-v/c)* in the denominator of the Lorentz profile function results from particles moving with velocity *v,* for which the rest-frame *frequency $\nu_{u\ell}$ is Doppler shifted to ν'= $\nu_{u\ell}$ (1 − v/c)* to lowest order in *v/c*. *For simplicity we have dropped the ν_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 where the *Doppler width* is much greater than the *natural width*, i.e.

$$(\Delta v)_{\text{FWHM}} \ll \sigma_v \Rightarrow \gamma_{u\ell} \ll (\sigma_v/c)\nu_{u\ell}$$

In this case the <u>*Lorentz profile is much more sharply peaked than the Doppler profile*</u> near *v = 0*, so for small velocities we can approximate it by a δ-function.

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

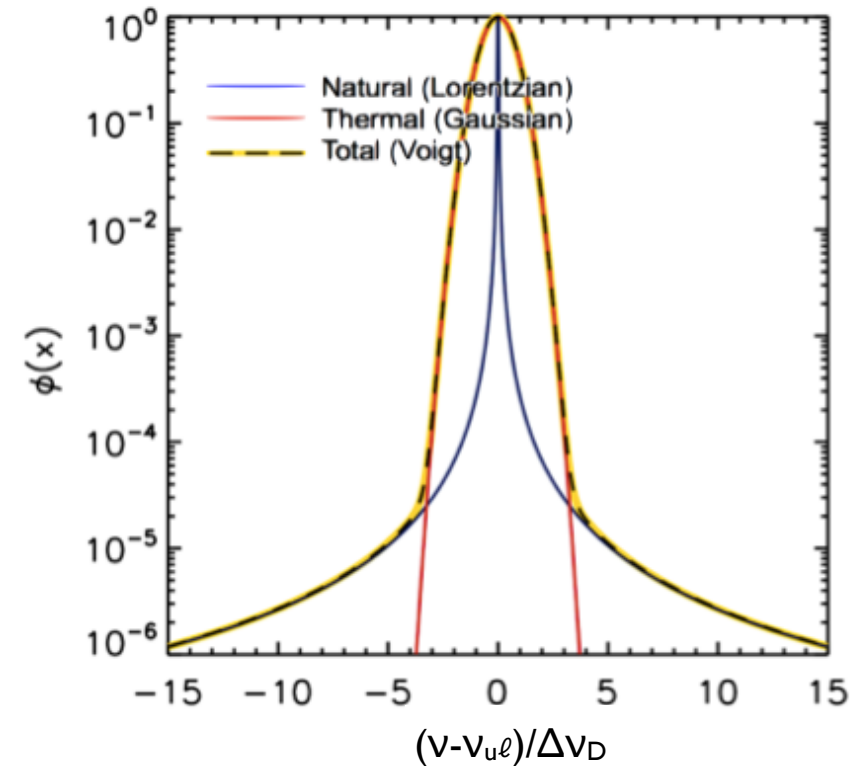In this case the integral is trivial, and reduces to

$$\phi_\nu = \frac{1}{\sqrt{\pi}\Delta\nu_D} e^{-(\nu-\nu_{u\ell})^2/\Delta\nu_D^2}$$

Gaussian profile valid in the line core

where the *Doppler width* **Δν$_D$** is defined by $\Delta\nu_D = \sqrt{2}\sigma_v/\lambda_{u\ell} = (2kT/m)^{1/2}/\lambda_{u\ell}$

The *line-center cross section* for absorption in the case of Doppler broadening is then

$$\sigma_{\ell u}(\nu_{u\ell}) = \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{u\ell}^2} A_{u\ell} \times \frac{1}{\sqrt{\pi}\Delta\nu_D}$$

$$= \frac{h\nu_{u\ell}}{4\pi} B_{\ell u} \times \frac{1}{\sqrt{\pi}\Delta\nu_D}$$

Natural (Lorentzian)
Thermal (Gaussian)
Total (Voigt)

$\phi(x)$

$(\nu-\nu_{u\ell})/\Delta\nu_D$

The Einstein coefficients can be calculated by quantum mechanics + classical electrodynamics calculation ➪

$f_{\ell u}$ = oscillator strength (dimensionless)

$$\frac{h\nu_{u\ell}}{4\pi} B_{\ell u} = \boxed{\frac{\pi e^2}{m_e c}} f_{\ell u}$$

classical result from electrodynamics = 0.02654 cm^2 s^{-1}

Plugging in we get:

$$\sigma_{\ell u}(\nu_{u\ell}) = \frac{\pi e^2}{m_e c} f_{\ell u} \times \frac{1}{\sqrt{\pi}\Delta\nu_D}$$

Numerically, this is

$$\sigma_{\ell u}(\nu_{u\ell}) = (1.42 \times 10^{-13}\ \mathrm{cm}^2)\, f_{\ell u} \sqrt{A/T_4}$$

In the case of hydrogen Lyα *A=1* and *f_{12}=0.4162*, so the line-center cross section is

$$\sigma_{\alpha}(\nu_{\alpha}) = 5.9 \times 10^{-14}\, T_4^{-1/2}\ \mathrm{cm}^2$$

This is 11 orders of magnitude larger than the Thomson cross-section! *That is, an electron bound to the proton is 11 orders of magnitude more efficient at scattering radiation than a free electron when the frequency of that radiation closely matches the natural frequency of the transition.*

This further emphasizes that bound electrons *resonantly scatter* the incoming radiation. To put these numbers in context, it is possible to measure the hydrogen column density, N_{HI}, in nearby galaxies. The observed intensity in the 21-cm line translates to typical HI column densities of order $N_{HI} \sim 10^{19} - 10^{21}$ cm^{-2}, which *translates to a number of scatterings for Lyα photons at line center of order $10^7 - 10^8$. This estimate highlights the importance of understanding the transport of Lyα photons out of galaxies.*

Note that the Lorentz profile falls off as $(\nu - \nu_{u\ell})^{-2}$ for frequencies far away from $\nu_{u\ell}$, whereas the Maxwellian profile falls off as $e^{-(\nu - \nu_{u\ell})^2/\Delta\nu_D^2}$, which is much faster. For frequencies far from $\nu_{u\ell}$, this means that we can instead think of the term $e^{-(\nu - \nu_{u\ell})^2/\Delta\nu_D^2}$ as a δ-function. In this case the integral is again trivial, and reduces to the Lorentz profile.

Thus the shape of the Voigt profile is simply a *core* that looks like a Doppler profile, but with broad *wings* that fall off as $1/(\nu - \nu_{u\ell})^2$, rather than exponentially as a pure Doppler profile would. We can 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 gives

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

where in the Lorentz profile we have written the difference in frequency $(\nu - \nu_{u\ell})$ as $(v/c)\nu_{u\ell}$. If we let $z = v/(\sigma_v\sqrt{2})$, then the solution to the resulting transcendental equation can be well approximated by

$$z^2 \approx 10.31 + \ln\left[\frac{7618\ \mathrm{cm\ s}^{-1}}{\gamma_{u\ell}\lambda_{u\ell}}\frac{\sqrt{2}\sigma_v}{10\ \mathrm{km\ s}^{-1}}\right]$$

where we have normalized to the value $\gamma_{u\ell}\lambda_{u\ell}$ for Lyα. Since the logarithmic term generally isn't large, the *Lorentzian shape (also referred to as the damping wings)* dominate the line profile for *z>3.2*, i.e. *for velocities of more than about 4.5 times the velocity dispersion.*

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.

Radiative transfer geometry. Figure from Draine.
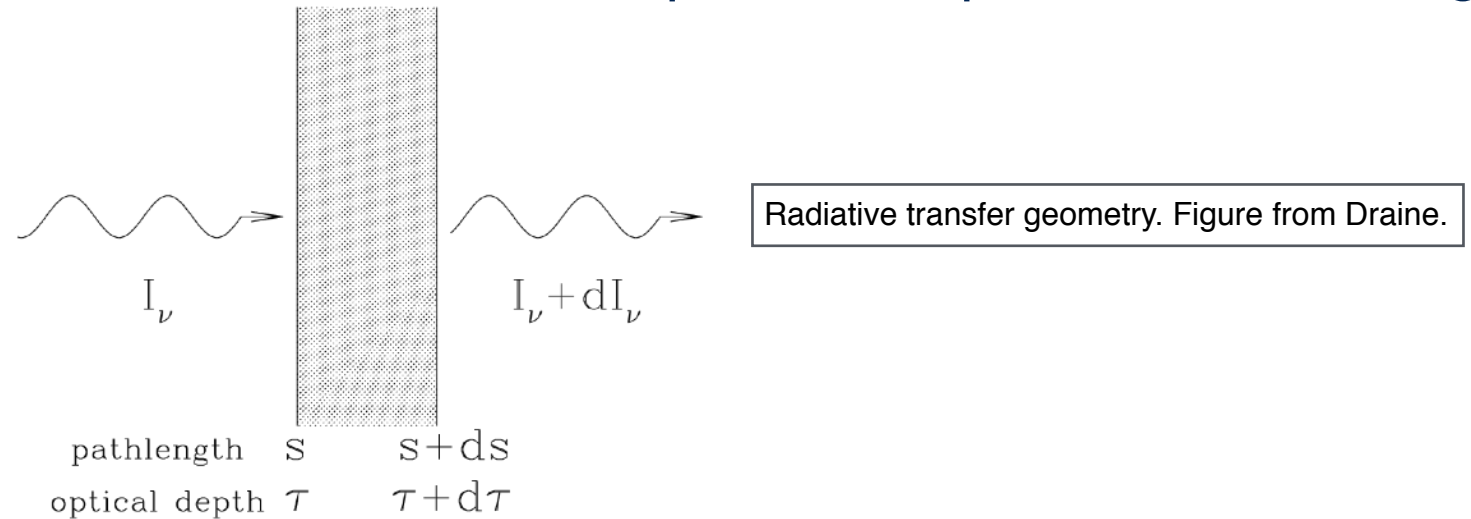
Consider a beam of radiation of intensity I_v entering a slab of material of thickness *ds*. On the far side of the slab, the intensity that emerges is $I_v + dI_v$. The equation of *radiative transfer* states that

$$dI_\nu = -I_\nu \kappa_\nu \, ds + j_\nu \, ds$$

where j_v is the *emissivity* of the material (with units of erg s^{-1} cm^{-3} Hz^{-1} sr^{-1}), and κ_v is the *absorption coefficient* (with units of cm^{-1}). This equation can be understood in terms of a microscopic model in which particles with density *n* each present an effective absorbing area, or cross section, of magnitude σ_v (cm^2), such that $\kappa_v = n\sigma_v$. Thus the mean free path of the radiation (which we discussed earlier for particle collisions) is $\lambda_{mfp} = (n\sigma_v)^{-1} = 1/\kappa_v$,

Suppose now that the dominant emission and absorption processes are line emission and absorption by atoms and molecules. We can write the *emissivity and absorption 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 <u>rate at a specific frequency</u> ν is $n_u A_{u\ell} \phi_\nu$. Each emission produces a photon of energy $h\nu$. Thus the specific power radiated per unit volume is $n_u A_{u\ell} \phi_\nu \, h\nu$. In the frame comoving with the emitting particles, the *emission is isotropic*, and thus is evenly directed over 4π sr. Thus the emissivity is

$$j_\nu = \frac{1}{4\pi} n_u A_{u\ell} h\nu \phi_\nu$$

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 <u>Einstein coefficients.</u> The rate at which *stimulated emission* produces new photons of frequency ν traveling in direction $\hat{n}$ is $n_u \, B_{u\ell} \, \phi_\nu \, (I_\nu/4\pi)$ 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 $n_\ell \, B_{\ell u} \, \phi_\nu \, (I_\nu/4\pi)$. Thus the <u>*net absorption minus emission rate*</u> is

$$\kappa_\nu = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \phi_\nu - \frac{h\nu}{4\pi} n_u B_{u\ell} \phi_\nu$$

Note that this has the right units: *length^{-1}* (recall that the B-coefficient has unit cm^2 erg^{-1} s^{-1} sr) . The I_ν is not included because of the way κ_ν is defined.

Recalling the relationship between the B coefficients from earlier *($g_\ell B_{\ell u} = g_u B_{u\ell}$)*, , we can rewrite this as

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

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

$$n_u = \frac{g_u}{g_\ell} n_\ell e^{-E_{u\ell}/kT} \qquad \Rightarrow \qquad \frac{g_\ell}{g_u} \frac{n_u}{n_\ell} = e^{-E_{u\ell}/kT}$$

Even if our two-level system is not in LTE, we can define the *excitation temperature* of the two levels by

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

The excitation temperature is not a *real temperature*; it is only a measure of the ratio of n_u to n_ℓ and is determined by a balance between radiative and collisional excitations and de-excitations. Clearly in LTE we have $T_{\text{exc}} = T$, but out of LTE this need not hold. With this definition, the attenuation coefficient becomes

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

Finally, using the relationships between the Einstein coefficients that we derived earlier, one can show that in general

$$S_\nu \equiv \frac{j_\nu}{\kappa_\nu} = B_\nu(T_{\text{exc}})$$

where $B_\nu(T_{\text{exc}})$ is the Planck function at the *excitation temperature*. The quantity S_ν is known as the *source function*.

Integrating the Transfer Equation: Formal Solution and Kirchoff's Law

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

$$d\tau_\nu = \kappa_\nu \, ds$$

which turns the transfer equation into

$$dI_\nu + I_\nu d\tau_\nu = S_\nu \, d\tau_\nu$$

The *dimensionless* quantity τ_ν is referred to as the *optical depth*. Recall that the $\lambda_{mfp} = 1/\kappa_\nu$, hence the optical depth is a coordinate that describes the *number of mean free paths traversed in the material*. Small values of $\tau_\nu \ll 1$ are referred to as *optically thin*, and large values of $\tau_\nu \gg 1$ are referred to as *optically thick*.

If we then multiply by $\exp(\tau_\nu)$ on both sides, we can integrate the equation:

$$e^{\tau_\nu} \left(dI_\nu + I_\nu \, d\tau_\nu \right) = e^{\tau_\nu} S_\nu \, d\tau_\nu$$

$$d \left(e^{\tau_\nu} I_\nu \right) = e^{\tau_\nu} S_\nu \, d\tau_\nu$$

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

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

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 further along the ray. This has two parts. The first is the intensity at the starting point, decreased by a factor of $exp\ (-\ \tau_\nu)$. 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 more than the radiation from the front.

Because the absorption and emission processes have not been specified, κ_ν and j_ν seem to be independent. However, they are not independent in *full thermodynamic equilibrium* (TE), whereby matter and radiation are in equilibrium at the same temperature *T*. An important relationship between them is known as *Kirchoff's law*, which we will now derive. Consider the thought experiment illustrated in the Figure on the right. *Two cavities made of different materials and containing different absorbers* are connected by a filter transparent only in the narrow frequency range ν to $\nu+d\nu$.
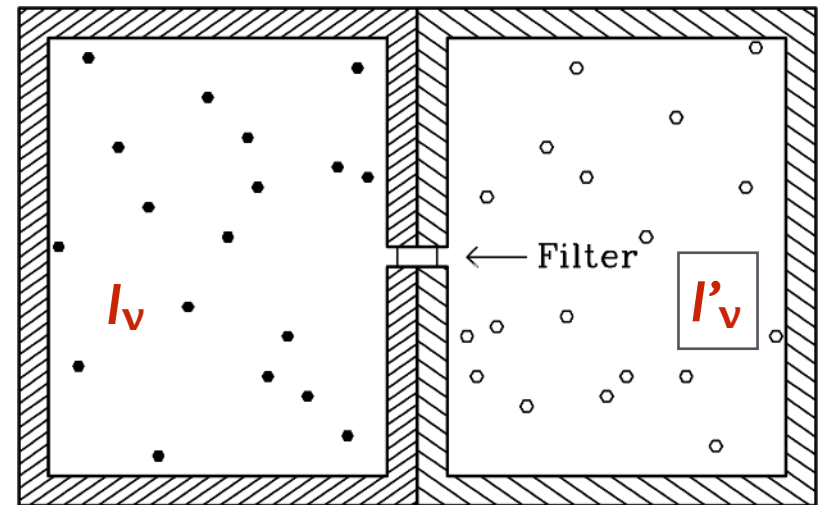
Kirchoff's thought experiment invokes two cavities in TE connected through a filter that passes radiation in the narrow frequency range ν to $\nu + d\nu$. The cavities may be made of different materials and contain different emitting/absorbing particles.

In *equilibrium at any temperature T*, radiation can *transfer no net power* from one cavity to the other, lest one cavity cool down and the other heat up. But that would violate the second law of thermodynamics because the two cavities at different temperatures could be used to drive a heat engine. Thus in full thermal equilibrium (TE) at temperature *T*,

$$\frac{dI_\nu}{ds} = 0 \quad \text{and} \quad I_\nu = B_\nu(T)$$

The equation of radiative transfer then implies

$$\frac{dI_\nu}{ds} = -\kappa_\nu B_\nu(T) + j_\nu = 0$$

or

$$S_\nu \equiv \frac{j_\nu}{\kappa_\nu} = B_\nu(T) \qquad \text{Kirchoff's law}$$

This law is remarkable because it connects the properties j_ν and κ_ν *at each frequency* for *any kind of matter* to the *single universal spectrum of equilibrium radiation $B_\nu(T)$*. Although Kirchhoff's law was derived for a system in TE, its applicability is not limited to blackbody radiation in full TE with its material environment.

Kirchoff's law also applies whenever the radiating/absorbing material is in thermal equilibrium (it has a well-defined temperature T) even if it is not in equilibrium with the radiation field, i.e. $I_\nu \neq B_\nu (T)$. This situation defines local thermodynamic equilibrium (LTE). For example, gas molecules in the Earth's lower atmosphere have a Maxwellian speed distribution, so the gas is in LTE with a well-defined kinetic temperature $T \sim 300$ K measurable with an ordinary thermometer. But the gas is in a non-equilibrium radiation field (anisotropic $T \sim 5800$ K blackbody spectrum of sunlight during the day, the cold dark sky at night, plus anisotropic emission from the ground) distinctly different from a blackbody at the gas temperature.

Kirchoff's law applies in LTE as well as in TE. Recall that $B_\nu (T)$ is a function of temperature only and does not depend on the microscopic properties of the radiating/absorbing material. In contrast, both j_ν and κ_ν depend only on the nature of the emitting/absorbing materials in the cavity and on the temperature of that material; *they do not depend on the ambient radiation field or its spectrum*. Thus the emissivity and absorption coefficient of all materials in LTE obey Kirchoff's law.

Kirchoff's law is not intuitively familiar to us because the optical brightness of room-temperature ($T \sim 300$ K) objects in our environment is nearly zero since $h\nu/kT \gg 1$. Thus, a glass of water might absorb 10% of the sunlight passing through it but not emit any detectable light because 10% of the optical brightness of a room-temperature blackbody is nearly zero. A familiar illustration of Kirchoff's law is a charcoal fire with flames and glowing coals. The infrared (heat) radiation from the black coals is much more intense than that of the even hotter but nearly transparent flames.

At this point it is helpful to reiterate the distinction between LTE and TE in terms of what we've learned about the radiative transfer equation. In LTE $S_\nu = B_\nu(T)$ and $I_\nu \neq B_\nu(T)$. Whereas in TE $S_\nu = B_\nu(T) = I_\nu$. This can be understood by considering our formal solution to the equation of radiative transfer for a slab of matter in LTE:

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

Since $S_\nu = B_\nu(T)$ is not a function of position s in the slab or τ_ν, it comes out of the integral and we can trivially integrate to get

$$I_\nu(\tau_\nu) = B_\nu(T) + e^{-\tau_\nu}[I_\nu(0) - B_\nu(T)]$$

For small τ_ν (optically thin), the $exp(-\tau_\nu)$ factor is nearly unity, so this gives $I_\nu = I_\nu(0)$. *Thus the radiation is the same as what it was on the far side of the slab, and it is clearly not in thermal equilibrium with the matter.* On the other hand, for large τ_ν (optically thick) the second term goes to zero and we see that the radiation field I_ν simply approaches the Planck function $B_\nu(T)$. Thus as the radiation passes through the matter, it becomes thermalized. In other words *thermal radiation* — for which $S_\nu = B_\nu(T)$ in LTE — becomes *blackbody radiation* — for which $I_\nu = B_\nu(T)$ — only for optically thick media. Or equivalently, full thermal equilibrium (TE) between the matter and the radiation field is achieved only for an optically thick medium.

Equation of Radiative Transfer for a Uniform Medium

Even if we are not in LTE, we have shown that for our simple two-level system we can define an excitation temperature such that

$$S_\nu \equiv \frac{j_\nu}{\kappa_\nu} = B_\nu(T_{\rm exc})$$

We showed this by simply using the relationships between the Einstein coefficients and our definition of excitation temperature. This looks like Kirchoff 's law $S_v = B_v(T)$ (which holds only in LTE), but evaluated at the *excitation temperature* $T_{\rm exc}$, rather than the *kinetic temperature T*. This is not surprising — since the source function S_v encodes the *emission/absorption properties of the matter*, and those properties depend only on the relative population of the *u* and *ℓ* levels of our two-level system, we can always choose to define a suitable temperature $T_{\rm exc}$ with the same relative populations, such that it looks just like we are seeing matter in LTE emitting/absorbing at that temperature. Since Kirchoff 's law tells you that the source function is $S_v = B_v(T)$ for matter in LTE, it thus also tells you how matter with the same relative level populations emits, i.e $S_v = B_v(T_{\rm exc})$. With this, our formal solution to the equation of radiative transfer becomes

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau)'} B_\nu(T_{\rm exc}) \, d\tau'$$

For the case of a uniform slab of material with T_{exc} = constant, we can immediately integrate this equation to obtain

$$I_\nu(\tau_\nu) = B_\nu(T_{\rm exc}) + e^{-\tau_\nu}[I_\nu(0) - B_\nu(T_{\rm exc})]$$

Example: Gunn-Peterson (1965) Effect

Consider radiation emitted at some frequency ν_e that lies blueward of Lyα by a source at redshift z_e, and observed at Earth at frequency $\nu_o = \nu_e/(1+z_e)$. At a redshift z such that $(1+z)\,\nu_o = \nu_\alpha$, the emitted photons will pass through the local Lya resonance as they propagates towards us through an *assumed smoothly* distributed sea of intergalactic neutral hydrogen of proper density $n_{HI}(z)$. They will be scattered *off the line-of-sight* with a cross-section (*neglecting stimulated emission*) of

$$\sigma(\nu) = \frac{\pi e^2}{m_e c} f_{12} \phi(\nu) \qquad \gamma({\rm Ly\alpha}) + {\rm H(1s)} \to {\rm H(2p)} \to {\rm H(1s)} + \gamma({\rm Ly\alpha})$$
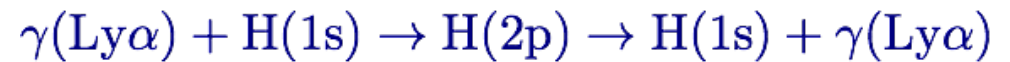
The probability of scattering of a photon in a *proper length interval cdt* at cosmic time t is

$$dP = n_{\rm HI}\,\sigma(\nu)\,cdt$$

The total optical depth for resonant scattering at the observed frequency ν_o is then given by,

$$\tau_{\rm GP} = \int_0^{z_e} dP = \int_0^{z_e} \sigma(\nu) n_{\rm HI}(z) \frac{cdt}{dz} dz$$

radial line element of FRW metric
$$\frac{dt}{dz} = \frac{1}{H(z)(1+z)};$$

$$H(z) = H_0[\Omega_m(1+z)^3 + \Omega_\Lambda]^{1/2}$$
Hubble parameter

The function ϕ_ν is sharply peaked around ν_α. Its width depends on the temperature of the IGM, but at 10^4 K its width is only $\Delta v_D/v_\alpha = c^{-1}\sqrt{2kT/m} = 4e\text{-}5$ (compared to redshift, which is of the order of $1\text{-}6$). We can then write

$$\sigma(\nu) = \frac{\pi e^2}{m_e c} f_{12} \, \delta(\nu - \nu_\alpha)$$

and

$$\tau_{\mathrm{GP}} = \int_0^{z_e} \left\{ \frac{\pi e^2 f_{12}}{m_e c} n_{\mathrm{HI}}(z) \frac{cdt}{dz} \right\} \delta[\nu_0(1+z) - \nu_\alpha] \, dz$$

$$= \int_1^{1+z_e} \left\{ \frac{\pi e^2 f_{12}}{m_e c} n_{\mathrm{HI}}(z) \frac{cdt}{dz} \frac{1}{\nu_0} \right\} \delta[\nu_0(1+z) - \nu_\alpha] \, \nu_0 d(1+z)$$

Thus we can take the factor in braces out of the integral, evaluated at $(1+z) = v_\alpha/v_o$; the integral that is left is unity, and we obtain $[\text{writing } n_{\mathrm{HI}}(z) = n_{\mathrm{H}}(z)x_{1s}(z)]$

$$\tau_{\mathrm{GP}}(z) = \left[\frac{\pi e^2 f_{12}}{m_e \nu_\alpha} \right] n_{\mathrm{H}}(z)x_{1s}(z) \frac{1}{H(z)}$$

The flux will be reduced, from the equation of radiative transfer, by a factor $\exp(-\tau_{GP})$.

Plugging in:

$$(...) = 1.3 \times 10^{-7}\,\mathrm{cm^3 s^{-1}}$$
$$H(z = 2) = H_0[\Omega_m(1+z)^3 + \Omega_\Lambda]^{1/2} = 6.7 \times 10^{-18}\,\mathrm{s^{-1}}$$
$$n_\mathrm{H}(z = 2) = 1.9 \times 10^{-7}(1+z)^3\,\mathrm{cm^{-3}} = 5.1 \times 10^{-6}\,\mathrm{cm^{-3}}$$

$$\Rightarrow \tau_\mathrm{GP}(z = 2) = 10^5\,x_{1s}$$

$x_{1s} = 10^{-3}$ ☞ **99.999%**
ionized ☞ $\tau_{GP} = 100$!

Complications:

$$n_\mathrm{H} \to n_\mathrm{H}\Delta_b$$
$$H(z)/(1+z) \to \frac{dv_\parallel}{dr}$$

= LOS physical velocity gradient at z

In an expanding Universe homogeneously filled with neutral hydrogen, the above equations apply to all parts of the source spectrum to the blue of Lyα. An *absorption trough* should then be detected in the level of the rest-frame UV continuum of the quasar; this is the so-called *Gunn-Peterson effect*.
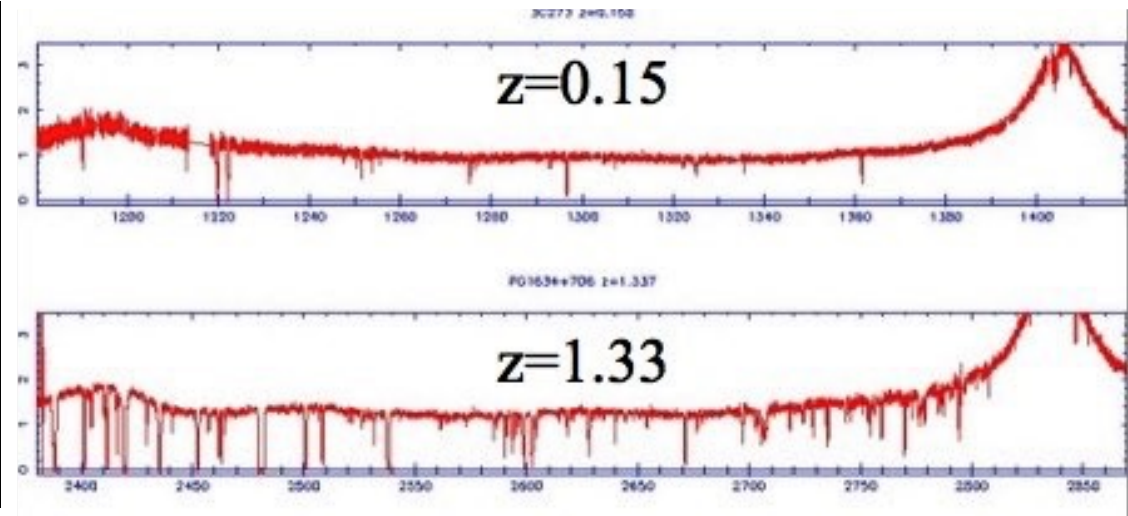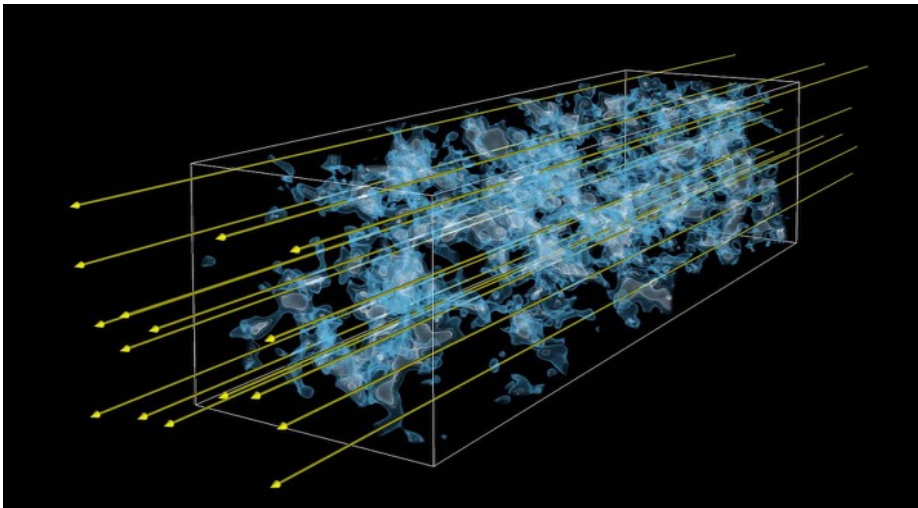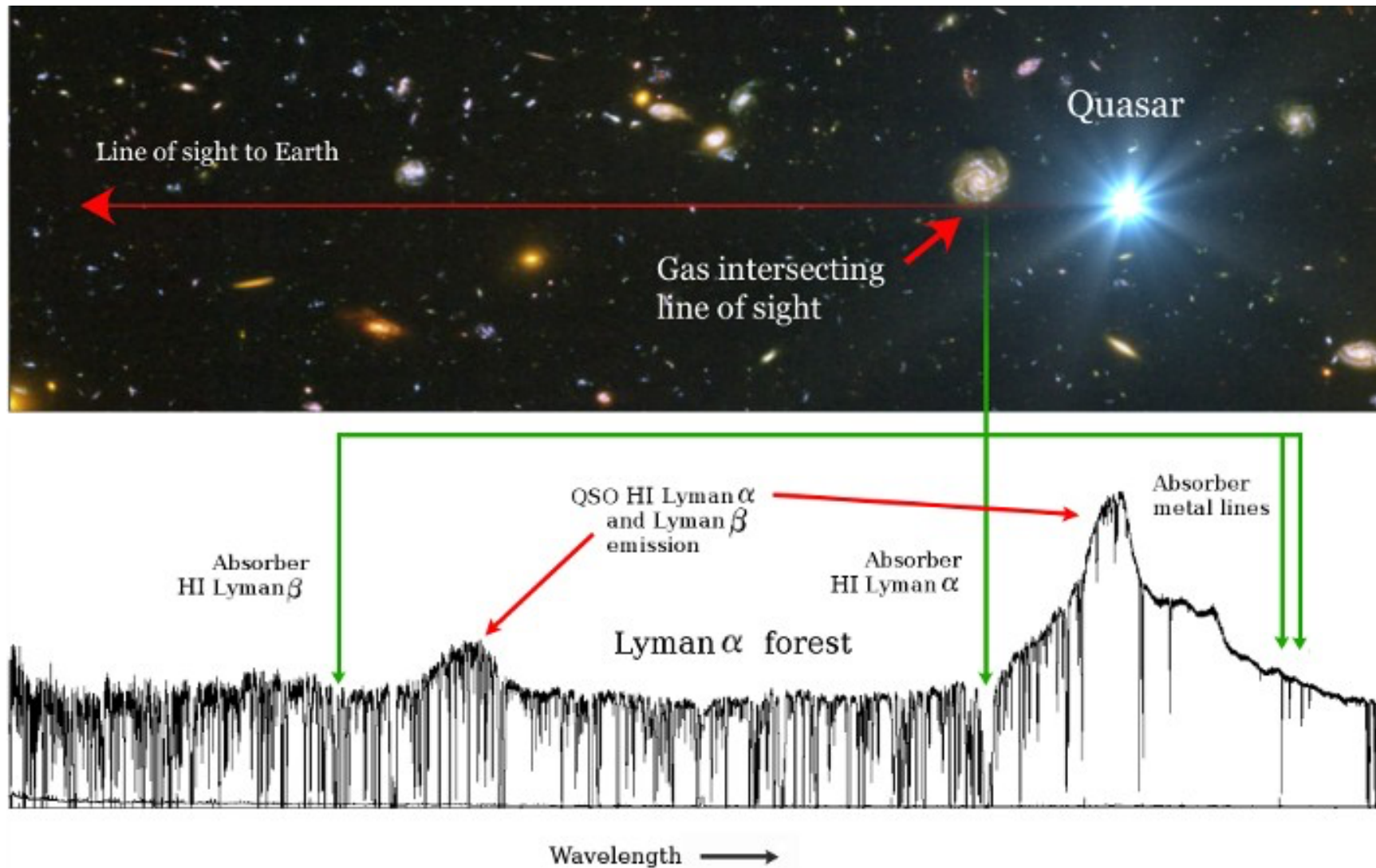
The *Lyman-α forest* is caused by hydrogen absorption. Lyα is the strongest absorption feature from hydrogen atoms. Due to the expansion of the Universe, the wavelength of light from the background quasar is stretched (or redshifted) as it travels towards us. A 'forest' of lines is observed, each at a different redshifted wavelength, each caused by a hydrogen gas cloud in the IGM at a different distance from the Earth. (Credit: N. Creighton)
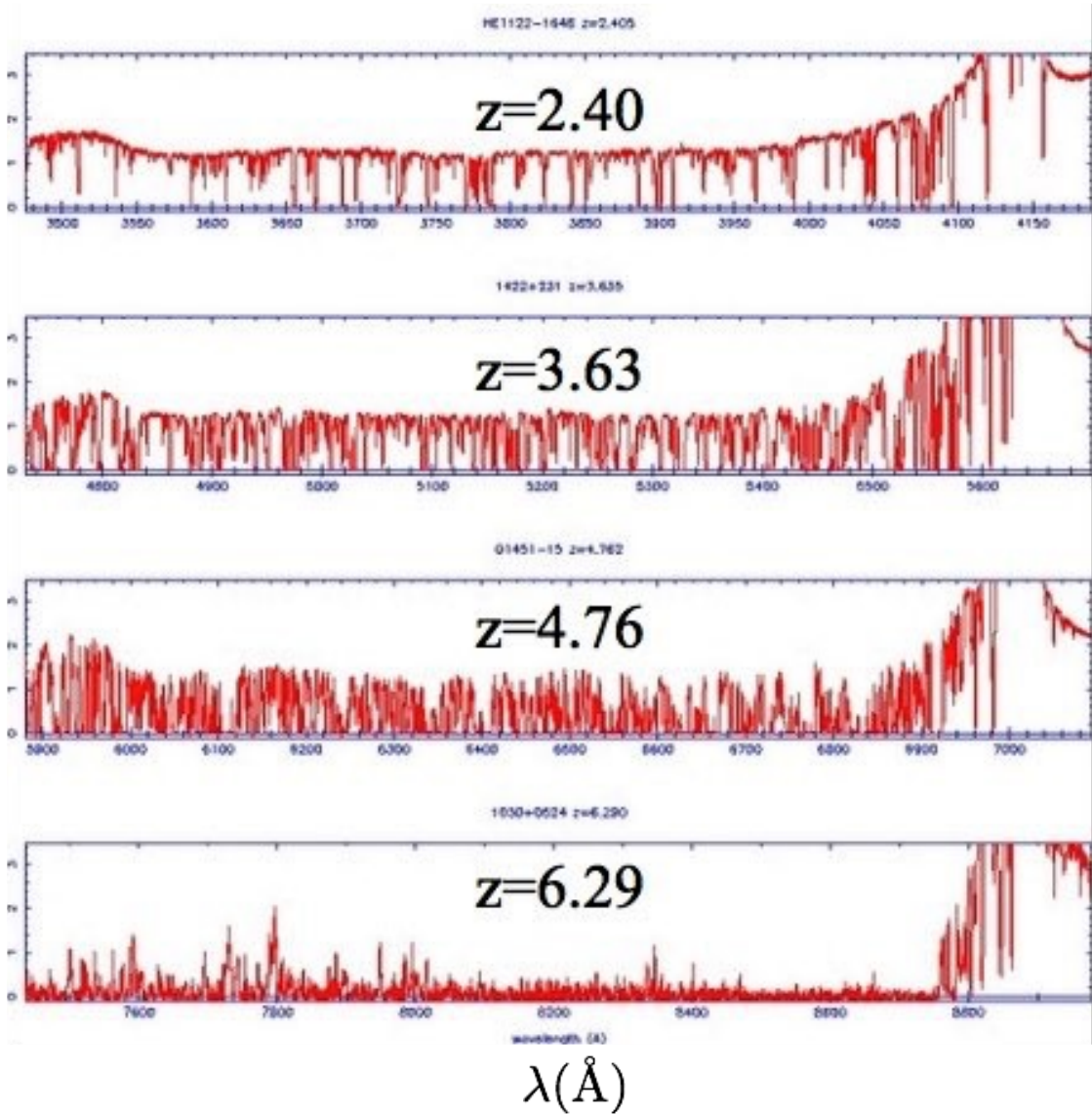
z	$\langle \exp(-\tau) \rangle$
2.75	0.74 ± 0.04
3.00	0.70 ± 0.02
3.89	0.48 ± 0.02
4.00	0.47 ± 0.03
5.00	$0.12^{+0.03}_{-0.04}$
5.50	$0.0.079^{+0.017}_{-0.013}$
6.00	< 0.006

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 $T_{exc} < 0$.*

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

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

If a *population inversion exists*, then the *term in parenthesis is negative*, and the attenuation coefficient is actually a *negative number*. For simplicity, let us consider *matter of negligible emissivity and constant, negative excitation temperature.*

In this case the transfer equation become

$$dI_\nu = -I_\nu \, d\tau_\nu \qquad \Longrightarrow \qquad I_\nu = I_\nu(0)e^{-\tau_\nu}$$

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 amplification 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 $exp(\tau_\nu)$ factor can be very large, and as a result the intensity can be huge. Many different masers occur in astrophysical environments. Amongst the most common are those of the molecules of *hydroxyl* (OH), *water* (H2O), *methanol* (CH3OH) and *silicon monoxide* (SiO). For some astrophysical sources the brightness temperature exceeds 10^{11} K!
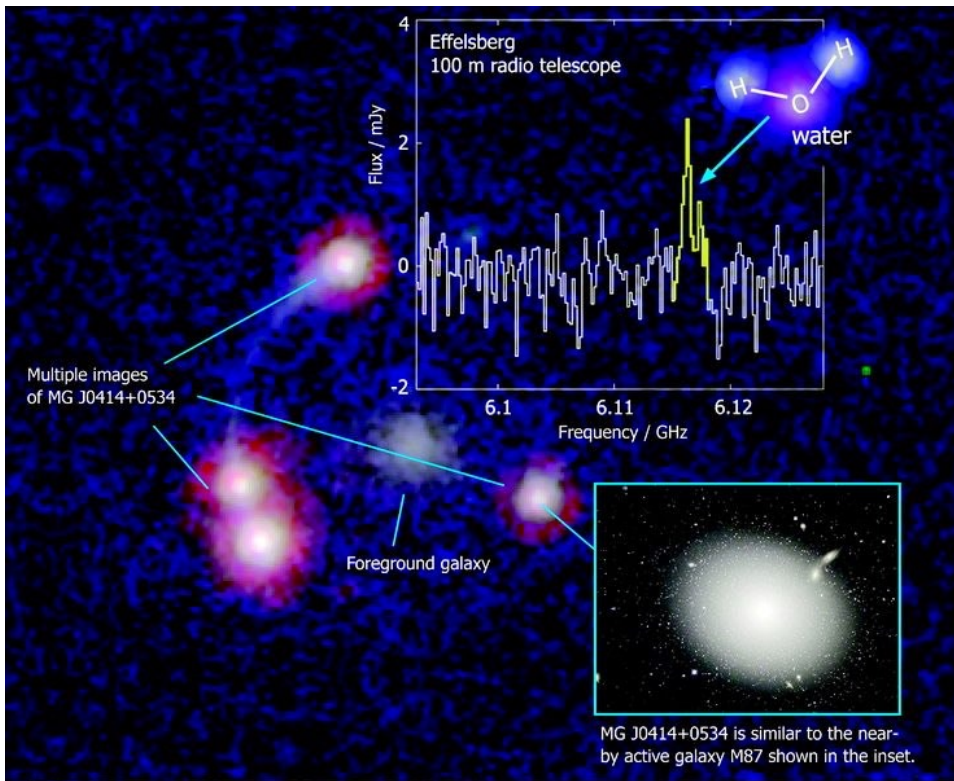
Discovery spectrum, showing water maser emission from the *z=2.64* quasar MG J0414+0534 (inset in an HST colour image of the quasar). The quasar appears broken up into four components by a foreground galaxy (diffuse source in the centre), acting as a *gravitational lens and strengthening the signal by a factor of 35*. The 22.23 GHz *rotational transition* $J_{K_aK_c}$ $6_{16} \rightarrow 5_{23}$ line of ortho-H_2O traces a warm and very dense ISM.

System of the rotational energy levels of ortho-molecule in the ground and first-excited (010) vibrational state. Arrows show the main cycles of the maser pumping in the following cases: Deguchi model (dot-dashed lines), de Jong model (solid lines), two-dust model (dashed lines).