School of Physics

Theory of line scattering and radiative transfer

Jonathan Higgins

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Abstract

Many problems in astrophysics require a quantification of the energy exchange between radiation and matter. This is obtained by formulating and solving an equation of radiative transfer, although how this is done will vary significantly based on the nature of the interactions in the system under investigation. In this pedagogical seminar I will describe some of these interactions with a focus on scattering by resonance lines. I will also describe the formulation of the associated radiative transfer and illustrate the inherent difficulty associated with treating scattering processes compared with e.g. thermal absorption/emission processes.

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1 Introductory theory and principles

This pedagogical seminar is concerned with the theory that describes energy exchange between radiation and matter, 'radiative transfer', particularly in the context of different mechanisms by which the two interact. This inroductory section will introduce much of the formalism and obtain some of the results necessary for what follows. The next section will comprise a detailed discussion of one particular mechanism, scattering by resonance lines, and some details of the associated radiative transfer. Finally, section three will focus on contrasting mechanisms at work in a particular scenario and attempt to draw attention to some of the differences apparent in the way radiative transfer in such an environment unfolds.

1.1 Radiative Transfer



Figure 1: The geometry used in defining the specific intensity of the radiation field

We begin by introducing the fundamental quantitative description of the radiation field, the *specific intensity*. The specific intensity I_{ν} is defined with reference to figure 1 as:

$$dE = I_{\nu}(\mathbf{r}, \mathbf{n}, t) \ dA \ d\omega \ d\nu \ dt \tag{1}$$

i.e. the specific intensity defines the energy dE transferred in time dt by radiation in frequency range $\nu \to \nu + d\nu$, contained in solid angle $d\omega$ about **n**, normal to area dA. We have made explicit the dependence of I_{ν} on position in space, direction and time.

Now consider the transfer of a beam of radiation through some material (see figure 2). The material can be decribed, in general, as a source of *opacity* - the interaction of the radiation with the material will cause some transfer of energy out of the beam. We describe the appropriate energy lost from the beam, which is proportional to both the incident specific intensity and the differential distance travelled through the material, via the *extinction coefficient* χ_{ν} :



Figure 2: Transfer of radiation through some source of opacity and/or emissivity

$$dE = \chi_{\nu} I_{\nu} \ dA \ ds \ d\omega \ d\nu \ dt \tag{2}$$

Similarly we can say that our generalised medium is a source of *emissivity*, interactions that cause the addition of energy to the beam. Such an addition of energy will build up along the path length travelled through the material, and is described via the *emission coefficient*:

$$dE = \eta_{\nu} \, dA \, ds \, d\omega \, d\nu \, dt \tag{3}$$

The emission and extinction coefficients will have forms dictated by the interactions that they represent (perhaps multiple kinds). The effect on the evolution of the specific intensity of radiation through the material can be quantified as follows (see figure 2):

$$[I_{\nu}(\mathbf{r} + \Delta \mathbf{r}, \mathbf{n}, t + \Delta t) - I_{\nu}(\mathbf{r}, \mathbf{n}, t)] dA d\omega d\nu dt = [-\chi_{\nu}I_{\nu}(\mathbf{r}, \mathbf{n}, t) + \eta_{\nu}] ds dA d\omega d\nu dt$$

Taylor expansion of the spatial and time arguments yields, for the left hand side:

$$\left[I_{\nu}(\mathbf{r},\mathbf{n},t) + (\Delta\mathbf{r}.\nabla)I_{\nu}(\mathbf{r},\mathbf{n},t) + \Delta t \frac{\partial}{\partial t}I_{\nu}(\mathbf{r},\mathbf{n},t) - I_{\nu}(\mathbf{r},\mathbf{n},t)\right] \ dA \ d\omega \ d\nu \ dt$$

If we note that $\Delta \mathbf{r} = \mathbf{n} \, ds$ and $\Delta t = ds/c$, we obtain the radiative transfer equation for the specific intensity:

$$\left[\frac{1}{c}\frac{\partial}{\partial t} + \mathbf{n}.\nabla\right] I_{\nu}(\mathbf{r},\mathbf{n},t) = -\chi_{\nu}(\mathbf{r},\mathbf{n},t)I_{\nu}(\mathbf{r},\mathbf{n},t) + \eta_{\nu}(\mathbf{r},\mathbf{n},t)$$
(4)

This is a completely general statement of the evolution of the specific intensity, but in this form it is of little practical use. A straightforward application is the calculation of radiative transfer through a static 1D cloud (1D in that we assume any variation in opacity and emissivity is constrained to lie along a single direction, that which the incident radiation passes along; subsequently the specific intensity will change along this direction only). For such a case we can write $\mathbf{n}.\nabla = d/ds$, the derivative w.r.t. the path-length *s* travelled through the cloud. If we now change variable to the *optical depth* defined such that $d\tau_{\nu} = \chi_{\nu} ds$, and define the *source function* $S_{\nu} \equiv \eta_{\nu}/\chi_{\nu}$, the transfer equation can be written:

$$\frac{dI_{\nu}(\tau_{\nu})}{d\tau_{\nu}} = -I_{\nu}(\tau_{\nu}) + S_{\nu}(\tau_{\nu}) \tag{5}$$

Thus in this simple setup the radiative transfer equation reduces to a first order ordinary differential equation, easily solved to give the solution (assuming a constant source function): $I_{\nu}(\tau_{\nu}) = I_{\nu}(0) e^{-\tau_{\nu}} + [1 - e^{-\tau_{\nu}}] S_{\nu}$. The equation and solution give some physical insight into τ_{ν} and S_{ν} ; the optical depth accumulated along the path of the incident ray will tend to suppress it exponentially, while the integrated source function will boost it in intensity.

Before proceeding we define the angle-averaged specific intensity (sometimes called the mean intensity) as:

$$J_{\nu}(\mathbf{r},t) = \frac{1}{4\pi} \oint I_{\nu}(\mathbf{r},\mathbf{n},t) \ d\omega$$

For an *isotropic* radiation field where I_{ν} is independent of direction, $J_{\nu} = I_{\nu}$. Another important quantity obtained from the specific intensity is the flux \mathbf{F}_{ν} (defined such that $\mathbf{F}_{\nu}.\mathbf{d}S$ is the rate of flow of energy across surface $\mathbf{d}S$), $\mathbf{F}_{\nu}(\mathbf{r}, t) = \oint I_{\nu}(\mathbf{r}, \mathbf{n}, t)\mathbf{n} d\omega$. The mean intensity and radiative flux are respectively the zeroth and first order angular moments of the specific intensity. We can integrate the transfer equation (4) over all solid angle to obtain its zeroth order angular moment:

$$\frac{1}{c}\frac{\partial J_{\nu}}{\partial t} + \frac{1}{4\pi}\nabla \mathbf{F}_{\nu} = -\chi_{\nu}J_{\nu} + \eta_{\nu}$$

where we have assumed the opacity and emissivity to be isotropic, as is often the case in the local rest frame of the material.

1.2 LTE and the thermal source function

Consider an isolated system comprised of a box of some material bathed in radiation. If the system is in thermodynamic equilibrium, the radiation field must be both homogeneous and isotropic (in accordance with the Second Law of Thermodynamics). Under such circumstances, there will be no net transfer of radiation between the radiation field and the material, thus we require:

$$\eta_{\nu} = \chi_{\nu} \ I_{\nu} \tag{6}$$

Also, the radiation is required to adopt a Planck spectrum corresponding to the thermal or kinetic temperature of the matter, T; this ensures that the matter and radiation in some sense have the same 'temperature', as required by thermal equilibrium. Thus $I_{\nu} \to B_{\nu}(T)$ in the equation above and we can describe the matter as having the source function:

$$S_{\nu} = B_{\nu}(T) \equiv \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}$$
(7)

Thermodynamic equilibrium also allows us to assume the Boltzmann distribution; if we take the example of atoms with ≥ 1 excited state(s), the level occupations n_i , n_j of two states of energy E_i , E_j and statistical weights g_i , g_j are given by:

$$\frac{n_i}{n_j} = \left[\frac{g_i}{g_j}\right] \exp\left[-\frac{(E_i - E_j)}{kT}\right] \tag{8}$$

Thus the distribution of atoms across the various excited states is determined simply by the temperature T and the total density $N = \sum_k n_k$. Allowing for the possibility of ionisation, similar determinations can be made for the distribution among states of ionisation using the Boltzmann-derived Saha equation.

If a system is in thermodynamic equilibrium, consideration of radiative transfer is redundant - $I_{\nu} = B_{\nu}$ everywhere - but we might apply the properties outlined above under an assumption of Local Thermodynamic Equilibrium (LTE), amounting to the following:

- Our medium has an inhomogeneous temperature, and we assume that the gradient of this temperature is sufficiently small that thermal equilibrium is in place locally at position \mathbf{r} with temperature $T(\mathbf{r})$ and density $N(\mathbf{r})$. The medium locally adopts all the properties associated with such a state.
- We are assuming thermal equilibrium of the matter only; the radiation spectrum need not be equal to the Planck spectrum and the radiative transfer equation remains to be solved.

To solve the radiative transfer problem we need to know the opacity and emissivity; these are in general determined by level populations, ionisation information etc. (the 'state' of the medium) which are in turn determined by equations of statistical equilibrium which generally involve the influence of the radiation field (see Mihalas [1978] ch. 5). Assuming LTE bypasses the process of solving the statistical equilibrium equations with the radiative transfer equation; the level populations are simply given by (8) and $\eta_{\nu} = \chi_{\nu} B_{\nu} \implies S_{\nu} = B_{\nu}$.

1.3 Bound-bound transitions in the 2-level atom



Figure 3: Radiative transitions in a 2-level atom; levels labelled 1 (ground state) and 2 (excited state), $(E_2 - E_1) = h\nu_0$

Consider the atomic energy level diagram shown in figure 3. The arrows correspond to 3 distinct kinds of radiative transition; these are, along with their corresponding *Einstein coefficients*:

• Spontaneous emission: a photon of frequency $\nu = \nu_0$ is emitted upon the radiative decay of the atom from state 2 to state 1. This process is characterised by the Einstein A coefficient, defined such that:

 $A_{21} \equiv$ transition rate for spontaneous emission

• Absorption: a photon of frequency $\nu = \nu_0$ is absorbed to excite the atom from state 1 to state 2. Characterised by the upwards Einstein B coefficient, defined such that:

 $B_{12}J_{\nu_0} \equiv \text{transition rate for absorption}$

• Stimulated emission: a photon of frequency $\nu = \nu_0$ is emitted upon the de-excitation of the atom from state 2 to state 1, induced by an interaction with an identical photon. This process is characterised by the downwards Einstein B coefficient, defined such that:

 $B_{21}J_{\nu_0} \equiv$ transition rate for stimulated emission

The Einstein coefficients A_{21} , B_{12} and B_{21} are properties of the transition between the 2 levels; they can be calculated using the relations derived below together with a semi-classical approach that treats a classical radiation field as a quantum mechanical perturbation to the states of the atom, see e.g. Rybicki and Lightman [1986] ch. 10.

At this stage we note that an assumption of thermodynamic equilibrium will allow us to derive relations between the Einstein coefficients. First we use the principle of *detailed balance*, that the net rate of upwards transitions from 1 to 2 is equal to the net rate of downwards transitions from 2 to 1, or:

$$n_1 B_{12} J_{\nu_0} = n_2 [A_{21} + B_{21} J_{\nu_0}] \tag{9}$$

We can also use that the level populations are given by the Boltzmann distribution (8); $n_2/n_1 = (g_2/g_1) \exp(-h\nu_0/kT)$, while the radiation field adopts the Planck spectrum and we can say $J_{\nu_0} = B_{\nu_0}(T)$. Together these statements allow us to show (without loss of generality, as the coefficients are intrinsic properties of the atomic transition):

$$B_{21} = \left[\frac{g_1}{g_2}\right] B_{12} \tag{10}$$

$$A_{21} = \frac{2h\nu_0^3}{c^2} B_{21} \tag{11}$$

These relations are of great importance; clearly the strength of radiative transitions in an atom can be characterised by a single quantity (i.e. any of the 3 Einstein coefficients or the more physically meaningful and dimensionless 'oscillator strength', see Rybicki and Lightman [1986]). Before moving on, we note that collisional transitions between the 2 atomic states in figure 3 are also possible; we can have collisional excitation, when the excitation energy is transferred to the atom by a collision with some other particle, and collisional de-excitation (the reverse process). Say that collisional excitations and de-excitations are described by the transition rates C_{12} and C_{21} respectively; detailed balance applied to the 2-level atom in the presence of some species of colliders of density n_c gives:

$$n_1 C_{12} = n_2 [C_{21} + A_{21}] \implies n_1 n_c \kappa_{12} = n_2 [n_c \kappa_{21} + A_{21}]$$
(12)

where we have assumed no radiation field is present, although spontaneous emission still occurs. We have implemented the definition $C_{ij} \equiv n_c \kappa_{ij}$; clearly the rate of collisions will be proportional to the density of colliders n_c , and so in defining the κ -coefficients we are simply factoring out this dependence. We can then choose n_c sufficiently high that collisional de-excitation happens much faster than radiative; we neglect the A-coefficient contribution and write:

$$C_{12} = \frac{n_2}{n_1} C_{21} = \left[\frac{g_2}{g_1} e^{-h\nu_0/kT}\right] C_{21}$$
(13)

As $C_{12}/C_{21} = \kappa_{12}/\kappa_{21}$ and the κ 's are properties of the atom (at fixed temperature), this relation holds true in general. Note that in this scenario the level populations obey the Boltzmann distribution; this can be interpreted as a by-product of the utility of collisions in ensuring LTE in high density situations.

2 Resonance Line Scattering

Resonance line scattering is a process that can be understood in the context of the 2-level atom model described in the previous section:



Figure 4: Sketch of scattering geometry

- A photon of frequency ν' travelling in direction \mathbf{n}' comes into contact with an atom of resonance frequency ν_0 , moving with a thermal velocity \mathbf{v} ; the photon causes radiative excitation of the atom i.e. promotes an electron from $1 \rightarrow 2$.
- The atom decays back to the initial state $(2 \rightarrow 1)$, emitting a photon of frequency ν in direction **n**; generally we will have $\mathbf{n} \neq \mathbf{n}'$ and thus $\nu \neq \nu'$ (due to Doppler shifting at the very least, see equation (23) later).

2.1 Photon redistribution

To describe radiative transfer of resonance line scattering we use the *redistribution function* $R(\nu', \mathbf{n}'; \nu, \mathbf{n})$, defined (in accordance with the conventions of Mihalas, see Mihalas [1978] ch. 13) such that the probability of scattering of a photon from frequency $\nu' \rightarrow \nu' + d\nu'$ and direction within solid angle $d\omega'$ about \mathbf{n}' to frequency $\nu \rightarrow \nu + d\nu$ and direction within solid angle $d\omega$ about \mathbf{n} is given by:

$$R(\nu', \mathbf{n}'; \nu, \mathbf{n}) \ d\nu' \ d\nu \ \frac{d\omega'}{4\pi} \ \frac{d\omega}{4\pi}$$
(14)

This function is normalised such that integration over all 4 variables (incoming direction and frequency, outgoing direction and frequency) gives unity. An extremely useful quantity that we can derive from the redistribution function is the *line absorption profile* $\varphi(\nu')$;

$$\varphi(\nu') = \frac{1}{4\pi} \oint d\omega \int_0^\infty d\nu \ R(\nu', \mathbf{n}'; \nu, \mathbf{n})$$
(15)

This acts a probability distribution function for the frequency at which the photon is absorbed; from the interpretation of the redistribution function, we can say that $\varphi(\nu') d\nu'$ is the probability of scattering from $\nu' \to \nu' + d\nu'$ to any other frequency (equivalently interpreted as the probability of absorption). Note that the line profile is normalised as follows: $\int_0^\infty \varphi(\nu) d\nu = 1$.

2.2 Physics of line absorption and scattering

For a resonance line centred on some frequency ν_0 , a first approximation to the line profile is provided by a delta function at the resonant frequency, $\varphi(\nu) = \delta(\nu - \nu_0)$; no photons are absorbed other than those with exactly the right frequency to excite the relevant atomic transition. However, in attempts to solve the transfer equation for line absorption/emission/scattering, it is usually necessary to consider a 'broadened' line profile, with a non-zero probability for absorption in some narrow region about ν_0 . There are several physical effects responsible for line broadening; we describe 2 such mechanisms below that are commonly applicable.

Natural broadening: Consider an isolated 2-level atom in its rest frame, with an excited state of finite lifetime τ and corresponding decay rate $\Gamma = \tau^{-1}$; $\Gamma = A_{21}$ as introduced in section 1.3. The uncertainty principle tells us that the excited state has a finite energy width $\Delta E \approx \hbar \Gamma$ - note that the ground state is assumed to have an infinite lifetime and therefore zero line width. An outline quantum mechanical justification for the shape of the naturally-broadened profile is given by Mihalas; the wavefunction of the excited state has time dependence $\sim \exp\left[-(i\omega_0 + \Gamma/2)t\right]$, with the $\exp\left[-(\Gamma/2)t\right]$ factor required by noting the corresponding probability of finding the atom in the excited state decays as $\exp\left(-\Gamma t\right)$. The probability distribution for the energy of the excited state is given by the modulus of the Fourier transform of the wavefunction, thus we can obtain the absorption line profile as follows:

$$P(\omega) \propto \left| \int_0^\infty e^{[i(\omega - \omega_0) - \Gamma/2]t} dt \right|^2 = [(\omega - \omega_0)^2 + (\Gamma/2)^2]^{-1}$$

$$\implies \varphi(\nu) = \frac{\Gamma}{4\pi^2} \left[\frac{1}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \right] \tag{16}$$

i.e. the line shape adopts a *Lorentz profile*, analogous to the scattering cross-section of a damped classical harmonic oscillator with damping constant Γ .

Doppler broadening: In typical astrophysical situations we have to deal with a further contribution to the line broadening arising when we consider the absorption profile of an ensemble of atoms with a Maxwellian thermal velocity distribution. Consider an atom seen to have thermal velocity component v_r along the line of sight from the observer; if the observer then sends a photon of frequency ν towards the atom, the atom (in its rest frame) will see the photon at frequency $\nu(1-v_r/c) \approx \nu - \nu_0(v_r/c)$. The resulting absorption profile then becomes a convolution of the rest-frame profile (which we denote $\varphi^{RF}(\nu)$) and the Maxwellian distribution of the thermal velocity component along the line of sight, for atoms of mass m at temperature T:

$$\varphi(\nu) = \int_{-\infty}^{\infty} \varphi^{RF} [\nu - (\nu_0/c)v_r] \ p(v_r) \ dv_r, \quad p(v_r) = \left[\frac{m}{2\pi kT}\right]^{1/2} e^{-mv_r^2/2kT}$$
(17)

In the case of an infinitely sharp excited state with resonant frequency ν_0 , the convolution yields a *Doppler profile*, a Gaussian centred on ν_0 :

$$\varphi(\nu) = \int_{-\infty}^{\infty} \delta[\nu - (\nu_0/c)v_r - \nu_0] p(v_r) dv_r$$
$$= \frac{c}{\nu_0} \times \left[\frac{m}{2\pi kT}\right]^{1/2} e^{-\frac{mc^2(\nu - \nu_0)^2}{2\nu_0^2 kT}}$$
(18)

At this stage a particularly useful change of variables becomes apparent; if we define the typical thermal velocity or equivalently the 'b parameter' $b \equiv (2kT/m)^{1/2}$, we see that we can write the width of the Doppler profile as $\Delta \nu_D = \nu_0 (b/c)$, defined such that the exponential in (18) becomes $\exp[-(\nu - \nu_0)^2/(\Delta \nu_D)^2]$. We now introduce the variable $x \equiv (\nu - \nu_0)/\Delta \nu_D$, the frequency offset from line centre in Doppler widths. We write the line absorption profile as a function of x, $\phi(x) = \varphi(\nu) \times \Delta \nu_D$, in the case of both the Doppler profile and the Lorentz profile:

(18)
$$\implies \phi_D(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}$$
 (19)

(16)
$$\implies \phi_L(x) = \frac{a}{\pi} \left[\frac{1}{a^2 + x^2} \right]$$
 (20)

where in the second equation we introduce the 'Voigt parameter' $a = \Gamma/(4\pi\Delta\nu_D)$, which gives a rough indication of the strength of natural broadening relative to Doppler broadening.

While it is useful to study both natural broadening and Doppler broadening in isolation, the most useful results come from studying the more applicable case of a naturally-broadened line profile that then undergoes Doppler broadening. Taking the Lorentz profile in equation (16) as the rest-frame profile $\varphi^{RF}(\nu)$ in equation (17), adopting the integration variable $y = v_r/b$, and finally taking x as the frequency variable, we obtain:

$$\phi(x) = \pi^{-1/2} H(a, x), \quad H(a, x) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{a^2 + (x - y)^2} dy \tag{21}$$

This form for the absorption line profile is called the *Voigt profile* (while H(a, x) is known as the Voigt function) and is plotted in figure 5, along with the Lorentz and Doppler profiles, for a Voigt parameter a = 0.015.



Figure 5: (Left) The normalised absorption line profiles with Voigt parameter a = 0.015; Voigt (solid line), Doppler (dashed line) and Lorentz (dot-dashed). (Right) Zoomed-in view to display behaviour in the wings

Clearly the Voigt profile resembles the Doppler profile near line centre (x = 0) and at large |x| begins to resemble the Lorentz profile. We describe the line as having a 'Doppler core' and 'Lorentz wings'; the prominence of the wings relative to the core will increase with larger a.

Before leaving the physics of the absorption profile behind, we note that other forms of line broadening are available, most notably collisional broadening which will dominate in very highdensity scattering media. See Mihalas ch. 9 for a detailed discussion of collisional broadening.

It makes sense to now try looking at extending our study of line absorption to line scattering. As mentioned previously, line scattering involves photon absorption followed by photon emission; a good starting point is to consider absorption and re-emission of a photon in the rest frame of the scattering atom. We can write the redistribution function for scattering in the rest frame as follows:

$$R^{RF}(\xi', \mathbf{n}'; \xi, \mathbf{n}) = \varphi^{RF}(\xi') \times p^{RF}(\xi|\xi') \times g(\mathbf{n}', \mathbf{n})$$
(22)

where we have used ξ to represent rest frame photon frequencies; the function $p^{RF}(\xi|\xi')$ acts as a conditional probability distribution function for the emission frequency ξ given absorption at frequency ξ' , while $g(\mathbf{n}', \mathbf{n})$ describes the directional redistribution. We can deduce the forms that these functions will take by interpreting a broadened excited state in terms of 'substates': the excited state (e.g. state 2 of the 2-level atom) is comprised of a continuum of substates, the probability density distribution of which in frequency space determines a range of frequencies at which a photon can be absorbed and is thus given by the line absorption profile. Now consider the form of the factorised redistribution function in the rest frame (we assume our atom to be excited from the ground state, and neglect collisional broadening):

- The upper level has finite width thus the absorption function (and therefore the substate distribution about the resonant frequency) adopts a Lorentz profile $\varphi(\xi') = (\Gamma/4\pi^2)[(\xi' \nu_0)^2 + (\Gamma/4\pi)^2]^{-1}$ (note: we do not use the Voigt profile as we are in the rest frame and have no thermal atomic velocities to average over).
- The atom absorbs at frequency ξ' ; thus the atom is excited to the substate of energy $h\xi'$. Upon return from this substate to the ground state a photon of frequency ξ is emitted, but as the ground state has fixed energy we know $\xi = \xi'$. Thus $p(\xi|\xi') = \delta(\xi - \xi')$.
- The function $g(\mathbf{n}', \mathbf{n})$ should really be written $g(\mathbf{n}'.\mathbf{n})$, as it is invariably a function of the angle between the 2 directions only; the form of the functional dependence is determined by the quantum numbers involved in the transition, but it is usual to assume isotropic scattering $(g(\mathbf{n}'.\mathbf{n}) = 1)$.

The single-atom redistribution function in the laboratory frame is then obtained by applying the following Doppler shifts to equation (22):

$$\nu' = \xi' + \nu_0 \left[\frac{\mathbf{v} \cdot \mathbf{n}'}{c} \right], \quad \nu = \xi + \nu_0 \left[\frac{\mathbf{v} \cdot \mathbf{n}}{c} \right]$$
(23)

where \mathbf{v} is the velocity of the atom in the lab frame due to thermal motions. Note that while the frequencies are transformed between the 2 frames, aberration of the photon direction vectors can be neglected. To obtain a redistribution function that will be applicable to a population of atoms it is then necessary to average over the Maxwellian thermal velocity distribution for \mathbf{v} . The result, written in terms of Doppler shifts from line centre x where $R(x', \mathbf{n}'; x, \mathbf{n}) = R(\nu', \mathbf{n}'; \nu, \mathbf{n}) \times (\Delta \nu_D)^2$, is:

$$R(x', \mathbf{n}'; x, \mathbf{n}) = \frac{g(\mathbf{n}', \mathbf{n})}{\pi \sin \theta} \exp\left[-\left(\frac{x' - x}{2}\right)^2 \csc^2(\theta/2)\right] \times H\left(a \sec(\theta/2), \frac{1}{2}(x' + x) \sec(\theta/2)\right)$$
(24)

where θ is the angle between the photon directions (see figure 4) and H is the Voigt function defined in (21). From this form we obtain the angle-averaged redistribution function $R(x', x) = \frac{1}{4\pi} \oint d\omega R(x', \mathbf{n}'; x, \mathbf{n})$:

$$R(x',x) = \frac{1}{\pi^{3/2}} \int_{(\bar{x}-\underline{x})/2}^{\infty} \left[\tan^{-1} \left(\frac{\underline{x}+u}{a} \right) - \tan^{-1} \left(\frac{\bar{x}-u}{a} \right) \right] e^{-u^2} du$$
(25)

where $\bar{x} = \max(x, x')$ and $\underline{x} = \min(x, x')$. Integration over all emitted frequencies will recover the absorption profile, $\phi(x') = \int_0^\infty R(x', x) \, dx$. Both forms of the redistribution function stated here describe what is referred to in the literature as 'Type II' redistribution; this label refers to the conditions under which the functions are applicable, namely the atom in the rest frame is excited from the ground state to some naturally broadened upper state with no collisional broadening. This is common in many astrophysical scattering problems, e.g. H I Ly α scattering in low-density media. It is worth noting that Type I redistribution is the limit of Type II when the upper state has zero energy width, something that does not occur in nature. There also exist types III and IV which correspond to redistribution with collisional broadening of the upper state (important in high density media), and natural broadening of both the upper and lower state (important if the transition occurs between 2 excited states) respectively. An indepth discussion of the various redistribution functions is provided by Hummer [Hummer, 1962] and Mihalas ch. 13 [Mihalas, 1978].

It is worthwhile to look at the conditional probability that a photon absorbed at x' will be re-emitted at x; this is obtained from the redistribution function by appropriate normalisation, $p(x|x') = R(x', x)/\phi(x')$. This function is plotted in figure 6 for a series of values of x'.



Figure 6: $p(x|x') = R(x',x)/\phi(x')$ for x' = 0, 1, 2, 3, 4, 5 (in order of peak value from left to right) with a = 0.015

Finally for this section, we quote approximate forms of the redistribution function intended to model some simple scattering scenarios:

Coherent redistribution: The photon is absorbed at lab frame frequency shift x' and reemitted at x = x'; we represent this via the angle-averaged redistribution function

$$R(x', x) = \phi(x') \ \delta(x' - x) = \phi(x) \ \delta(x' - x)$$
(26)

Complete redistribution: The photon is absorbed at x' and re-emitted at frequency shift x, entirely uncorrelated with x':

$$R(x', x) = \phi(x') \ \phi(x) \tag{27}$$

Complete and coherent redistribution describe Type-II redistribution fairly well for absorption in the core and the wings of the line respectively. Photons absorbed in the wings (typically only possible for large *a*) scatter in a roughly coherent manner, while photons absorbed in the core $(|x'| \leq x_c \approx 2.6 \text{ for } a = 0.015 \text{ - boundary at } x_c \text{ determined by solution to } \phi_D(x_c) = \phi_L(x_c))$ undergo a random frequency reshuffling.

2.3 The line source function

We want a general expression for the source function to use in a calculation of the radiative transfer accounting for resonance line scattering - we assume isotropy of the radiation field. Here we begin by writing expressions for the extinction and emission coefficients:

$$\chi_{\nu} = \left[n_1 B_{12} \varphi(\nu) - n_2 B_{21} \psi(\nu) \right] \frac{h\nu_0}{4\pi}$$
(28)

$$\eta_{\nu} = n_2 A_{21} \psi(\nu) \; \frac{h\nu_0}{4\pi} \tag{29}$$

These equations follow from definitions of the Einstein coefficients in terms of transition rates, given in section 1.3, or at least a more robust version accounting for the spread in frequency space of the excited state. Consider that atoms in state 1 will absorb photons with a frequency distribution $\varphi(\nu)$, thus the transition rate for absorption becomes $B_{12}J_{\nu} \varphi(\nu)d\nu$. The rates for spontaneous emission and stimulated emission will become $A_{21} \psi(\nu)d\nu$ and $B_{21}J_{\nu} \psi(\nu)d\nu$; note that we have introduced an emission profile $\psi(\nu) \ (\neq \varphi(\nu)$ in general).

The emission profile profile describes the distribution in frequency of the occupancy of the excited state, i.e. the total excited state occupancy n_2 becomes a distribution $n_2(\nu) = n_2\psi(\nu)$. $n_2(\nu)$ is formally determined from the equation of statistical equilibrium for the excited state; we do not discuss the relevant equation here, but we note that it must account for the possibility of resonant scattering causing redistribution from ν' to ν for frequencies in the upper state. We can attain a form for $\psi(\nu)$ by a physical argument for the form of the emission coefficient (we ignore stimulated emission):

- The energy removed from a beam of mean intensity $J_{\nu'}$ at frequency ν' is proportional to $\chi_{\nu'}J_{\nu'} d\nu'$, where $\chi_{\nu'} = \chi_l \varphi(\nu')$ is the extinction coefficient and $\chi_l = n_1 B_{12} h \nu_0 / (4\pi)$. Let's call this energy $E(\nu') d\nu'$.
- The energy of photons from this frequency ν' subsequently scattered to frequency ν is given by the previous quantity multiplied by the conditional probability $p(\nu|\nu') = R(\nu',\nu)/\varphi(\nu')$. Let's call this quantity $E(\nu',\nu)$.
- The total energy of photons scattered to frequency ν is given by integrating the previous quantity over all ν' . Let's call this quantity $E(\nu)$; it's given by:

$$E(\nu) = \int d\nu' \ E(\nu', \nu)$$

= $\int d\nu' \ E(\nu') \times \frac{R(\nu', \nu)}{\varphi(\nu')}$
 $\propto \int d\nu' \ \chi_l \varphi(\nu') J_{\nu'} \times \frac{R(\nu', \nu)}{\varphi(\nu')}$

• The quantity $E(\nu)$ is proportional to the emissivity. The proportionalities are such that we can write:

$$\eta_{\nu} = \chi_l \int R(\nu', \nu) J_{\nu'} \, d\nu$$

We can see that the emissivity has a non-trivial frequency dependence; it is in fact dependent upon the radiation field across the entire resonance line, not just at the frequency in question. If we now return to the expression (29), consistency with our physical argument along with the normalisation condition $\int \psi(\nu) d\nu = 1$ requires that we say:

$$\psi(\nu) = (\bar{J})^{-1} \int R(\nu', \nu) J_{\nu'} \, d\nu', \quad \bar{J} = \int \varphi(\nu) J_{\nu} \, d\nu \tag{30}$$

We can write the equation of radiative transfer analogous to equation (4) for a homogeneous, isotropic medium giving rise to resonance line scattering as:

$$\frac{1}{c}\frac{\partial J_{\nu}}{\partial t} = \chi_l \left[-\varphi(\nu)J_{\nu} + \int R(\nu',\nu)J_{\nu'} \, d\nu' \right]$$
(31)

Finally, we quote the general result for the source function arising from resonance line scattering, using the equations (28) and (29):

$$S_{l} = \frac{n_{2}A_{21}\psi(\nu)}{n_{1}B_{12}\varphi(\nu) - n_{2}B_{21}\psi(\nu)} = \frac{2h\nu_{0}^{3}}{c^{2}} \left[\frac{n_{1}g_{2}\varphi(\nu)}{n_{2}g_{1}\psi(\nu)} - 1\right]^{-1}$$
(32)

where, as we are including stimulated emission, we must use the full form of $\psi(\nu)$ determined from statistical equilibrium of the excited state, i.e. not equation (30). Note that upon the reinclusion of stimulated emission the transfer equation as written in (31) is still accurate (more specifically the RHS ($\eta_{\nu} - \chi_{\nu} J_{\nu}$) is unchanged).

3 Radiative transfer in a 'stellar atmosphere'

In this section we return to the general radiative transfer equation (4) and adapt it to formulate and attempt to solve time-independent radiative transfer in a particular geometry, for different varieties of opacity and emissivity. This geometry is a standard application of the time-independent radiative transfer equation; the *plane parallel semi-infinite atmosphere*, often used to approximate the atmosphere of a star.

All properties of the atmosphere become functions of the height z and the angle from the normal, $\theta = \cos^{-1} \mu$ (isotropic quantities will then become functions of z only). The optical depth scale is defined by $d\tau_{\nu} = -\chi_{\nu} dz$; the minus sign ensures that the optical depth increases into the atmosphere. Now we write the appropriate time-independent transfer equation:

$$(\mathbf{n}.\nabla)I_{\nu} = \frac{\partial}{\partial s}I_{\nu} = \mu \frac{\partial I_{\nu}}{\partial z} = -\chi_{\nu}\mu \frac{\partial I_{\nu}}{\partial \tau_{\nu}}$$
$$\implies \mu \frac{\partial I_{\nu}}{\partial \tau_{\nu}} = I_{\nu} - S_{\nu}$$
(33)



Figure 7: Geometry of plane-parallel semi-infinite atmosphere; the optical depth is taken to be zero at the boundary (z = 0) and increases without limit for decreasing z

where $I_{\nu} = I_{\nu}(\tau_{\nu}, \mu)$ and $S_{\nu} \equiv \eta_{\nu}/\chi_{\nu} = S_{\nu}(\tau_{\nu})$. This equation can be integrated after multiplication by an appropriate integrating factor; if we integrate from τ_1 to τ_2 , we obtain:

$$I_{\nu}(\tau_1,\mu) = I_{\nu}(\tau_2,\mu)e^{-(\tau_2-\tau_1)/\mu} + \frac{1}{\mu}\int_{\tau_1}^{\tau_2} S_{\nu}(\tau)e^{-(\tau-\tau_1)/\mu} d\tau$$
(34)

This solution offers a complete understanding of the problem if we know the source function S_{ν} , along with any suitable boundary conditions. Now consider the problem of determining the mean (angle-averaged) intensity at a depth τ_{ν} within the atmosphere; we want to determine the intensity at τ_{ν} as a function of μ and integrate over solid angle. We divide the intensity at the depth of interest into that which builds up from the stellar surface ('incoming' radiation) and that which builds up from infinite depth ('outgoing' radiation):

• Incoming $(\pi \ge \theta \ge \pi/2)$: $I_{\nu}(0,\mu) = 0$ for $\mu \le 0$; the intensity entering the atmosphere at the surface is zero. There are no sources capable of producing such radiation, the only radiation at the surface will be exiting it with $\mu \ge 0$. Thus, the solution (34) for incoming radiation will be given by (integrate from $\tau = 0$ to $\tau = \tau_{\nu}$):

$$I_{\nu}(\tau_{\nu},\mu) = \frac{1}{-\mu} \int_{0}^{\tau_{\nu}} S_{\nu}(\tau) e^{-(\tau-\tau_{\nu})/\mu} d\tau, \quad -1 \le \mu \le 0$$

• Outgoing $(\pi/2 \ge \theta \ge 0)$: $\lim_{\tau_{\nu}\to\infty} [I_{\nu}(\tau_{\nu},\mu)e^{-\tau_{\nu}/\mu}] = 0$ for $\mu \ge 0$; a beam of radiation from infinite optical depth that encounters no source, only sinks (opacity), will be killed off completely. The solution from (34) for outgoing radiation will then be given by (integrate from $\tau = \infty$ to $\tau = \tau_{\nu}$):

$$I_{\nu}(\tau_{\nu},\mu) = \frac{1}{\mu} \int_{\tau_{\nu}}^{\infty} S_{\nu}(\tau) e^{-(\tau-\tau_{\nu})/\mu} d\tau, \quad 0 \le \mu \le 1$$

We now integrate from $-1 \le \mu \le 1$ to obtain the mean intensity at optical depth τ_{ν} as:

$$J_{\nu}(\tau_{\nu}) = \frac{1}{2} \int_{-1}^{1} I_{\nu}(\tau_{\nu},\mu) d\mu$$

$$= \frac{1}{2} \left[\int_{-1}^{0} d\mu \int_{0}^{\tau_{\nu}} S_{\nu}(\tau) e^{-(\tau_{\nu}-\tau)/(-\mu)} \frac{d\tau}{(-\mu)} + \int_{0}^{1} d\mu \int_{\tau_{\nu}}^{\infty} S_{\nu}(\tau) e^{-(\tau-\tau_{\nu})/\mu} \frac{d\tau}{\mu} \right]$$

$$= \frac{1}{2} \left[\int_{0}^{\tau_{\nu}} d\tau S_{\nu}(\tau) \int_{1}^{\infty} w^{-1} e^{-(\tau_{\nu}-\tau)w} dw + \int_{\tau_{\nu}}^{\infty} d\tau S_{\nu}(\tau) \int_{1}^{\infty} w^{-1} e^{-(\tau-\tau_{\nu})w} dw \right]$$

$$= \frac{1}{2} \int_{0}^{\infty} d\tau S_{\nu}(\tau) E_{1}(|\tau-\tau_{\nu}|), \quad E_{n}(x) = \int_{1}^{\infty} t^{-n} e^{-xt} dt \qquad (35)$$

where the change of variables $w = 1/|\mu|$ has been made in going from the second line to the third line. This equation was derived by Schwarzschild (see Menzel [1967]) and is often called the 'Schwarzschild-Milne equation', while the E_1 function is one of a set of functions $\{E_n\}$ known as 'exponential integrals'. Many similar expressions exist for the moments of the radiation field such as the flux in terms of integration over higher-order exponential integrals. Using such expressions, it can be shown that we should expect $J_{\nu}(\tau_{\nu}) \to S_{\nu}(\tau_{\nu})$ for $\tau_{\nu} \to \infty$ (see Mihalas [1978] ch. 2 for details).

3.1 Thermal absorption/emission vs scattering

We can divide the many different mechanisms by which radiation and matter interact into those that allow a net exchange of radiant / photon energy and the thermal / kinetic energy of the particles comprising the transferring medium, and those that do not. The former can be described as 'true' absorption (emission) processes as they involve the destruction (creation) of a photon such that it's energy is added to (extracted from) the medium's pool of thermal energy; an example would be the absorption of a photon by an atom which subsequently decays by collisional de-excitation, transferring its excitation energy to kinetic energy distributed among the particles. The other case in which photons are conserved describes scattering processes e.g. resonance line scattering, see section 2.

For interaction processes between radiation and matter that come under true absorption and/or emission, the medium actively exchanges energy with the radiation field such that the radiation field will locally become *coupled*, to some extent, to the properties of the medium. For such processes the assumption of LTE is often a good approximation and we take our source function to be equal to the Planck function $(S_{\nu} = B_{\nu})$. Thus, from the analysis outlined before we would get a mean intensity of $J_{\nu} = B_{\nu}$ in the limit of large optical depth, travelling into the star.

As a simpler example of scattering (beyond the discussion in section 2) consider the case where we have some continuum scattering mechanism, such as Thomson scattering of photons by electrons, at work in the atmosphere of our star. The scattering is 'continuum' in that it occurs at all frequencies, a good approximation in Thomson scattering. Assume that this mechanism brings about coherent, isotropic scattering (no change in frequency but random directional redistribution); we can obtain the source function as follows:

- Write $\chi_{\nu} = n\sigma$, σ is the cross-section for scattering e.g. $\sigma = \sigma_T$ for Thomson scattering.
- The emission coefficient is given by the isotropic power emitted per unit frequency interval per unit solid angle, per unit volume: $\eta_{\nu} = P_{\nu}/(4\pi) \times n$. Noting that $P_{\nu} = c\sigma u_{\nu}$ and $J_{\nu} = u_{\nu} \times c/(4\pi)$, we get $\eta_{\nu} = n\sigma J_{\nu}$.

Thus we can write the source function as $S_{\nu} = J_{\nu}$; in contrast to the LTE case, emission is now decoupled from the properties of the local medium and strongly dependent on the radiation field itself; this is a consequence of the passive role that the medium plays in scattering processes. The radiation field at any given point can be strongly dependent on distant properties of the scattering medium (e.g. due to boundary conditions enforced by the stellar surface) and thus scattering acts to *delocalise* the radiative transfer problem.

Returning to the continuum coherent scattering example, we need to solve the following radiative transfer equation:

$$\mu \frac{\partial I_{\nu}}{\partial \tau_{\nu}} = I_{\nu} - J_{\nu} \tag{36}$$

As $J_{\nu} = \frac{1}{2} \int_{-1}^{1} d\mu \ I_{\nu}$ we see that the transfer equation has gone from a partial differential equation in the LTE case to an integral equation. The evolution of the radiation field at some depth in a particular direction now depends on the solution itself in all directions at that depth. Note that the 'solution' in equation (35) with $S_{\nu} \to J_{\nu}$ is still an accurate statement, but it is no longer an explicit statement of the solution $J_{\nu}(\tau_{\nu})$; we now have an integral equation for J_{ν} which is not easily solved.

In the combined case involving both thermal absorption / emission and scattering, we can write for the source function:

$$S_{\nu} = (1 - \rho_{\nu})B_{\nu} + \rho_{\nu}J_{\nu}, \quad \rho_{\nu} = \frac{n\sigma_{\nu}}{\chi_{\nu}^{(thermal)} + n\sigma_{\nu}}$$
(37)

Once again, the solution J_{ν} can be stated as in (35) as an integral equation. We can develop (35) into an iterative method known as 'A-iteration' (see Mihalas [1978] ch. 6) that can be used to converge to the correct solution if the parameter ρ_{ν} is small enough through the atmosphere.

4 Conclusions

We conclude with some general comments about the effects of scattering in radiative transfer. Interactions that allow net exchange of thermal energy between the radiation field and the transfer medium will generally tend to induce a coupling of the properties of the radiation field to those of the medium (i.e. LTE, the radiation field tends to a Planck spectrum with a radiation temperature equal to the kinetic temperature of the matter). In contrast to this, scattering allows a decoupling of these properties in which the radiation field itself, nonlocal to the direction or frequency for which it is being computed, affects its own development. We can at least say that scattering produces problems in radiative transfer, and its application throughout various areas of astrophysics, that are often non-trivial.

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