

Lecture Notes:

INTRODUCTION TO NON-LTE RADIATIVE TRANSFER
AND ATMOSPHERIC MODELING

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July 2008

Basic Equations

The specific intensity of radiation I_ν (erg cm⁻²s⁻¹sr⁻¹Hz⁻¹) is the energy passing through unit area per unit time, per unit solid angle Ω , and per unit frequency ν . The intensity depends on position, direction, and frequency (also on time and polarization, not considered here).

Assume azimuthal symmetry, let θ be the angle between the direction of I and the outward direction, with $\mu = \cos\theta$, and let r measure position, so that $I_\nu = I_\nu(r, \mu)$.

The mean intensity J_ν is the angle average of I_ν :

$$J_\nu = (1/4\pi) \int I_\nu d\Omega = (1/2) \int_{-1}^{+1} I_\nu d\mu.$$

The monochromatic energy density is $U_\nu = (4\pi/c)J_\nu$.

The monochromatic flux is defined by

$$\pi F_\nu = \int I_\nu \cos\theta d\Omega = 2\pi \int_{-1}^{+1} I_\nu \mu d\mu.$$

Note that $(\pi F_\nu)4\pi R^2 = L$ is the luminosity, or the net energy per unit time and per unit frequency, in erg s⁻¹Hz⁻¹, passing outward through a spherical surface of radius R , while F_ν is equal to I_ν provided that I_ν is both isotropic outward and zero inward. Thus the surface flux πF_ν is π times the μ -weighted average of I_ν . The effective temperature T_{eff} is defined by $\pi F = \sigma T_{eff}^4$ where $F = \int_0^\infty F_\nu d\nu$, and $\sigma = 2\pi^5 k^4 / 15c^2 h^3$ is Stefan's constant. The integral of the Planck function $B_\nu(T)$ over all ν is $\sigma T^4 / \pi$.

In analogy with J_ν , another flux definition in the literature is

$$H_\nu = (1/2) \int_{-1}^{+1} I_\nu \mu d\mu = (\pi F_\nu) / 4\pi.$$

The equation of radiative transfer is

$$dI_\nu / d\ell = -\kappa_\nu I_\nu + \eta_\nu,$$

where κ_ν is the absorption coefficient, in cm⁻¹, η_ν is the emission coefficient in erg cm⁻³s⁻¹sr⁻¹Hz⁻¹, and ℓ is distance in cm in the direction of I . Here it is assumed that κ_ν and η_ν are not explicitly dependent on I_ν . The source function is $S_\nu = \eta_\nu / \kappa_\nu$ and the optical depth τ_ν , measured inward from the surface, is defined by $d\tau_\nu = -\kappa_\nu \mu d\ell$. Here we consider plane geometry in which μ is constant with height along the direction of I_ν . Then the transfer equation becomes

$$\mu dI_\nu / d\tau_\nu = I_\nu - S_\nu,$$

where τ_ν at a given depth is the integral of κ_ν along the inward normal from the surface to the given depth. Often κ_ν is expressed as $\kappa_\nu = \rho k_\nu$ where ρ is the gas density in g cm^{-3} and k_ν is the mass absorption coefficient in $\text{cm}^2 \text{g}^{-1}$. We can integrate the transfer equation over μ to obtain $dH_\nu/d\tau = J_\nu - S_\nu$.

The transfer equation has the following formal solution, where, for simplicity, we omit the frequency subscript. The intensity at a given value of τ in the inward direction ($\mu < 0$) is given by

$$I(\tau, \mu) = I(0, \mu)e^{\tau/\mu} - (1/\mu) \int_0^\tau e^{(\tau-t)/\mu} S(t) dt,$$

where $I(0, \mu)$ is any given incident intensity at the $\tau = 0$ boundary. In the outward direction ($\mu > 0$) the solution is

$$I(\tau, \mu) = I(\tau_m, \mu)e^{-(\tau_m-\tau)/\mu} + (1/\mu) \int_\tau^{\tau_m} e^{-(t-\tau)/\mu} S(t) dt,$$

where $I(\tau_m, \mu)$ is any given incident intensity at an inner boundary where $\tau = \tau_m$. In the case of a semi-infinite atmosphere the first term is zero provided that $I(\tau_m, \mu)$ does not increase exponentially. Thus for $\mu > 0$,

$$I(\tau, \mu) = (1/\mu) \int_\tau^\infty e^{-(t-\tau)/\mu} S(t) dt.$$

The emergent intensity in this semi-infinite case is

$$I(0, \mu) = (1/\mu) \int_0^\infty e^{-t/\mu} S(t) dt, \text{ for } \mu > 0.$$

If S is a linear function of t it is easily shown that $I(0, \mu) = S(\tau = \mu)$. This is called the Eddington-Barbier relation.

We can use these equations for $I(\tau, \mu)$ to express the mean intensity $J(\tau)$ as an integral over the source function $S(t)$. This involves the first exponential integral

$$E_1(x) = \int_x^\infty (1/y)e^{-y} dy$$

which behaves as $(1/x)e^{-x}$ at large x and as $-\log x$ as x approaches 0. Apart from incident radiation terms, the result is

$$J(\tau) = (1/2) \int_0^{\tau_m} E_1(|t - \tau|) S(t) dt.$$

This equation is often written as

$$J(\tau) = \Lambda\{S\}, \text{ where } \Lambda \text{ is called the Lambda operator.}$$

The E_1 function has the property $\int_0^\infty E_1(t) dt = 1$ so that when S is constant in the semi-infinite case with no incident radiation, $J = S$ at large τ , and $J = (1/2)S$ at the surface.

The flux quantity H defined above depends on the source function according to

$$H(\tau) = (1/2) \int_0^{\tau_m} E_2(|t - \tau|) \text{sgn}(t - \tau) S(t) dt, \text{ where } \text{sgn}(t - \tau) \text{ is the sign of } (t - \tau), \text{ and } E_2 \text{ is the second exponential integral}$$

$$E_2(x) = \int_x^\infty (1/y^2) e^{-y} dy.$$

This equation for H is often written as $H(\tau) = \Phi\{S\}$, where Φ is called the Phi operator. The E_2 function has the property $\int_0^\infty E_2(t)dt = 1/2$ so that when S is constant in the semi-infinite case with no incident radiation, $H = 0$ at large τ , and $H = (1/4)S$ at the surface. Another property of the flux equation is that if $S(\tau) = C_0 + C_1\tau$ where C_0 and C_1 are constants, then H approaches $(1/3)C_1$ at large τ .

Within an enclosure in thermodynamic equilibrium at temperature T , the intensity I_ν is isotropic and equal to the Planck function

$$B_\nu(T) = (2h\nu^3/c^2)[e^{h\nu/kT} - 1]^{-1} \text{ in erg cm}^{-2}\text{s}^{-1}\text{sr}^{-1}\text{Hz}^{-1}.$$

Also, all particles have Maxwellian velocity distributions, excitations are governed by the Boltzmann equation, and ionizations by the Saha-Boltzmann equation (both equations given later), all at the same temperature T .

Local thermodynamic equilibrium (LTE) refers to the assumption that velocities, excitations, and ionizations are all in equilibrium corresponding to the local temperature, which may vary with depth in the medium. In general this means that $S_\nu = B_\nu$ at each depth, but the intensity I_ν must be calculated from the transfer equation with $S_\nu = B_\nu$. LTE is a good approximation at sufficiently large optical depths such as in stellar photospheres at continuum frequencies or in relatively weak lines. Here we discuss general non-LTE case in which $S_\nu \neq B_\nu$, which includes the special case of LTE.

Monochromatic Scattering

If every photon encountering an atom (or an electron) is scattered isotropically with no change in frequency (or if this is the net effect of successive scatterings), then $S_\nu = J_\nu$. We can consider a combination of LTE and scattering by writing the transfer equation as

$$dI/d\ell = -\kappa^{ab}(I - B) - \kappa^{sc}(I - J)$$

where the frequency subscript has been omitted for simplicity.

Let $d\tau = -(\kappa^{ab} + \kappa^{sc})\mu d\ell$ and $\epsilon = \kappa^{ab}/(\kappa^{ab} + \kappa^{sc})$. Then

$$\mu dI/d\tau = I - S \text{ where } S = (1 - \epsilon)J + \epsilon B.$$

In this last equation we can introduce the Lambda operator, given above, and write

$$S = (1 - \epsilon)\Lambda\{S\} + \epsilon B.$$

To demonstrate some simple solutions of this equation we replace the $E_1(x)$ function by the first-order approximation $\sqrt{3}e^{-\sqrt{3}x}$ so that we have the integral equation

$$S(\tau) = (1 - \epsilon) \int_0^\infty (\sqrt{3}/2)e^{-\sqrt{3}|t-\tau|} S(t)dt + \epsilon B$$

in the semi-infinite case with no incident radiation. This equation has the following solution when ϵ and B are constant:

$$S(\tau) = B[1 - (1 - \sqrt{\epsilon})e^{-\sqrt{3\epsilon}\tau}]$$

as can be verified by substitution. This result shows that 1) $S(0) = \sqrt{\epsilon}B$, and 2) for $\epsilon \ll 1$, S approaches B only for $\tau > 1/\sqrt{\epsilon}$, which is referred to in this case as the thermalization depth.

These two results illustrate the physical nature of the scattering process. The parameter ϵ is small when a photon is much more likely to be scattered than thermally absorbed, even though LTE is assumed for the absorption. Such scattering decouples S from B so that the photons escaping through the boundary effectively originate deep in the atmosphere rather than at τ of order unity. This is the case of simple monochromatic scattering, but a very similar interpretation applies to photons in a spectral line as described in the next section. The thermalization depth is $1/\sqrt{\epsilon}$ for monochromatic scattering, but, as discussed in the next section, is $1/\epsilon$ in the case of scattering in a line with complete frequency redistribution, i.e., with a common frequency probability for both absorption and emission within the line.

Line Radiation

In the case of line radiation, the Einstein coefficient A_{21} represents the number of spontaneous radiative transitions from the upper atomic level 2 to the lower level 1, per atom in level 2, per unit time.

$B_{12}\bar{J}$ is the number of transitions from 1 to 2 due to the absorption of line radiation, per atom in level 1, per unit time. Here $\bar{J} = \int_0^\infty J_\nu \phi_\nu d\nu$, where J_ν is the mean intensity of line radiation and ϕ_ν is the line profile function (the probability within the line of an absorption or of an emission, here considered the same) normalized so that $\int_0^\infty \phi_\nu d\nu = 1$. This rate is proportional, through \bar{J} , to the number of available photons that can cause the 1 to 2 transition.

$B_{21}\bar{J}$ is the number of 2 to 1 radiative transitions stimulated by radiation at line frequencies. (In this case the emitted photon travels in the same direction as the one causing the emission, as in a laser, but this property does not affect the development here.)

n_1 and n_2 are the number densities (level populations) in cm^{-3} for levels 1 and 2.

$n_2(A_{21} + B_{21}\bar{J})$ equals the number of downward radiative transitions ($\text{cm}^{-3}\text{s}^{-1}$).

$n_1B_{12}\bar{J}$ equals the number of upward radiative transitions ($\text{cm}^{-3}\text{s}^{-1}$) resulting from the absorption of photons.

A_{21} , B_{21} , and B_{12} are the Einstein coefficients for spontaneous emission, stimulated emission, and absorption.

If these transitions are the only effective ones (i.e., no collisions), then in a steady state, i.e., in statistical equilibrium, we have $n_2(A_{21} + B_{21}\bar{J}) = n_1B_{12}\bar{J}$.

This equation allows us to derive relationships between the Einstein coefficients.

In thermodynamic equilibrium \bar{J} is equal to the Planck function B_ν at the line frequency ν (which is essentially constant throughout the line), and $n_2/n_1 = n_2^*/n_1^*$ where this equilibrium ratio is given by the Boltzmann equation $n_2^*/n_1^* = (g_2/g_1)e^{-h\nu/kT}$. Here g_1 and g_2 are the statistical weights of levels 1 and 2, so that $n_2^*(A_{21} + B_{21}B_\nu) = n_1^*B_{12}B_\nu$. Solving this equation for B_ν gives

$$B_\nu = (A_{21}/B_{21})[e^{h\nu/kT}(g_1B_{12}/g_2B_{21}) - 1]^{-1}.$$

Since the Einstein coefficients and the statistical weights are independent of T it follows that

$$A_{21}/B_{21} = 2h\nu^3/c^2 \text{ and } g_1B_{12} = g_2B_{21}.$$

Now suppose there are collisional transitions between levels 1 and 2 in addition to the radiative transitions. Let n_2C_{21} and n_1C_{12} be, respectively, the number of downward and upward collisional transitions per unit volume and time ($\text{cm}^{-3}\text{s}^{-1}$). These collision rates will depend on temperature and will be proportional to the number density of particles inducing the collisional transition, usually the electron number density.

The statistical equilibrium equation with both radiative and collisional transitions is then $n_2(A_{21} + B_{21}\bar{J} + C_{21}) = n_1(B_{12}\bar{J} + C_{12})$.

Since C_{21} and C_{12} are independent of n_2 , n_1 , and \bar{J} , we can consider the case of thermodynamic equilibrium, so that the radiative terms drop out, and we obtain the relationship $n_2^*C_{21} = n_1^*C_{12}$ between the downward and upward collision rates. This relationship assumes that the particle velocities have Maxwellian distributions. When $n_2/n_1 = n_2^*/n_1^*$, the two levels are said to be in detailed balance.

We will return to this statistical equilibrium equation after first considering line absorption and emission in the radiative transfer equation.

Here we assume that the normalized profile function ϕ_ν represents the probability that a photon is emitted at a given frequency ν within a given line, as well as the probability that a photon is absorbed at frequency ν within the line. In the simple case of only thermal Doppler broadening due to a Maxwellian distribution of velocities, with negligible intrinsic line broadening, ϕ_ν is given by $\phi_\nu = (\Delta\nu_D\sqrt{\pi})^{-1}e^{-[(\nu-\nu_0)/\Delta\nu_D]^2}$ where ν_0 is the line center frequency and $\Delta\nu_D$ is the thermal doppler width $\Delta\nu_D = (\nu_0/c)\sqrt{2kT/m_a}$, in which m_a is the mass of the atoms that absorb and re-emit the line radiation.

This use of the same ϕ_ν for absorption and emission is the case of complete redistribution. In the more general case of partial redistribution, the frequency of an emitted photon is correlated with that of the absorbed photon that caused the atomic excitation. See Hubeny, I. & Lites, B. W. 1995, Partial redistribution in multilevel atoms. I. Method and application to the solar hydrogen line formation, *ApJ*, 455, 376, and the Appendix in Avrett, E. H. & Loeser, R. 2008, Models of the solar chromosphere and transition region from SUMER and HRTS observations: Formation of the extreme-ultraviolet spectrum for hydrogen, carbon, and oxygen, *ApJS*, 175, 229.

The number of spontaneous photon emissions per unit volume, time, and frequency is $n_2A_{21}\phi_\nu$. Since each emission contributes energy $h\nu$ distributed over solid angle 4π , the emission coefficient is $\eta_\nu = (h\nu/4\pi)n_2A_{21}\phi_\nu$. The line absorption coefficient is similarly $\kappa_\nu = (h\nu/4\pi)n_1B_{12}\phi_\nu$ such that $\kappa_\nu I_\nu$ is the absorbed energy in the units $\text{erg cm}^{-3}\text{s}^{-1}\text{sr}^{-1}\text{Hz}^{-1}$. The stimulated emission term in the same units is $(h\nu/4\pi)n_2B_{21}\phi_\nu I_\nu$.

The stimulated emission and absorption terms can be combined (since both are proportional to I_ν), finally giving the line transfer equation

$$dI_\nu/d\ell = -(h\nu/4\pi)\phi_\nu[(n_1B_{12} - n_2B_{21})I_\nu - n_2A_{21}].$$

This equation can be put in the form considered earlier, i.e.,

$$\mu dI_\nu/d\tau_\nu = I_\nu - S_\nu$$

by defining the monochromatic optical depth $d\tau_\nu = -\kappa_\nu\mu d\ell$ in terms of the line absorption coefficient

$$\kappa_\nu = (h\nu/4\pi)(n_1B_{12} - n_2B_{21})\phi_\nu = (h\nu/4\pi)n_1B_{12}[1 - (n_2g_1/n_1g_2)]\phi_\nu,$$

and with the source function given by

$$S_\nu = (2h\nu^3/c^2)[(n_1g_2/n_2g_1) - 1]^{-1}$$

which is equal to the Planck function when $n_2/n_1 = n_2^*/n_1^*$.

Note that in this case of complete redistribution, S does not depend on ϕ_ν and is essentially frequency independent over the bandwidth of the line.

Now we return to the statistical equilibrium equation which expresses n_2/n_1 in terms of \bar{J} , the collision rates, and the Einstein coefficients. Substituting this ratio into the equation for S gives the result

$$S = (\bar{J} + \varepsilon B)/(1 + \varepsilon),$$

where

$$\varepsilon = (C_{21}/A_{21})(1 - e^{-h\nu/kT}),$$

thus writing the statistical equilibrium equation as an equation for the line source function.

Using the notation $\epsilon = \varepsilon/(1 + \varepsilon)$, this equation for S becomes

$$S = (1 - \epsilon)\bar{J} + \epsilon B,$$

which has the same form as the earlier expression in the case of coherent scattering together with thermal absorption and emission, except that J_ν in the earlier expression now becomes the line-integrated function \bar{J} . Combining $\bar{J} = \int_0^\infty J_\nu\phi_\nu d\nu$ with $J_\nu = \Lambda\{S\}$ from the transfer equation gives, in the semi-infinite case,

$$\bar{J} = \int_0^\infty K(|t - \tau|)S(t)dt \text{ where } K(p) = \int_0^\infty \phi_\nu^2 E_1(\phi_\nu p) d\nu.$$

This function has the normalization $\int_0^\infty K(p)dp = 1/2$.

Two-Level-Atom Solutions

We now show numerical solutions of the equation

$$S = (1 - \epsilon) \int_0^\infty K(|t - \tau|)S(t)dt + \epsilon B.$$

in which the statistical equilibrium and transfer equations have been combined.

For simplicity we introduce the dimensionless frequency variable x defined by

$$x = (\nu - \nu_0)/\Delta\nu_D,$$

i.e., the frequency displacement from line center in units of the Doppler width, so that the profile function is $\phi_\nu = \phi(x)/\Delta\nu_D$, where

$\phi(x) = (1/\sqrt{\pi})e^{-x^2}$, which has the normalization $\int_0^\infty \phi(x)dx = 1$.

We use the optical depth τ defined by

$$d\tau = (1/\Delta\nu_D)(h\nu/4\pi)n_1B_{12}[1 - (n_2g_1/n_1g_2)]\mu dl.$$

This τ is $\sqrt{\pi}$ times the line-center optical depth.

Then the transfer equation can be written in the simple form $\mu dI_x/d\tau = \phi_x(I_x - S)$.

The left panel of Figure 1 below shows a set of calculated solutions $S(\tau)$ in the semi-infinite case with $B = 1$ and for different constant values of ϵ . Note that $S(0) = \sqrt{\epsilon}B$ in each case, as was noted earlier in the case of monochromatic scattering. Here it should be noted that $S \rightarrow B$ for $\tau \sim 1/\epsilon$ rather than for $\tau \sim 1/\sqrt{\epsilon}$ as in the monochromatic case. This depth where $S \rightarrow B$ is called the thermalization length, and is much greater here because photons in the line wings can travel greater distances between scatterings than those at line center, and photons absorbed in the line core can be re-emitted in the wings.

The right panel of Fig. 1 shows the Doppler line absorption profile $\phi(x)$ and the emergent line intensity $I_x(\tau = 0)$ in the normal direction ($\mu = 1$) in each case as functions of x . Half of the symmetric line profile is plotted. Here, $I_x = \int_0^\infty \phi_x e^{-\phi_x \tau} S(\tau) d\tau$.

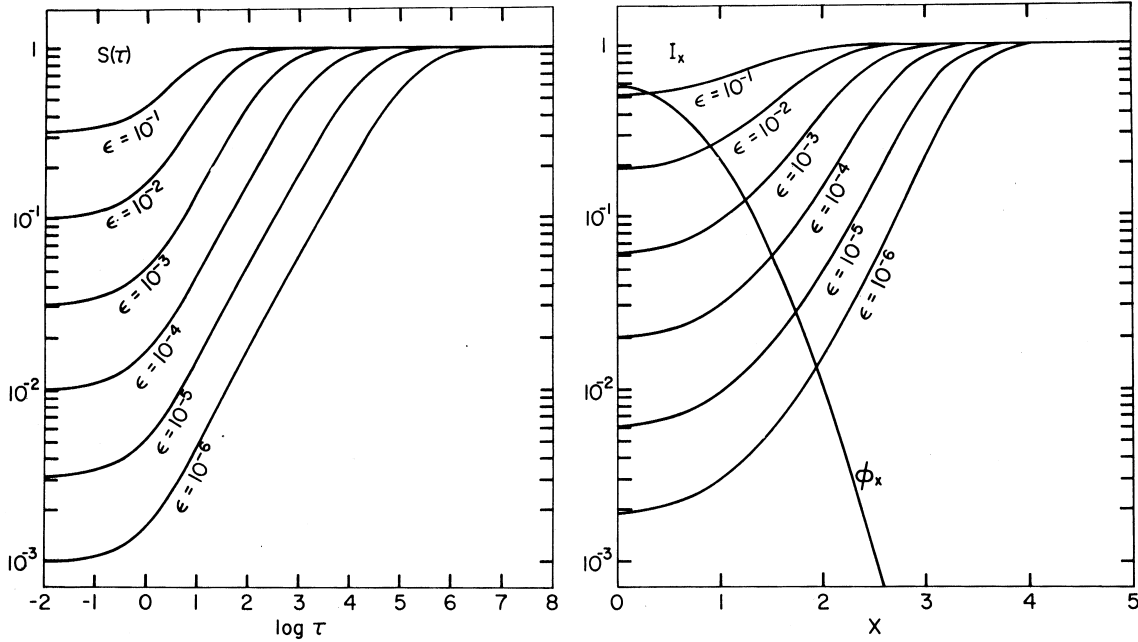


Figure 1: $S(\tau)$ and I_x for $B = 1$ and different values of ϵ .

These results demonstrate how the central intensity decreases and the line width increases as the parameter ϵ decreases. Here ϵ is essentially C_{21}/A_{21} , the ratio of collisional to radiative de-excitation, when this ratio is small. Conversely, $\epsilon \rightarrow 1$ for $C_{21} \gg A_{21}$.

We now show solutions when $B(\tau)$ is not constant. Figure 2 shows results for $\epsilon = 10^{-4}$ and $B(\tau) = 1 + 100e^{-C\tau}$ with $C = 10^{-2}, 10^{-3}$, and 10^{-4} . Here the Doppler width is still assumed to be constant with depth for simplicity.

The previous variation of S relative to $B = 1$ for $\epsilon = 10^{-4}$ now is changed to a variation of S relative to a characteristic depth-dependent average of B over a thermalization length. Note that while the calculated central intensity is smaller than the continuum in each case, emission peaks occur in the wings as a consequence of the rise in $B(\tau)$ toward the surface.

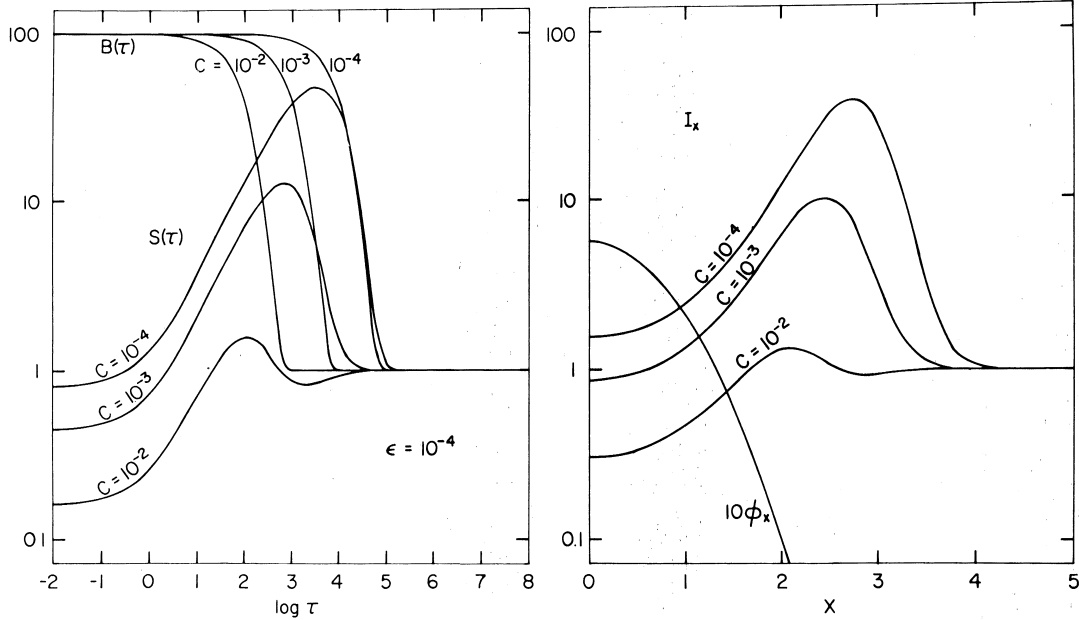


Figure 2: Solutions with $\epsilon = 10^{-4}$ and $B(\tau) = 1 + 100e^{-C\tau}$ with $C = 10^{-2}, 10^{-3}$, and 10^{-4}

Figure 3 below shows solutions with a given $B(\tau) = 1 + 100e^{-0.001\tau}$ and $\epsilon = 10^{-2}, 10^{-4}$, and 10^{-6} . These figures show that the emergent profiles range from absorption lines to centrally-reversed emission lines, depending on $B(\tau)$ and ϵ .

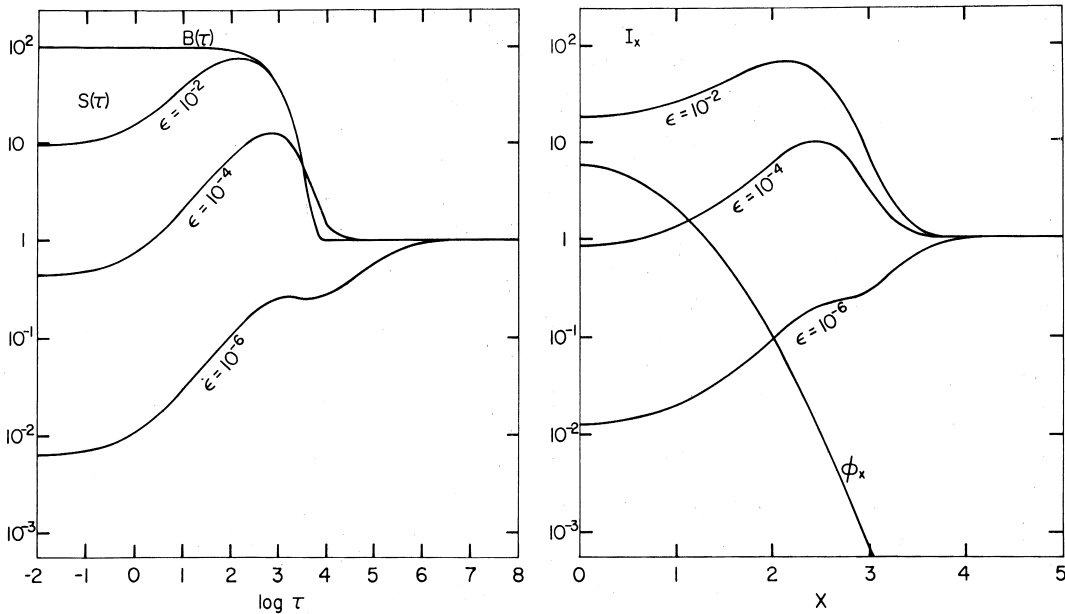


Figure 3: Solutions with $B(\tau) = 1 + 100e^{-0.001\tau}$ and $\epsilon = 10^{-2}, 10^{-4}$, and 10^{-6} .

The two-level atom that we have considered allows for radiative and collisional excitation and de-excitation between the two levels. Such atoms absorb and emit photons having frequencies within the bandwidth of the line transition. Photons also can be absorbed and emitted at the same frequencies by other constituents in the gas. To illustrate some of these effects we consider the more general form of the transfer equation

$$\mu dI_x/d\tau = \phi_x(I_x - S) + r(I_x - S^c)$$

where the additional terms represent absorption and emission of photons by a “continuum” source. Here r is the ratio of continuum to line opacity and S^c is the continuum source function, which in some cases is the Planck function.

In Figure 4 below we show results with $S^c = B = 1$ and various values of ϵ , and now with $r = 10^{-4}$ in addition to $r = 0$. Note that the solution becomes independent of ϵ when $\epsilon \ll r$. In this case photons are coupled to the thermal medium through continuum absorption and emission rather than by means of the collisional transitions we have considered, and $S \rightarrow S^c$ and not B . When r greatly exceeds ϵ the thermalization length generally lies between $1/r$ and $1/\sqrt{r}$.

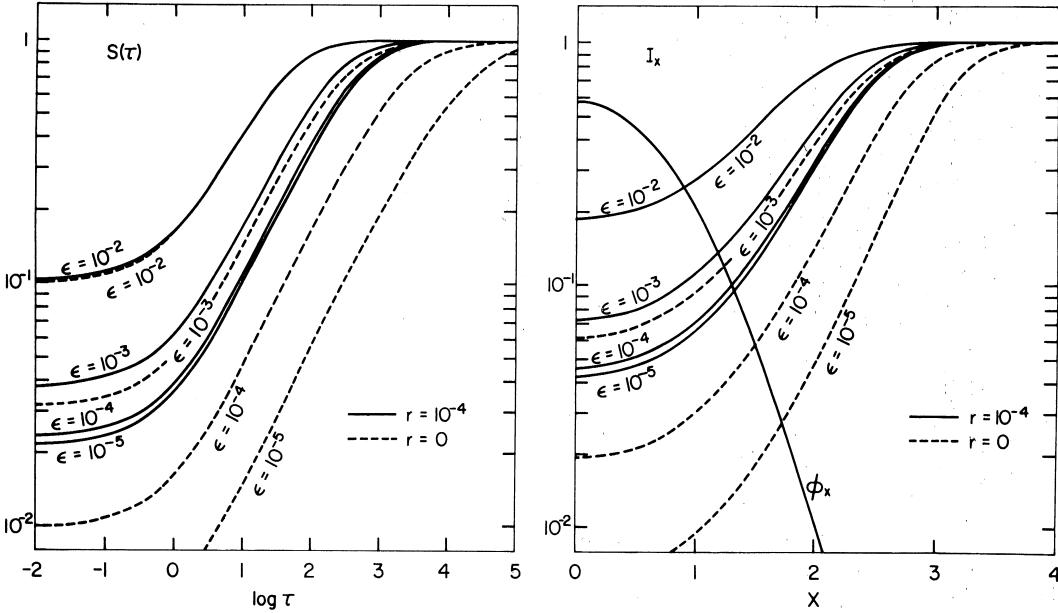


Figure 4: Solutions with constant ϵ and r (and $a = 0$, discussed below). r is unimportant when $r \ll \epsilon$. ϵ is unimportant when $\epsilon \ll r$.

So far we have considered only Doppler line broadening and have not included broadening in the atom’s rest frame. When Lorentz broadening is combined with Doppler broadening we need to replace our Gaussian profile function $\phi_x = (1/\sqrt{\pi})e^{-x^2}$ by the Voigt function

$$\phi_x = (a/\pi^{3/2}) \int_{-\infty}^{+\infty} [a^2 + (x - y)^2]^{-1} e^{-y^2} dy,$$

which reduces to the Gaussian profile when $a = 0$. Here $a = \Gamma/4\pi\Delta\nu_D$ where in the two-level case $\Gamma = A_{21}$ for natural broadening alone.

Figure 5 shows the solutions with $B = 1, \epsilon = 10^{-4}, r = 0$ and three values of a . As a becomes larger the opacity in the line wings decreases more slowly, and the far wings of the line intensity profile become broader.

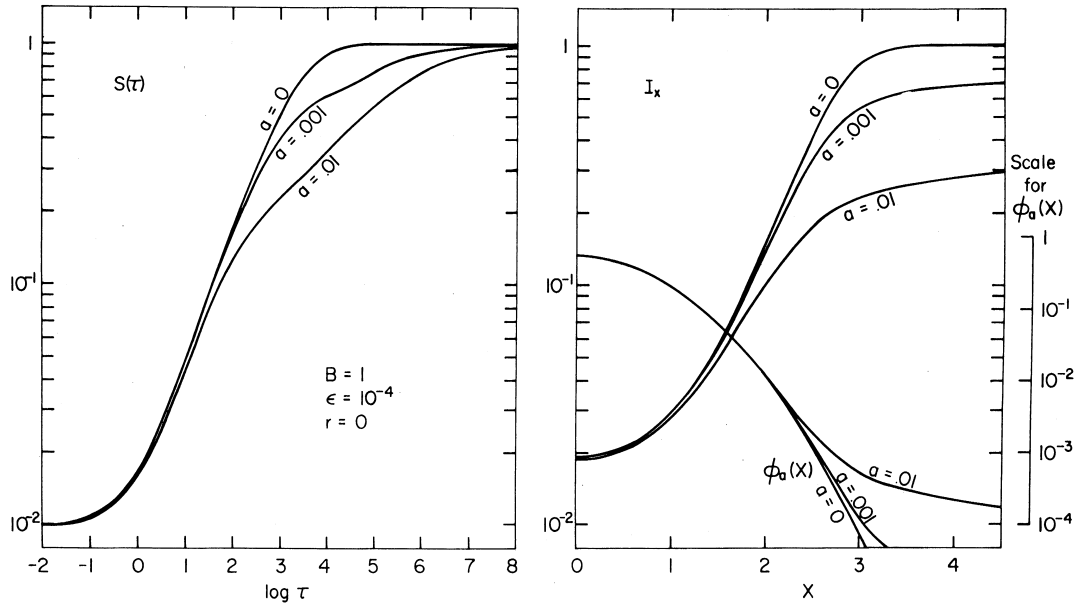


Figure 5: Solutions with Doppler and Voigt profiles.

Figure 6 shows the corresponding results for $B(\tau) = 100e^{-0.001\tau}$. In this case the peak of the centrally reversed emission line is diminished as a increases.

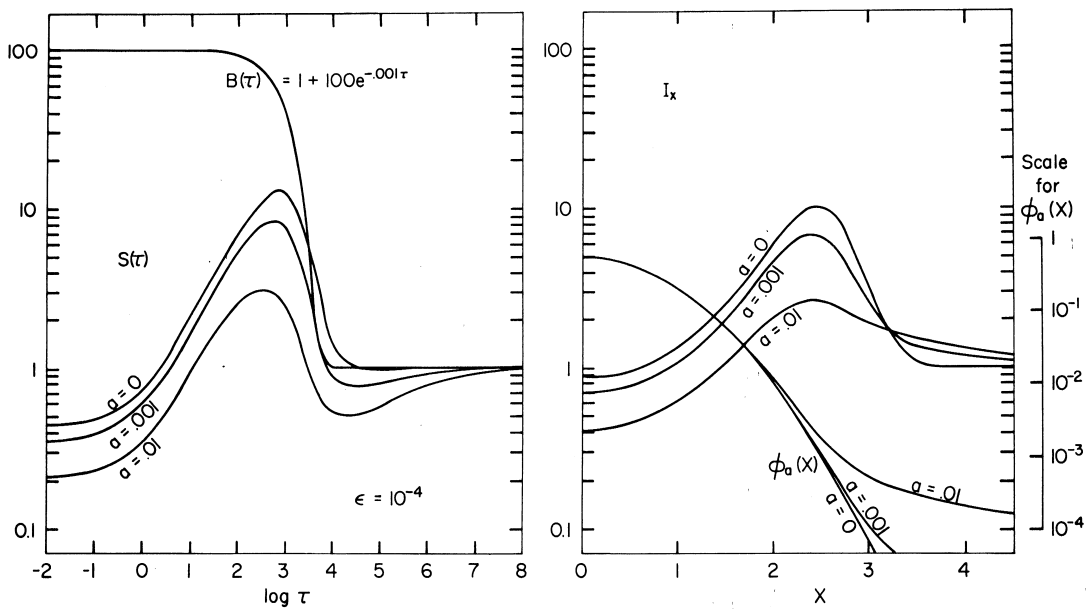


Figure 6: Solutions with Doppler and Voigt profiles and variable B .

The results in Fig. 4 indicate that for $a = 0$, the solution is mostly determined by the larger of the two parameters ϵ and r . Figure 7 shows that when $a > 0$ the line wing can be quite sensitive to r even when $r \ll \epsilon$. For a Voigt profile, extended line wings can develop when r is several orders of magnitude smaller than ϵ .

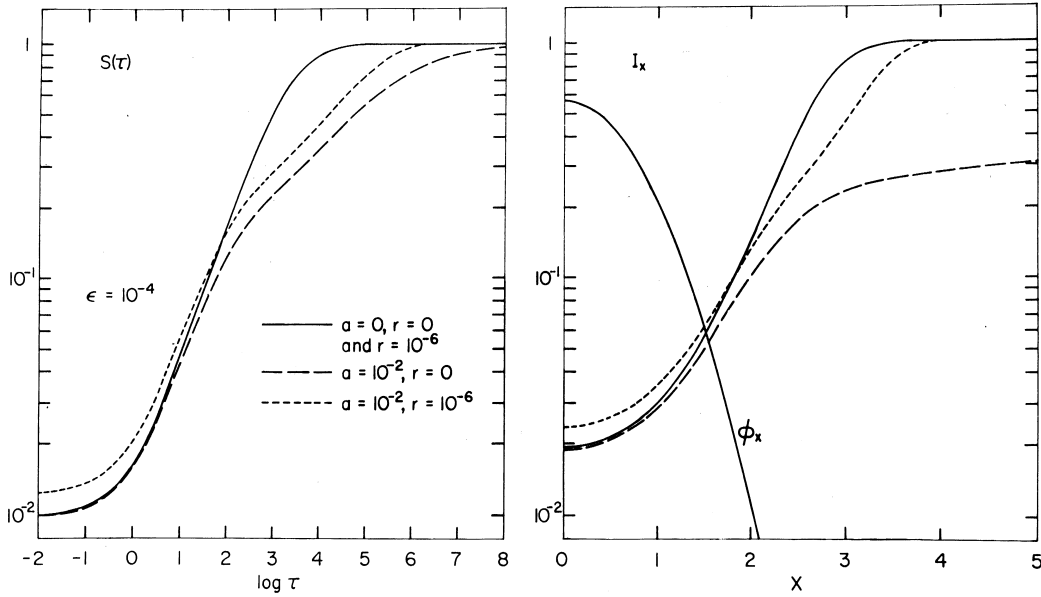


Figure 7: Solutions with Doppler and Voigt profiles and with $r = 0$ and 10^{-6} .

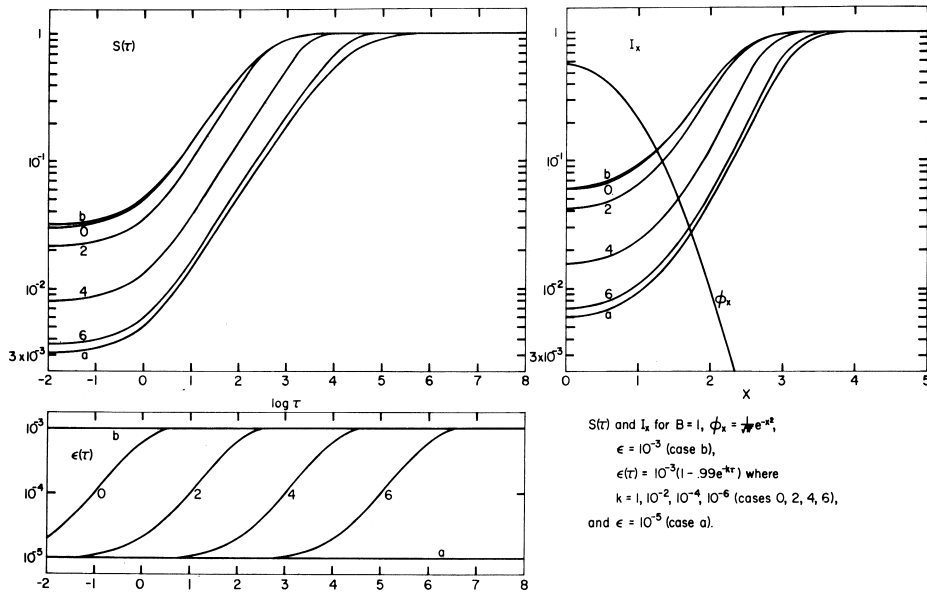


Figure 8: Solutions with $\epsilon(\tau)$ varying between 10^{-5} and 10^{-3} .

For completeness we conclude this discussion with results in Figure 8 showing the effects of depth variations in ϵ . For $B = 1$, $a = 0$, $r = 0$ we let ϵ vary with τ between 10^{-5} and 10^{-3} as indicated in the bottom panel. The results suggest that the scale of the variation of S is roughly determined by the values of ϵ at thermalization-length depths.

These eight figures illustrate solutions corresponding to variations of $B(\tau)$ and $\epsilon(\tau)$ and to different values of the parameters r and a , which, along with the Doppler width, also depend on depth in general. These are idealized cases, but they can provide help in understanding more complex calculations. These and other illustrations are from Avrett, E. H. 1965, The Formation of Spectral Lines, Second Harvard-Smithsonian Conference on Stellar Atmospheres, SAO Spec. Rept. 174, pp. 101-140.

Numerical Methods

These results have been obtained by numerical methods since in only very simple cases is it possible to obtain analytic solutions. To simplify the discussion of numerical solutions we can consider again the special case given earlier: $S(\tau) = (1 - \epsilon) \int_0^\infty (\sqrt{3}/2) e^{-\sqrt{3}|t-\tau|} S(t) dt + \epsilon B$ which has the known solution $S(\tau) = B[1 - (1 - \sqrt{\epsilon})e^{-\sqrt{3}\epsilon\tau}]$. Note that this equation was obtained by combining the equation for S in terms of J with the solution of the transfer equation for J in terms of S . A solution can be found iteratively by simply starting with $S(\tau) = (1 - \epsilon)J(\tau) + \epsilon B$ from an initial $J(\tau)$, using this $S(\tau)$ in the transfer equation to obtain a new $J(\tau)$, i.e., evaluating $J(\tau) = \int_0^\infty (\sqrt{3}/2) e^{-\sqrt{3}|t-\tau|} S(t) dt$, and continuing iteratively. This is called a solution by "lambda iteration". For small values of ϵ , roughly $1/\sqrt{\epsilon}$ iterations are required in this particular case. Acceleration procedures can be used to reduce the number of iterations. This simple case, with $E_1(x)$ instead of $K(x)$, and then $E_1(x)$ approximated by $\sqrt{3}e^{\sqrt{3}x}$, presents a severe test of the lambda iteration method. The general case for the calculation of a line source function with complete and partial frequency redistribution is discussed by Hubeny, I. 2003, Accelerated Lambda iteration: An overview, in Stellar Atmosphere Modeling, ed. I. Hubeny, D. Mihalas, & I. Werner, ASP Conf. Ser. 288, 17. See also Avrett, E. H. 2008, Rapidly-converging methods for solving multilevel transfer problems, 2008, in Numerical Methods for Multidimensional Radiative Transfer, ed. E. Meinköhn, G. Kanschat, R. Rannacher, & R. Wehrse (Heidelberg: Springer), in press.

Alternatively, this integral equation can be solved directly by means of a system of simultaneous equations. We can choose a set of optical depths τ_i at which we want to calculate S_i . For simplicity we can assume that $S(t)$ varies linearly in each interval $t_j \leq t \leq t_{j+1}$, so that $S(t) = (t_{j+1} - t_j)^{-1}[(t_{j+1} - t)S_j + (t - t_j)S_{j+1}]$ in that interval. Then the integral equation can be written as the following set of N equations in the N unknowns S_i :

$S_i = (1 - \epsilon_i) \sum_{j=1}^N W_{i,j} S_j + \epsilon_i B_i$, $i = 1, 2, \dots, N$ where the weighting coefficients $W_{i,j}$ are independent of the values of S . From this equation we can obtain $S_i = \sum_{j=1}^N M_{ij} B_j$, where M_{ij} depends only on the set of τ_i values. We have found that such solutions can be used successfully to solve a wide range of non-LTE radiative transfer problems, but lambda iterations, accelerated or not, can be used whenever the needed optical depth range is not $\gg 1$.

This short section does not do justice to the extensive literature on numerical methods. See the two conference volumes cited above: Stellar Atmospheric Modeling; and Numerical Methods for Multilevel Radiative Transfer.

Including Bound-Free Transitions The discussion so far has been largely limited to bound-bound transitions in atoms with only two energy levels. Before considering multi-level cases we need to include the equations for bound-free transitions, i.e., for ionization and recombination.

Consider an atom with two bound levels and a continuum. The level-2 statistical equilibrium equation is

$$n_2(A_{21} + B_{21}\bar{J} + C_{21} + P_{2c}) = n_1(B_{12}\bar{J} + C_{12}) + n_c P_{c2}.$$

The statistical equilibrium equation for the continuum is

$$n_c(P_{c1} + P_{c2}) = n_1 P_{1c} + n_2 P_{2c},$$

and the sum of these two equations is the statistical equilibrium equation for level 1.

It is convenient to use the continuum equation to eliminate n_c from the level-2 equation, giving the result

$$n_2(A_{21} + B_{21}\bar{J} + C_{21} + \mathcal{P}_{21}) = n_1(B_{12}\bar{J} + C_{12} + \mathcal{P}_{12}),$$

where

$$\mathcal{P}_{12} = P_{1c}P_{c2}/(P_{c1} + P_{c2}) \text{ and } \mathcal{P}_{21} = P_{2c}P_{c1}/(P_{c1} + P_{c2}).$$

\mathcal{P}_{ij} , which is added to C_{ij} , is thus the rate from i to j through the continuum.

Each P is $R + C$ where, for each level l , R_{lc} is the photoionization rate, C_{lc} is the collisional ionization rate, R_{c1} is the radiative recombination rate, and C_{c1} is the collisional recombination rate, all per initial-state atom or ion.

The photoionization rate is given by

$$R_{lc} = 4\pi \int_{\nu_l}^{\infty} (1/h\nu)\alpha_l(\nu)J_\nu d\nu$$

where $\alpha_l(\nu)$ is the bound-free absorption coefficient and ν_l is the threshold frequency for ionization.

Utilizing equilibrium relationships in the same way as we did before in relating the Einstein coefficients for line radiation, it is easily shown that the radiative recombination rate is given by

$$R_{cl} = (n_l/n_c)^* R_{lc}^\dagger, \text{ where } R_{lc}^\dagger = 4\pi \int_{\nu_l}^{\infty} (1/h\nu)\alpha_l(\nu)e^{-h\nu/kT}[(2h\nu^3/c^2) + J_\nu]d\nu.$$

and where the equilibrium ratio $(n_l/n_c)^*$ is given by the Saha-Boltzmann equation

$$(n_l/n_c)^* = n_e(h^2/2\pi m_e kT)^{3/2}(g_l/2U_c)e^{h\nu_{cl}/kT}.$$

Here n_e is the electron number density, m_e is the electron mass, g_l is the statistical weight of level l , U_c is the ion partition function, and $h\nu_{cl}$ is the ionization energy from level l . (The ion partition function appears here because n_c represents the total number of ions in all excitation states.)

Note that $R_{lc}^\dagger = R_{lc}$ when J_ν is the Planck function.

The collisional ionization and collisional recombination rates are related to each other by this equilibrium ratio:

$$C_{cl} = (n_l/n_c)^* C_{lc}.$$

Recall that for the two-level atom without a continuum, we had the following equation for the line source function:

$$S = (\bar{J} + \varepsilon B)/(1 + \varepsilon),$$

where

$$\varepsilon = (C_{21}/A_{21})(1 - e^{-h\nu/kT}).$$

The corresponding result when the continuum is included is

$$S = (\bar{J} + \tilde{\varepsilon} \tilde{B})/(1 + \tilde{\varepsilon}),$$

where

$$\tilde{\varepsilon} = [(C_{21} + \mathcal{P}_{21})/A_{21}]\{1 - [(C_{21} + \mathcal{P}'_{21})/(C_{21} + \mathcal{P}_{21})]e^{-h\nu/kT}\},$$

and

$$\tilde{B} = (2h\nu^3/c^2)\{[(C_{21} + \mathcal{P}_{21})/(C_{21} + \mathcal{P}'_{21})]e^{h\nu/kT} - 1\}^{-1}$$

where

$$\mathcal{P}'_{21} = (n_1^*/n_2^*)\mathcal{P}_{12}.$$

Note that $\tilde{\varepsilon}$ and \tilde{B} reduce to ε and B when both \mathcal{P}_{21} and \mathcal{P}'_{21} are much smaller than C_{21} .

On the other hand, when photoionization and recombination rates dominate, $\tilde{\varepsilon}$ and \tilde{B} depend on J_ν in the two continua, and are insensitive to the local temperature. This is the so-called photoionization-dominated case.

Before discussing the general multilevel equations, we consider a particularly simple 3-level atom, without a continuum, with $A_{31} \neq 0$ and $A_{21} = A_{32} = 0$. The statistical equilibrium equations for levels 3 and 1 are

$$n_3(A_{31} + B_{31}\bar{J} + C_{31} + C_{32}) = n_1(B_{13}\bar{J} + C_{13}) + n_2C_{23}$$

and

$$n_1(B_{13}\bar{J} + C_{13} + C_{12}) = n_3(A_{31} + B_{31}\bar{J} + C_{31}) + n_2C_{21}.$$

Eliminating n_2 from these equations gives

$$n_3(A_{31} + B_{31}\bar{J} + C_{31} + \mathcal{C}_{31}) = n_1(B_{13}\bar{J} + C_{13} + \mathcal{C}_{13})$$

where

$$\mathcal{C}_{ij} = C_{i2}C_{2j}/(C_{21} + C_{23}),$$

This example shows that we have the same equation as in the two-level case except that level 2 provides an additional collisional path between levels 3 and 1.

Multilevel Atoms

Finally we consider multilevel cases with more than one line transition. It is useful to define the net radiative rate coefficient ρ , sometimes called the net radiative bracket, by the equation

$$n_u(A_{ul} + B_{ul}\bar{J}_{ul}) - n_l B_{lu}\bar{J}_{ul} = n_u A_{ul} \rho_{ul}$$

where u and l refer to the upper and lower levels of a line transition.

The statistical equilibrium equation for level m is then

$$n_m(\sum_i A_{mi}\rho_{mi} + \sum_k C_{mk} + P_{mc}) = \sum_j n_j A_{jm}\rho_{jm} + \sum_k n_k C_{km} + n_c P_{cm}$$

where levels i lie below m , levels j lie above m , and levels k include i and j .

The sum of these equations for $m = 1, 2, \dots, N$ is the continuum equation $n_c \sum_k P_{ck} = \sum_k n_l P_{kc}$. We use this continuum equation to eliminate n_c , and obtain

$$n_m(\sum_i A_{mi}\rho_{mi} + \sum_k Z_{mk}) = \sum_j n_j A_{jm}\rho_{jm} + \sum_k n_k Z_{km}, \text{ where } Z_{ab} = C_{ab} + P_{ac}P_{cb}/\sum_k P_{ck}.$$

This equation for n_m applies to each level of an N -level atom, but any one of these equations is the sum of all the others (because of our use of the continuum equation). We can exclude the n_1 equation, divide the others by n_1 , and have $N - 1$ equations for the $N - 1$ unknown ratios $n_2/n_1, n_3/n_1, \dots, n_N/n_1$.

Suppose that we know the total number density n_{tot} , representing $n_1 + n_2 + \dots + n_N + n_c$, and that we have separately calculated the ratio n_c/n_1 , which is discussed in the next section. Then n_1 is given by

$$n_1 = n_{tot}/(1 + n_2/n_1 + n_3/n_1 + \dots + n_N/n_1 + n_c/n_1)$$

so that the ratios determined from the statistical equilibrium equations allow us to obtain all of the number densities.

The term $A_{ul}\rho_{ul}$ represents the net number of radiative transitions from level u to level l . Since $\rho \rightarrow 0$ at large optical depths, a useful starting approximation is to set all ρ values equal to zero. The coefficients in the set of equations then depend only on the collision rates, and on photoionization rates.

The definition above for ρ_{ul} involving n_u , n_l , and \bar{J}_{ul} is equivalent to

$$\rho_{ul} = 1 - (\bar{J}_{ul}/S_{ul}),$$

$$\text{where } S_{ul} = (2h\nu^3/c^2)\{[(n_l g_u)/(n_u g_l)] - 1\}^{-1}.$$

When S_{ul} and \bar{J}_{ul} are related by

$$S = (\bar{J} + \epsilon\mathcal{B})/(1 + \epsilon),$$

for any \mathcal{B} , it then follows that

$$\rho = \epsilon[(\mathcal{B}/S) - 1].$$

This equation shows that ρ is of order ϵ when S differs from \mathcal{B} , and that $\rho \rightarrow 0$ as $S \rightarrow \mathcal{B}$. Given S_{ul} from n_u/n_l , the corresponding ρ can be determined from this equation.

The statistical equilibrium equations above for the n_m/n_1 ratios are used in two ways, 1) to determine at each depth the number densities, given ρ for every line transition, and 2) to set up the equations for ϵ and \mathcal{B} for each line transition which are used to obtain ρ for that transition. We iterate between these two steps, but these iterations readily converge because we directly solve the coupled transfer and statistical equilibrium equations for each line transition and iterate only on the coupling between transitions. This is sometimes called the equivalent two-level atom method.

The general ϵ and \mathcal{B} equations can be obtained without difficulty but are somewhat lengthy and are not included here. The detailed equations for a three-level atom are given by Avrett, E. H. & Loeser, R. 1987, Iterative solution of multilevel transfer problems, in Numerical Radiative Transfer, ed. W. Kalkofen, Cambridge University Press, 135. See also the Appendix of Avrett & Loeser 2008 (cited p.5).

Solving the Bound-Free Equations

The derivation of the expressions for the photoionization and radiative recombination rates given on page 13 involves the radiative transfer equation for bound-free radiation. For level l this equation has the form

$$dI_\nu/d\ell = -n_l\alpha_l(\nu) + n_c\alpha_l^{sr}(\nu)I_\nu + n_c\alpha_l^{rr}(\nu)$$

where the rates for radiative recombination (α^{rr}), stimulated recombination (α^{sr}), and photoionization (α) are related by

$$\alpha^{rr} = (2h\nu^3/c^2)\alpha^{sr} \text{ and } \alpha^{sr} = \alpha(n_l/n_c)^*e^{-h\nu/kT}.$$

We define the departure coefficient b_l for level l by the equation

$$b_l = (n_l/n_c)/(n_l/n_c)^*,$$

or

$$b_l = (n_l/n_l^*)/(n_c/n_c^*),$$

so that b_l is the level- l number density not only relative to n_l^* but also relative to (n_c/n_c^*) .

Then the continuum transfer equation is

$$dI_\nu/d\ell = -n_l\alpha_l(\nu)(1 - b_l^{-1}e^{-h\nu/kT})[I_\nu - S_l(\nu)],$$

where

$$S_l(\nu) = (2h\nu^3/c^2)(b_l e^{h\nu/kT} - 1)^{-1}.$$

Let $d\tau_\nu = -n_l\alpha_l(\nu)\mu d\ell$, and, for simplicity, ignore stimulated recombination, which is usually negligible, so that $S_\nu = B'_\nu/b_l$ and $B'_\nu = (2h\nu^3/c^2)e^{-h\nu/kT}$. Then the transfer equation for level l is

$$\mu dI_\nu/d\tau_\nu = I_\nu - S_\nu,$$

from which we can write $J_\nu = \Lambda\{S_\nu\}$.

We need to calculate the departure coefficient b_1 for level 1 in order to determine the ratio of ions to neutral atoms. Consider first the simplest case of a 1-level atom with a continuum for which the statistical equilibrium equation is

$$n_1(R_{1c} + C_{1c}) = n_c(R_{c1} + C_{c1}).$$

Using b_1 , and R_{1c}^\dagger from page 13, this becomes

$$b_1(R_{1c} + C_{1c}) = R_{1c}^\dagger + C_{1c}$$

or

$$(1/b_1) = [(R_{1c}/R_{1c}^\dagger) + \epsilon]/(1 + \epsilon)$$

where in this case

$$\epsilon = C_{1c}/R_{1c}^\dagger.$$

When the stimulated recombination term in R_{1c}^\dagger is ignored, we have

$$R_{1c}/R_{1c}^\dagger = \int_{\nu_1}^{\infty} (1/h\nu) J_\nu d\nu / \int_{\nu_1}^{\infty} (1/h\nu) B'_\nu d\nu.$$

When $h\nu/kT \gg 1$, most of the contributions to both integrals occur near ν_1 , and this ratio is approximately J_{ν_1}/B'_{ν_1} .

$$\text{Then } S_{\nu_1} = (J_{\nu_1} + \epsilon B'_{\nu_1})/(1 + \epsilon).$$

As in our earlier discussion of monochromatic scattering, a first-order approximation for $J_\nu = \Lambda\{S_\nu\}$ is

$$J_{\nu_1}(\tau) = (\sqrt{3}/2) \int_0^\infty e^{-\sqrt{3}|t-\tau|} S_{\nu_1}(t) dt.$$

Then, when B'_{ν_1} and ϵ are constant with depth, we have the analytic solution

$$S_{\nu_1}(\tau) = B'_{\nu_1} [1 - (1 - \sqrt{\epsilon}) e^{-\sqrt{3\epsilon}\tau}],$$

where $\epsilon = \epsilon/(1 + \epsilon)$,

$$\text{and finally, } b_1(\tau) = 1/[1 - (1 - \sqrt{\epsilon}) e^{-\sqrt{3\epsilon}\tau}].$$

To obtain a numerical solution we can write the $1/b_1$ equation above as

$$(1/b_1) = [\int_{\nu_1}^{\infty} (1/h\nu) \Lambda\{B'_\nu/b_1\} d\nu / \int_{\nu_1}^{\infty} (1/h\nu) B'_\nu d\nu + \epsilon]/(1 + \epsilon)$$

and solve the set of simultaneous equations for $1/b_1$ corresponding to a set of depths in the atmosphere.

This solution in the 1-level case shows how b_1 is determined from the combined transfer and statistical equilibrium equations. The mathematical problem here is similar to the cases of monochromatic scattering and resonance line scattering considered earlier.

The ϵ parameter in this one-level case is $\epsilon = C_{1c}/R_{1c}^\dagger$, but this is not the appropriate result when there are more levels, since collisional ionization from level-1 is usually small compared with processes involving higher levels, as discussed below.

Consider again the two-level atom with a continuum. The equations for the continuum and level 1 are

$$n_c(P_{c1} + P_{c2}) = n_1P_{1c} + n_2P_{2c}$$

and

$$n_1(P_{1c} + C_{12}) = n_cP_{c1} + n_2(A_{21}\rho_{21} + C_{21}).$$

Eliminating n_2 we obtain a result similar to that for a single level:

$$n_1(R_{1c} + C_{1c}^\dagger) = n_c(R_{c1} + C_{c1}^\dagger)$$

where

$$C_{1c}^\dagger = C_{1c} + C_{12}P_{2c}/D_2,$$

$$C_{c1}^\dagger = C_{c1} + P_{c2}(A_{21}\rho_{21} + C_{21})/D_2, \text{ and}$$

$$D_2 = P_{2c} + A_{21}\rho_{21} + C_{21}.$$

Thus, in addition to R_{1c} and C_{1c} , ionization can occur by collisional excitation to level 2 followed by ionization from that level. In addition to R_{c1} and C_{c1} , recombination to level 1 can occur by recombination to level 2 followed mainly by collisional and radiative de-excitation.

We can obtain $1/b_1$ from the solution of a set of simultaneous equations as before, with expressions for ϵ and B' that include these additional rates.

Before continuing with the general equations for an N -level atom, we consider the limiting case in which $\tau_\nu \gg 1$ in the level-1 continuum. For such large optical depths, $J_\nu \rightarrow S_\nu = B'_\nu/b_1$ (again ignoring stimulated recombination), and $n_1P_{1c} \rightarrow n_cP_{c1}$. Also, we neglect C_{1c} and C_{c1} . Then J_ν in the level-1 continuum is not needed, and

$$n_1/n_c \rightarrow [(A_{21}\rho_{21} + C_{21})/C_{12}]/(P_{c2}/P_{2c}), \text{ or}$$

$$b_1 \rightarrow [(A_{21}\rho_{21} + C_{21})/C_{21}](R_{2c}^\dagger/R_{2c}),$$

where we have ignored C_{2c} .

This case will be considered further in the following section.

The On-The-Spot Approximation

In the first section of these notes we included terms representing a specified incident intensity at the boundary at $\tau = 0$ or at $\tau = \tau_m$ in either incident direction.

In general, the mean intensity J_ν at any depth in the atmosphere can be written as

$$J_\nu = J_\nu^{int} + J_\nu^{ext}$$

where $J_\nu^{int} = \Lambda\{S_\nu\}$ is the mean intensity produced within the atmosphere, and J_ν^{ext} is the mean intensity at the given depth from the attenuated surface illumination, given by the incident surface value times $E_2(\tau_\nu)$ or $E_2(t_m - \tau_\nu)$, depending on which surface is illuminated. Here we assume angle-independent incident intensity (rather than, for example, a narrow pencil beam from a distant star), and use the E_2 function rather than exponential attenuation to account for the range of μ values.

Consider an illuminated low-density interstellar cloud in which the collision rates are all negligible, and

$$n_1 R_{1c} \gg n_2 R_{2c} + n_3 R_{3c} + \dots$$

Then

$$n_1 (R_{1c}^{int} + R_{1c}^{ext}) = n_c (R_{c1} + R_{c2} + R_{c3} + \dots).$$

As noted at the end of the previous section, $n_1 R_{1c}^{int} \rightarrow n_c R_{c1}$ at large optical depths in the level-1 continuum. This is called the “on the spot” approximation for an optically thick medium, since each photon produced by a direct recombination to level 1 is assumed to be balanced by a photoionization at the same spot.

Then

$$n_1/n_c = (R_{c2} + R_{c3} + \dots)/R_{1c}^{ext},$$

where

$$R_{1c}^{ext} = 4\pi \int_{\nu_1}^{\infty} (1/h\nu) \alpha_1(\nu) J_{\nu}^{ext} d\nu.$$

Note that each $R_{cl} = (n_l/n_c)^* R_{cl}^{\dagger}$ where $(n_l/n_c)^*$ depends on n_e . Tabulations of $\alpha_l = R_{cl}/n_e$ for the levels of hydrogen and temperatures 5000, 10000, and 20000 K are given in Table 2.1 of Osterbrock, D. E., & Ferland, G. J., *Astrophysics of Gaseous Nebulae and Active Galactic Nuclei*, Univ. Science Books, 2006. The hydrogen ionization ratio thus depends on T , n_e , and the illuminating radiation, and does not require radiative transfer solutions.

The Strömgen Radius

Consider the mean intensity at the distance r from the center of a star of radius R . For simplicity let the intensity at the stellar surface be independent of μ . As viewed from the position at r , let θ_s be the angle between the center and outer edge of the star, so that $\sin \theta_s = R/r$. For a given frequency ν , the mean intensity at r is

$$J = (1/4\pi) I \int d\Omega = (1/2) I \int_0^{\theta_s} \sin \theta d\theta = (1/2) I (1 - \cos \theta_s)$$

or

$$J = (1/2) I (1 - \sqrt{1 - (R/r)^2}).$$

When $r \gg R$ this reduces to $J = (1/4) I (R/r)^2$.

Since the flux πF at the surface of the star is π times I , the mean intensity at r is

$$J = (1/4\pi) (\pi F) (R/r)^2.$$

At optical depth τ_{ν} into a nebula at distance r from a star with this flux,

$$J_{\nu} = (1/4\pi) (\pi F_{\nu}) (R/r)^2 e^{-\tau_{\nu}}.$$

Then the term R_{1c}^{ext} in the previous section becomes

$$R_{1c}^{ext} = (R/r)^2 \int_{\nu_1}^{\infty} (1/h\nu) \pi F_{\nu} \alpha_1(\nu) e^{-\tau_{\nu}} d\nu.$$

The optical depth in this expression is given by

$$\tau_\nu(z) = \int_0^z \alpha_1(\nu)n_1(z')dz'$$

where z is the geometrical depth into the nebula from its illuminated boundary, and where, for hydrogen,

$$\alpha_1(\nu) \approx 6.3 \times 10^{-18}(\nu_1/\nu)^3 \text{ (cm}^2\text{)}.$$

The on-the-spot equation given above can be written as

$$n_1/n_c = n_e f(T)/R_{1c}^{ext}.$$

Consider a hydrogen nebula with $n_c = n_p = n_e$ that is fully ionized at the illuminated boundary. For given values of temperature, illumination, and $n_H = n_1 + n_p$ we can calculate n_1/n_H at the boundary, given the assumption that $n_e = n_H$ there.

Then, at successive depths into the nebula we can then calculate n_1/n_H , and the corresponding n_p/n_H , based on the integrated values of n_1 in the expression for $\tau_\nu(z)$.

Table 2.2 of Osterbrock & Ferland lists the ratios n_1/n_H calculated in this way vs. the radial distance from the star r in parsecs for a nebula of uniform temperature $T = 7500$ K and density $n_H = 10 \text{ cm}^{-3}$ illuminated by a star having the radius of an O6 main sequence star, emitting the flux $\pi F_\nu = \pi B_\nu(40,000 \text{ K})$.

These calculations indicate that hydrogen is mostly ionized within a radius r_1 between 9.9 and 10.0 pc ($1 \text{ pc} = 3.086 \times 10^{18} \text{ cm}$), and is mostly neutral beyond r_1 .

This r_1 is called the Strömgen radius, and can be calculated approximately as follows.

The on-the-spot equation above can be written as

$$n_1 R_{1c}^{ext} = n_p^2 f(T).$$

Using $d\tau_\nu = n_1 \alpha_1(\nu) dr$ we obtain

$$R^2 \int_{\nu_1}^{\infty} (1/h\nu) \pi F_\nu e^{-\tau_\nu} d\tau_\nu d\nu = n_p^2 f(T) r^2 dr.$$

Integrating over ν on the left and r on the right gives

$$R^2 \int_{\nu_1}^{\infty} (1/h\nu) \pi F_\nu d\nu = \int_0^{\infty} n_p^2 f(T) r^2 dr.$$

Since the luminosity of the star is $L_\nu = (4\pi R^2) \pi F_\nu$, this becomes

$$\int_{\nu_1}^{\infty} (1/h\nu) L_\nu d\nu = 4\pi \int_0^{\infty} n_p^2 f(T) r^2 dr.$$

The left side of this equation is the total number of ionizing photons.

Suppose T is constant and $n_p = n_H$ for $r \leq r_1$, and $n_p = 0$ for $r > r_1$. Then the right side of this equation becomes the product of two terms:

$$\{n_H^2 f(T)\} \{(4\pi/3)r_1^3\}.$$

The first of these terms is the number of recombinations per unit volume. The second term is the volume of the ionized region, with r_1 as its radius. Thus r_1 can be determined from

the temperature and density of the nebula and the luminosity of the star. The Strömgen radius gives a useful estimate of the distance from the star where ionization ends and the gas becomes neutral, but detailed calculations show that there is not a sharp boundary between these two regions.

***N*-Level Resonance Continuum Equations**

For hydrogen, determining the degree of ionization is often the most critical part of the overall number density calculation. We have discussed how n_c/n_1 is found for 1-level and 2-level atoms. We now consider the general case with N levels.

In the 2-level case we showed how the $n = 2$ statistical equilibrium equation was used to eliminate n_2 from the continuum equation. For N levels we can use the set of $n = 2, 3, \dots, N$ equations to eliminate n_2, n_3, \dots, n_N from the continuum equation. However, we have found that in many applications, the continuum equation combined with the $n = 1$ equation, as shown below, gives a result with better convergence properties.

The continuum equation

$$n_c \sum_{l=1}^N P_{cl} = \sum_{l=1}^N n_l P_{lc}$$

may be written as

$$n_c [P_{c1} + (n_1^*/n_c^*) P_{cL}] = n_1 P_{1c} + Q_{Lc}.$$

where

$$P_{cL} = \sum_{l=2}^N (n_l^*/n_1^*) (R_{lc}^\dagger + C_{lc})$$

and

$$Q_{Lc} = \sum_{l=2}^N n_l (R_{lc} + C_{lc}).$$

The level-1 equation can be written as

$$n_1 (P_{1L} + P_{1c}) = Q_{L1} + n_c P_{c1}$$

where

$$P_{1L} = \sum_{l=2}^N C_{1l}$$

and

$$Q_{L1} = \sum_{l=2}^N n_l (A_{l1} \rho_{l1} + C_{l1}).$$

Using b_1 as defined on page 16, the combination of these two equations leads to the result

$$b_1 (R_{1c} + T_{1c}) = R_{1c}^\dagger + T_{c1}$$

where

$$T_{1c} = C_{1c} + P_{1L} (Q_{Lc}/Q_{L1c})$$

and

$$T_{c1} = C_{1c} + P_{cL} (Q_{L1}/Q_{L1c})$$

where $Q_{L1c} = Q_{L1} + Q_{Lc}$.

In order to retain the stimulated emission terms in a convenient way we define

$$R_{1c}^* = 4\pi \int_{\nu_1}^{\infty} (1/h\nu)\alpha_1(\nu)(2h\nu^3/c^2)e^{-h\nu/kT} d\nu$$

and

$$R'_{1c} = 4\pi \int_{\nu_1}^{\infty} (1/h\nu)\alpha_1(\nu)J_{\nu}(1 - b_1^{-1}e^{-h\nu/kT})d\nu.$$

Then

$$b_1(R'_{1c} + T_{1c}) = R_{1c}^* + T_{c1},$$

which finally becomes

$$(1/b_1) = (U + \epsilon_2)/(1 + \epsilon_1),$$

where

$$U = R'_{1c}/R_{1c}^*, \quad \epsilon_1 = T_{c1}/R_{1c}^*, \quad \text{and} \quad \epsilon_2 = T_{1c}/R_{1c}^*.$$

If we define

$$\gamma_{\nu} = 1 - (1/b_1)e^{-h\nu/kT},$$

then

$$U = \int_{\nu_1}^{\infty} (1/\nu)\alpha_1(\nu)\gamma_{\nu}J_{\nu}d\nu / \int_{\nu_1}^{\infty} (1/\nu)\alpha_1(\nu)(2h\nu^3/c^2)e^{-h\nu/kT} d\nu$$

This γ_{ν} , which is close to unity, has a second-order dependence on b_1 and is considered known from a previous iterative cycle. The $1/b_1$ equation above has been derived from the statistical equilibrium equations for the continuum and level 1, and expresses b_1 in terms of: J_{ν} in the level-1 continuum, the number densities n_2, n_3, \dots, n_N , the photoionization rates from these levels, and the net radiative rate coefficients ρ for the resonance lines. We determine b_1 as a function of depth by combining this equation with the radiative transfer equation for $\nu \geq \nu_1$.

This equation is

$$\mu dI_{\nu}/d\ell = -n_1\alpha_1(\nu)\gamma_{\nu}[I_{\nu} - S_1(\nu)] - \kappa'_{\nu}[I_{\nu} - S'(\nu)]$$

where

$$S_1(\nu) = (2h\nu^3/c^2)/(b_1e^{h\nu/kT} - 1)$$

and where the term $\kappa'_{\nu}[I_{\nu} - S'(\nu)]$ represents the absorptions and emissions from all processes other than those for the level-1 continuum. These other processes include the $\nu \geq \nu_1$ portions of the higher hydrogen continua, and the continua and lines of all other atoms and ions in this wavelength range. These other processes may depend to some extent on the b_1 solution. For example, κ'_{ν} may include Thomson scattering by free electrons, and n_e has a dependence on n_p which in turn depends on hydrogen ionization, and thus on b_1 . While it may appear that everything depends on everything else, we attempt in this development to derive equations for primary quantities, with secondary terms calculated from previous iterative steps.

The optical depth τ_ν is defined by

$$d\tau_\nu = -[n_1\alpha_1(\nu)\gamma_\nu + \kappa'_\nu]\mu d\ell.$$

Unless hydrogen is mostly neutral so that $n_1 \approx n_H$, n_1 will depend on hydrogen ionization and hence on b_1 . In practice, the iterative determination of τ_ν is usually very well behaved.

The transfer equation then becomes

$$\mu dI/d\tau_\nu = I_\nu - S_\nu$$

where

$$S_\nu = (1 - \delta_\nu)S_1(\nu) + \delta_\nu S'_\nu$$

or

$$S_\nu = (1 - \delta_\nu)(1/b_1)\gamma_\nu^{-1}(2h\nu^3/c^2)e^{-h\nu/kT} + \delta_\nu S'_\nu.$$

Here

$$\delta_\nu = \kappa'_\nu/[\kappa_1(\nu) + \kappa'_\nu], \text{ and } \kappa_1(\nu) = n_1\alpha_1(\nu)\gamma_\nu.$$

This equation for S_ν has the form $S_\nu = a_\nu(1/b_1) + c_\nu$, so that in the expression for U we can write

$$J_\nu = \Lambda\{a_\nu(1/b_1) + c_\nu\}.$$

As before, we can obtain a set of linear equations for the values of $1/b_1$ at a given set of depths in the atmosphere. The explicit coefficients in this set of equations are easily derived.

It is of interest to examine these equations in the $\tau \gg 1$ limit, for which $J_\nu \rightarrow S_\nu$. For simplicity let δ_ν and S'_ν be frequency independent. Then

$$U \rightarrow (1 - \delta)(1/b_1) + \delta(S'/\overline{B})$$

where

$$\overline{B} = \int_{\nu_1}^{\infty} (1/\nu)\alpha_\nu B'_\nu d\nu / \int_{\nu_1}^{\infty} (1/\nu)\alpha_1(\nu)\gamma_\nu d\nu.$$

This leads to the result

$$1/b_1 = [\epsilon_2 + \delta(S'/\overline{B})]/(\epsilon_1 + \delta).$$

Then $1/b_1 \rightarrow S'/\overline{B}$ when δ is much smaller than ϵ_1 and ϵ_2 , and $1/b_1 \rightarrow T_{1c}/T_{c1}$ when δ can be neglected.

Resonance Continuum With Incident Radiation

In the earlier discussion of the on-the-spot approximation we let $J_\nu = J_\nu^{int} + J_\nu^{ext}$. When this second term is added, the general equation given above for $1/b_1$ becomes

$$1/b_1 = (U + U^{ext} + \epsilon_2)/(1 + \epsilon_1),$$

where U depends on J_ν^{int} , and U^{ext} depends on J_ν^{ext} .

Since this equation is the same as before except that U^{ext} is added to ϵ_2 , it follows that in the $\tau \gg 1$ limit (with δ and S' frequency independent),

$$1/b_1 \rightarrow [U^{ext} + \epsilon_2 + \delta(S'/\overline{B})]/(\epsilon_1 + \delta).$$

In typical chromospheric applications the bound-free collision rates can be neglected. Then this equation reduces to

$$1/b_1 \rightarrow [R_{1c}^{ext} + C_{21}f_{2c} + R_{1c}^\dagger\delta(S'/\overline{B})]/(R_{2c}^\dagger f_{21} + \delta R_{1c}^\dagger)$$

where

$$R_{1c}^{ext} = 4\pi \int_{\nu_1}^{\infty} (1/h\nu)\alpha_1(\nu)J_\nu^{ext}d\nu,$$

$$f_{2c} = (n_2^*/n_1^*)R_{2c}/(R_{2c} + A_{21}\rho_{21} + C_{21}),$$

and

$$f_{21} = (n_1^*/n_1^*)(A_{21}\rho_{21} + C_{21})/(R_{2c} + A_{21}\rho_{21} + C_{21}).$$

This equation for $1/b_1$ shows the relative dependence of incident radiation, the collisional and radiative transitions between levels 1 and 2, and the influence of absorption and emission by other processes.

When $R_{1c}^{ext} = \delta = 0$, this equation reduces to

$$b_1 \rightarrow [(A_{21}\rho_{21} + C_{21})/C_{21}](R_{2c}^\dagger/R_{2c})$$

as we derived earlier.

It is important to note that when $\delta = 0$ and R_{1c}^{ext} dominates, b_1 still depends on $A_{21}\rho_{21} + C_{21}$, unless $R_{2c} \ll (A_{21}\rho_{21} + C_{21})$. The simple derivation of the Strömgen radius given earlier has no reference to ρ_{21} or C_{21} .

Determining the Electron Density

In the Saha-Boltzmann equation for level-1 of hydrogen, $g_1/2U_c = 1$, so that

$$n_1 = b_1 n_e n_p \Psi(T),$$

where

$$\Psi(T) = (h^2/2\pi m_e kT)^{3/2} e^{h/\nu_{c1}/kT}$$

where ν_{c1} is the threshold frequency.

The electron density is the sum of the proton density and the number of electrons contributed by the ionization of other constituents. We write

$$n_e = n_p + Zn_H$$

where n_H is the total hydrogen number density

$$n_H = \sum_{l=1}^N n_l + n_p.$$

For the moment we ignore hydrogen in molecular form.

Defining Z in this way is convenient since Z is roughly the fraction, relative to hydrogen, of elements that are singly ionized. In the 3000 to 6000 K temperature range Z generally has values between 10^{-4} and 10^{-3} . Here we assume that Z , as a function of depth, is given from a separate determination of the ionization equilibrium of constituents other than hydrogen.

We define $\sigma = \sum_{l=2}^N n_l$, and combine $n_1 + \sigma + n_p = n_H$ with the equations for n_1 and n_e above. The result is a quadratic equation with the solution

$$n_e = \{ \sqrt{(1 + b_1 \Psi Z n_H)^2 + 4b_1 \Psi (n_H - \sigma)} + b_1 \Psi Z n_H - 1 \} / 2b_1 \Psi$$

As $T \rightarrow 0$, $\Psi \rightarrow \infty$, and $n_e \rightarrow Z n_H$, as we expect when hydrogen is neutral but other atoms are ionized. For high temperatures we get $n_e \rightarrow n_p + Z n_H$, as we expect when hydrogen is fully ionized.

At low temperatures a significant fraction of hydrogen can be in molecular form. Here we consider only H_2 , but in general we should include molecules consisting of hydrogen combined with other atoms. The equations for n_{CH} , n_{OH} , and n_{CO} as well as for n_{H_2} are discussed in §5 of Avrett & Loeser 2008 (cited p. 5)

Then the n_H equation is

$$n_H = n_1 + \sigma + n_p + 2n_{H_2}.$$

In LTE at the temperature T , n_{H_2} and n_1 are related by

$$n_{H_2} = C(T)n_1^2$$

where $C(T)$ is a tabulated function (e.g., see Tsuji, T. 1973, Molecular abundances in stellar atmospheres. II. A&A, 23, 411).

This n_H equation is then quadratic in n_1 , with the solution

$$n_1 = \{ \sqrt{8C(n_H - \sigma - n_p) + 1} - 1 \} / 4C$$

which reduces to $n_1 = n_H - \sigma - n_p$ as $C \rightarrow 0$.

For large C , $n_1 = \sqrt{(n_H - \sigma - n_p)/2C}$, for which

$$n_{H_2} = Cn_1^2 = (n_H - \sigma - n_p)/2,$$

showing that all hydrogen is in molecular form.

Given n_H , T , b_1 , Z , and σ , the equations given above can be used to determine n_e , n_1 , n_p , and n_{H_2} .

The Negative Hydrogen Ion

The rate equations that describe the coupling between hydrogen atoms and ions with the negative hydrogen ion H^- , and with H_2 , and H_2^+ are given in detail by Lites, B. W., & Mihalas, D. 1984, The H^- equilibrium using coupled rate equations for H^- , H , H^+ , H_2 , and H_2^+ , Solar Phys., 93, 23. Below we give the basic equations for H^- , which dominates the opacity in the photospheres of solar-type stars.

The bound-free absorption coefficient for H^- is given by

$$\kappa_\nu(\text{H}_{\text{bf}}^-) = n_{\text{H}^-} \alpha_\nu(\text{H}^-) [1 - (1/b_{\text{H}^-}) e^{-h\nu/kT}].$$

The cross section $\alpha_\nu(\text{H}^-)$ is zero for wavelengths greater than the threshold value $1.64 \mu\text{m}$, and has a maximum near $0.85 \mu\text{m}$. Values of the cross section vs. wavelength are given by Wishart, A. W. 1979, The bound-free photo-detachment cross-section of H^- , MNRAS, 187, 59P. The H^- number density is

$$n_{\text{H}^-} = b_{\text{H}^-} n_{\text{H}^-}^*$$

where the equilibrium expression in this case is

$$n_{\text{H}^-}^* = n_{\text{H1}} n_e (h^2/2\pi m_e kT)^{3/2} (1/4) e^{h\nu_{\text{H}^-}/kT}$$

and ν_{H^-} is the threshold frequency corresponding to $1.64 \mu\text{m}$.

Before giving the equations for the H^- departure coefficient b_{H^-} we note that the H^- free-free absorption coefficient has the form

$$\kappa_\nu(\text{H}_{\text{ff}}^-) = n_{\text{H1}} n_e F_\nu(T)$$

where values of the function $F_\nu(T)$ are given by Stilley, J. L. & Callaway, J. 1970, Free-free absorption coefficient of the negative hydrogen ion, ApJ, 160, 245. In both of these equations n_{H1} is the number density of neutral hydrogen in the ground state.

At a temperature of 6000 K (typical of the solar photospheric layers where the visible and near infrared spectrum is formed) the H^- bound-free and H^- free-free opacities, multiplied by $10^{-38} n_{\text{H1}} n_e$, depend on wavelength λ as indicated below.

$\lambda(\mu\text{m})$	bound-free	free-free	total	
0.50	2.82	0.15	2.97	
0.85	3.86	0.39	4.25	maximum
1.20	2.78	0.76	3.54	
1.60	0.13	1.32	1.45	
1.65	0.00	1.40	1.40	minimum
2.00	0.00	2.40	2.40	

Even when all other opacities are included, the total opacity for solar-type stars has a minimum near $1.65 \mu\text{m}$, where the H^- bound-free opacity is zero and the H^- free-free opacity has not yet increased to large values. At this wavelength, monochromatic optical depth unity is located at the greatest geometrical depth in the atmosphere. The opacity has a secondary minimum near $0.4 \mu\text{m}$ and then continually increases at shorter wavelengths, due to other opacity sources, as it continually increases longward of $1.65 \mu\text{m}$, due mainly to H^- free-free opacity, and to H free-free opacity at much longer wavelengths.

The H^- departure coefficient b_{H^-} is close to unity in the deep layers, but differs from unity higher in the atmosphere, and is determined as follows.

The photodetachment rate for the process $\text{H}^- + h\nu \rightarrow \text{H} + e$ is $n_{\text{H}^-} R$, where

$$R = 4\pi \int_{\nu_{\text{H}^-}}^{\infty} (1/h\nu) \alpha_\nu J_\nu d\nu.$$

The inverse rate depends on

$$R^\dagger = 4\pi \int_{\nu_{H^-}}^{\infty} (1/h\nu)\alpha_\nu e^{-h\nu/kT}(2h\nu^3/c^2 + J_\nu)d\nu.$$

The electron collisional detachment rate for the process $H^- + e \rightarrow H + 2e$ is $n_{H^-}n_e C_{H^-,e}$, and we define

$$r_e = n_e C_{H^-,e}.$$

We let $n_{H^-}n_H C_{H^-,H}$ be the rate of associative detachment $H^- + H \rightarrow H_2 + e$, and define

$$r_H = n_H C_{H^-,H}.$$

Finally, we let $n_H^3 C_{3H}$ be the rate for the three-body collision process $3H \rightarrow H_2 + H$, and define

$$r_{3H} = n_H^3 C_{3H}.$$

The statistical equilibrium equation for H^- then can be written as

$$n_{H^-}(R + r_e + r_H) = n_{H^-}^*(R^\dagger + r_e + b_{H_2}r_H).$$

The departure coefficient b_{H_2} can be found from the H_2 statistical equilibrium equation

$$r_{3H} + n_{H^-}r_H = b_{H_2}(r_{3H} + n_{H^-}^*r_H).$$

Solving for $b_{H^-} = n_{H^-}/n_{H^-}^*$ gives the result, in the familiar form,

$$1/b_{H^-} = (R + \epsilon)/(R^\dagger + \epsilon),$$

where

$$\epsilon = r_e + r_H(1 + a)$$

and

$$a = n_{H^-}^*r_H/r_{3H}.$$

The parameter ϵ depends on n_H , n_e , and T , while R and R^\dagger depend on integrals over J_ν and on T . Given these quantities, vs. depth, we can calculate the corresponding b_{H^-} and H^- opacity. Here it is sufficient to solve the transfer equation for J_ν , solve this $1/b_{H^-}$ equation and obtain the H^- opacity, obtain a new J_ν from the transfer equation, etc., since J_ν and b_{H^-} are not strongly coupled together.

A detailed discussion of H^- non-LTE effects in the solar atmosphere is given by Vernazza, J. E., Avrett, E. H., & Loeser, R. 1981, Structure of the solar chromosphere. III. Models of the EUV brightness components of the quiet Sun, ApJS, 45, 635.

Energy Balance Equations

We have shown that

$$R_{lc} = 4\pi \int_{\nu_l}^{\infty} (1/h\nu)\alpha_l(\nu)J_\nu d\nu$$

is the number of photoionizations from level l per atom in level l per unit time, and that

$$R_{cl} = (n_l^*/n_c^*)4\pi \int_{\nu_l}^{\infty} (1/h\nu)\alpha_l(\nu)e^{-h\nu/kT}(2h\nu^3/c^2 + J_\nu)d\nu$$

is the number of recombinations to level l per ion per unit time.

In order to deal with energy rather than the number of transition we need to remove the $1/h\nu$ term from these two expressions. Recalling that $b_l = (n_l/n_l^*)/(n_c/n_c^*)$, we can write

$$\Phi_l = 4\pi n_l [(1/b_l) \int_{\nu_l}^{\infty} \alpha_l(\nu) e^{-h\nu/kT} (2h\nu^3/c^2 + J_\nu) d\nu - \int_{\nu_l}^{\infty} \alpha_l(\nu) J_\nu d\nu]$$

as the net radiative cooling rate for the level- l continuum, or the energy per unit volume and time transferred from ions into photons by recombinations to level- l , minus the amount that photons return by ionizations from level- l .

This equation also applies to the net radiative cooling rate for H^- by simply changing the subscript l to H^- .

The continuum transfer equation given earlier can be written in the form

$$\mu dI_\nu/dh = -n_l \alpha_l(\nu) [I_\nu - (1/b_l) e^{-h\nu/kT} (2h\nu^3/c^2 + I_\nu)],$$

where on the left side we have introduced $dh = \mu d\ell$ to change from distance ℓ in the direction of I_ν to height h in the outward direction.

Since $J_\nu = (1/2) \int_{-1}^{+1} I_\nu d\mu$ and $\pi F_\nu = 2\pi \int_{-1}^{+1} I_\nu \mu d\mu$ we can integrate the transfer equation over direction to obtain

$$d(\pi F_\nu)/dh = -4\pi n_l \alpha_l(\nu) [J_\nu - (1/b_l) e^{-h\nu/kT} (2h\nu^3/c^2 + J_\nu)].$$

Finally, consider the integral of this equation over the l continuum, with the integrated flux defined as

$$\pi F_l = \int_{\nu_l}^{\infty} \pi F_\nu d\nu.$$

It then follows that

$$d(\pi F_l)/dh = \Phi_l,$$

so that the net radiative cooling rate for the level- l continuum is the derivative of the integrated flux πF_l with respect to height. Constant flux implies a zero net radiative cooling rate.

The derivation above is for the level- l continuum for which the bound-free absorption coefficient is given by $\kappa_l(\nu) = n_l \alpha_l(\nu)$. The results are applicable for cases with other forms of the absorption coefficient. For example, the hydrogen free-free absorption coefficient at any frequency ν is given by

$$\kappa_\nu^{ff} = 3.7 \times 10^8 T^{-1/2} Z^2 n_e n_i \nu^{-3} (1 - e^{-h\nu/kT}) \bar{g}_{ff}$$

(see Rybicki, G. B. & Lightman, A. P. 1979, Radiative Processes in Astrophysics, Wiley, p. 162). For free-free processes the departure coefficient b is unity. The hydrogen free-free net radiative cooling rate at a given atmospheric depth is then

$$\Phi^{ff} = 4\pi [\int_0^\infty \kappa_\nu^{ff} e^{-h\nu/kT} (2h\nu^3/c^2 + J_\nu) d\nu - \int_0^\infty \kappa_\nu^{ff} J_\nu d\nu].$$

For a line transition between upper and lower levels u and l , the net radiative cooling rate is

$$\Phi_{ul} = h\nu_{ul}[n_u(A_{ul} + B_{ul}\bar{J}) - n_l B_{lu}\bar{J}].$$

and then

$$\Phi_{ul} = h\nu_{ul}n_u A_{ul} \rho_{ul}$$

in terms of the net radiative rate coefficient $\rho_{ul} = (1 - \bar{J}/S_{ul})$

The sum of Φ_l , Φ^{ff} , and Φ_{ul} for all bound-free, free-free, and bound-bound transitions for all important atoms, ions, and molecules represents the net energy transferred from the gas into radiation. In radiative equilibrium, i.e., in a steady state with only radiative transport, we should have $\sum \Phi = 0$. This is equivalent to having the integrated flux be constant with depth.

Outer regions of stellar atmospheres are often not in radiative equilibrium but are heated by the dissipation of mechanical wave energy or by magnetohydrodynamic effects. Let W represent such heating (in $\text{erg cm}^{-3}\text{s}^{-1}$) at a given depth in the atmosphere. Then we should have $\sum \Phi = W$ at that depth in a steady state. It is possible by means of successive trial solutions of the equations discussed here to arrive at a distribution of temperature and density for which this constraint is satisfied.

The Grey Atmosphere

For completeness we include a brief discussion of the special case of LTE radiative equilibrium in a semi-infinite atmosphere where the absorption coefficient κ has no frequency dependence. The $\Phi = 0$ equation then reduces to $B = J$ where $B = \int_0^\infty B_\nu d\nu$ and $J = \int_0^\infty J_\nu d\nu$. Thus $B(\tau)$ is given by the integral equation

$$B(\tau) = \int_0^\infty E_1(|t - \tau|)B(t)dt.$$

Here τ is defined by $d\tau = -\kappa \mu d\ell$, and the transfer equation is

$$\mu dI/d\tau = I - B.$$

It was noted on page 3 that at large τ the flux H , which is constant in this case, is $(1/3)dB/d\tau$ (since $S = B$). Thus $B(\tau) \rightarrow 3H\tau + \text{constant}$ at large τ . This result supplies the multiplier needed to determine B from the integral equation above.

If as before we replace $E_1(x)$ by the first-order approximation $\sqrt{3}e^{-\sqrt{3}x}$, then the integral equation has the solution

$$B(\tau) = 3H(\tau + 1/\sqrt{3}).$$

Without this approximation, the solution is

$$B(\tau) = 3H[\tau + q(\tau)]$$

where $q(\tau)$ is called the Hopf function, which can be determined numerically. Representative values are

$$q(0) = 1/\sqrt{3} = 0.5773..$$

$$q(1) = 0.6985..$$

$$q(2) = 0.7079..$$

$$q(\infty) = 0.7104..$$

We noted on page 1 that B , the Planck function integrated over all ν , is $\sigma T^4/\pi$, and that $\pi F = 4\pi H = \sigma T_{eff}^4$ where T_{eff} is the effective temperature of the atmosphere. Then the solution in this case can be expressed as

$$T(\tau) = T_{eff}\{(3/4)[\tau + q(\tau)]\}^{1/4}.$$

which gives the LTE radiative equilibrium temperature distribution when κ has no frequency dependence.

Continuum Opacities

We have referred to $\alpha_\ell(\nu)$ as the photoionization cross section, or the bound-free absorption coefficient, for an atom in energy level ℓ . We have also given expressions for the H and H⁻ free-free absorption coefficients. Model atmosphere calculations require such absorption coefficients or opacities for all atoms, ions, and molecules. A discussion of the principal sources of opacity in stellar atmospheres can be found in Novotny, E. 1973, *Introduction to Stellar Atmospheres and Interiors*, Oxford Univ. Press, Oxford. Expressions for the photoionization cross sections corresponding to the $\ell = 1$ ground state of an extensive list of atoms and ions is given by Verner, D. A., Ferland, G. J., & Korista, K. T. 1996, *Atomic data for astrophysics. II. New analytic fits for photoionization cross sections of atoms and ions*, *ApJ*, 465, 487.

Line Opacities

While bound-free continua are the important opacity sources for hot stars, line opacity dominates the spectra of cooler stars. Model atmospheres for cool stars need to include the opacity due to millions of lines. Extensive line lists are available from several web sites:

<http://www-amdis.iaea.org/AMDIS>,

http://acldata/nist/gov/nist_atomic_spectra.html,

<http://wwwsolar.nrl.navy.mil/chianti.html>,

and particularly <http://kurucz.harvard.edu>.

The Kurucz website lists the wavelengths and strengths of roughly 50 million atomic lines and 100 million molecular lines, mostly the result of calculations, since only a small fraction of the total have been measured in the laboratory.

The compilation of line opacities has been a major undertaking which has been successful in matching spectra from a variety of stellar photospheres. To interpret spectra formed in chromospheric and higher layers we need not only line opacities but also to be able to determine the departures from LTE for each atom and ion. This is a further major undertaking. See Short, C. I., & Hauschildt, P. H. 2005, *A non-LTE line blanketed model of a solar-type star*, *ApJ*, 618, 926, and Fuhrmeister, B., Schmitt, J. H. M. M., & Hauschildt, P. H. 2006, *PHOENIX model chromospheres of mid- to late-type M Dwarfs*, *A&A*, 436, 677.

Hydrostatic Equilibrium

The equation of hydrostatic equilibrium relating the pressure gradient and density in a gravitational field is

$$dp/dx = g\rho$$

where p is the total pressure, x is geometrical depth that increases in the direction of the pull of gravity, g is the gravitational constant within the atmosphere, and ρ is the mass density. In the atmosphere of a star of mass M_* and radius R_* we would have the surface value $g = GM_*/R_*^2$.

The mass density can be written as

$$\rho = m_{\text{H}}(1 + 4Y)n_{\text{H}}$$

where we ignore the small contribution of electrons and elements other than hydrogen and helium. Here m_{H} is the hydrogen atomic mass, n_{H} is the total number density of hydrogen in all forms (i.e., the proton density), and Y is the helium-to-hydrogen abundance ratio $n_{\text{He}}/n_{\text{H}}$. For simplicity we have used 4 instead of 4.0026 for $m_{\text{He}}/m_{\text{H}}$. n_{H^-} is usually too small to affect the density or pressure, even though the H^- opacity can be significant.

We write the total pressure as $p = p_{\text{gas}} + p_{\text{turb}} + p_{\text{exp}}$.

The gas pressure is given by

$$p_{\text{gas}} = (n_{\text{H1}} + n_{\text{p}} + n_{\text{H2}} + n_{\text{He}} + n_{\text{e}})kT$$

where n_{H1} is the neutral hydrogen density and n_{H2} is the molecular hydrogen density. Since the total hydrogen density is given by $n_{\text{H}} = n_{\text{H1}} + n_{\text{p}} + 2n_{\text{H2}}$, it follows that

$$p_{\text{gas}} = (n_{\text{H}} - n_{\text{H2}} + n_{\text{He}} + n_{\text{e}})kT.$$

Turbulent motions in the atmosphere can give rise to the turbulent pressure

$$p_{\text{turb}} = (1/2)\rho V_{\text{turb}}^2.$$

If the gas expands due to a flow velocity, normally satisfying the continuity equation $V_{\text{exp}}n_{\text{H}} = \text{constant}$, we add the expansion pressure

$$p_{\text{exp}} = \rho V_{\text{exp}}^2.$$

Here we do not include a radiation pressure term, which can be significant for hot stars. Then we can write the total pressure as

$$p = n_{\text{H}}F$$

where

$$F = [1 + Y - (n_{\text{H2}}/n_{\text{H}}) + n_{\text{e}}/n_{\text{H}}]kT + m_{\text{H}}(1 + Y)[(1/2)V_{\text{turb}}^2 + V_{\text{exp}}^2].$$

Eliminating n_{H} between these equations for p and ρ gives

$$\rho = [m_{\text{H}}(1 + 4Y)/F]p.$$

We define

$$G = gm_{\text{H}}(1 + 4Y)/F,$$

so that the hydrostatic equilibrium equation becomes

$$dp/dx = Gp.$$

Let $p = p_r$ at the reference depth x_r . Then the solution of this equation is

$$p(x) = p_r e^{H(x)}$$

where $H(x)$ is the pressure scale height

$$H(x) = \int_{x_r}^x G(x') dx',$$

which represents the distance over which p changes by the factor e (assuming constant G).

The following are typical values of H for the solar surface gravity. In the temperature range 4000-5000 K, hydrogen is mostly neutral so that $n_e/n_{\text{H}} \ll 1$, and $H \approx 100$ km for $V_{\text{turb}} = 0$, and $H \approx 130$ km for $V_{\text{turb}} = 4 \text{ kms}^{-1}$. In the temperature range 10,000-15,000 K, hydrogen is mostly ionized so that $n_e/n_{\text{H}} \approx 1$, and $H \approx 500$ km for $V_{\text{turb}} = 0$, and $H \approx 900$ km for $V_{\text{turb}} = 10 \text{ kms}^{-1}$.

For a stellar surface gravity 1/10 of the solar value, the scale heights will be 10 times larger.

An alternative to choosing the pressure p_r at the reference depth x_r is to specify a given value for the optical depth at x_r at a given wavelength. A typical choice is for the optical depth in the continuum at 500 nm to be unity at $x = 0$. This is a convenient way to determine the arbitrary multiplicative constant in the equation $dp/dx = Gp$. This constraint can be applied by starting with a value of p_r at $x = 0$, determining $p(x)$, and integrating to get τ_{500} at $x = 0$. The calculation is then repeated with a smaller or larger p_r if this τ value is, respectively, larger or smaller than unity.

If T , n_e/n_{H} , $n_{\text{H}_2}/n_{\text{H}}$, V_{turb} , and V_{exp} are given vs. x (along with Y , which is normally assumed constant), then we can obtain $p(x)$ and $n_{\text{H}}(x)$. Note that n_e/n_{H} and $n_{\text{H}_2}/n_{\text{H}}$ are determined as part of the overall model calculation.

For flow velocities that satisfy mass conservation, V_{exp} is proportional to $1/n_{\text{H}}(x)$. Since the pressure depends on V_{exp}^2 , the scale height is increased by flows in either the outward or the inward direction. Non-zero values of V_{turb} also cause an increase in scale height. Solar limb observations indicate that the chromosphere is more extended than calculations with $V_{\text{turb}} = 0$ predict, and for this reason many atmospheric models assume a given $V_{\text{turb}}(x)$.

The height of the top of the solar chromosphere, just below the chromosphere- corona transition region, can be determined by limb observations of the neutral helium line at 1083 nm. The observed bright narrow ring around the outer edge of the Sun, except in coronal hole regions, is caused by helium ionization due to coronal illumination, and is not greatly affected by spicules and other projections of chromospheric material into the corona. See Avrett, E. H., Fontenla, J. M., & Loeser, R. 1994, Formation of the solar 10830 A line, in *Infrared Solar Physics*, ed. D. M Rabin, J. T. Jefferies, & C. Lindsey, (Dordrecht: Kluwer), 35.

$V_{turb}(x)$ is often identified with the non-thermal line broadening velocity V_{nt} in the expression for the Doppler width

$$\Delta\nu_D = (\nu_0/c)\sqrt{(2kT/m_a) + V_{nt}^2}.$$

This equation was given earlier (p. 5), without V_{nt} , as the thermal Doppler width.

In principle, $V_{nt}(x)$ can be determined as part of the atmospheric modeling procedure from a comparison between calculated and observed central line widths. If the Doppler core of a line is calculated to be formed at depth x and temperature T and if the observed Doppler core is broader, then the V_{nt} needed for agreement is the non-thermal velocity at that x .

In practice, it is not always possible to distinguish between small-scale motions that produce Doppler broadening and a number of macroscopic effects. A stellar line flux profile is clearly affected by variations across the entire stellar disk. Solar intensity profiles often represent averages over inhomogeneous regions except at the highest spatial and temporal resolution near disk center.

Thus, there is considerable uncertainty in determining $V_{nt}(x)$, and in setting $V_{turb}(x) = V_{nt}(x)$. The forces that increase the scale height and extend the atmosphere might not have the form of an addition to the gas pressure. An alternative is to let $V_{turb} = 0$ and to replace the constant g by the effective gravity $g_{eff}(x) \leq g$ in the hydrostatic equilibrium equation, so that

$$dp/dx = g_{eff}(x)\rho.$$

This approach is discussed in a recent paper by Fontenla, J. M., Balasubramaniam, K. S., & Harder, J. 2007, Semiempirical models of the solar atmosphere. II. The quiet-Sun low chromosphere at moderate resolution, ApJ 667, 1243. Their chromospheric model has $g_{eff}(x)$ varying from the solar gravitational constant $g = 0.274 \text{ km s}^{-2}$ to a minimum of 0.174 km s^{-2} in the upper chromosphere.

Time Variations, Mass Flows, and Particle Diffusion In the absence of time variations, mass flows, and diffusion effects, the *local* statistical equilibrium equation for the level m number density is

$$0 = \sum_{l \neq m} (n_l P_{lm} - n_m P_{ml}) + n_c P_{cm} - n_m P_{mc},$$

where P_{ij} is the transition rate (s^{-1}) from i to j per particle in the initial state. When these three effects are included, this equation becomes

$$\partial n_m / \partial t + d[n_m(U + V_m)] / dz = \sum_{l \neq m} (n_l P_{lm} - n_m P_{ml}) + n_c P_{cm} - n_m P_{mc},$$

where t is time, z is geometrical depth, U is the fluid or center of mass velocity, and V_m is the diffusion velocity. V_m has an effect similar to U except that neutral atoms and ions move in opposite directions. The diffusion velocity can be calculated given the local temperature and temperature gradient and the neutral and ion number densities and their gradients.

The terms on the left side of the statistical equilibrium equation cause the number density at one depth to depend on the number densities at other depths, and cause the number densities to vary with time. These are non-local effects that are in addition to the non-local radiative transfer effects. These are important when there are large temperature variations over small distances, as in the solar chromosphere-corona transition region, or if dU/dz or $\partial n_m/\partial t$ are significant, since they cause changes in the ionization of hydrogen, helium, and other elements.

A numerical approach to the solution of this more general problem is to define the function

$$G = (1/n_m)\{\partial n_m/\partial t + d[n_m(U + V_m)]\}$$

so that the statistical equilibrium equation can be written in the standard form

$$n_m(\sum_{l \neq m} P_{ml} + P_{mc} + G_m) = \sum_{l \neq m} n_l P_{lm} + n_c P_{cm},$$

which allows the non-LTE equations to be solved in the same way as before, by simply adding G_m to the ionization rate P_{mc} . The calculation of G_m is, of course, non-trivial, but has been discussed at length in four papers by Fontenla, Avrett, and Loeser: 1990, Energy balance in the solar transition region. I. Hydrostatic thermal models with ambipolar diffusion, *ApJ*, 355, 700; ...II. Effects of pressure and energy input on hydrostatic models, *ApJ*, 377, 712; ...III. Helium emission in hydrostatic, constant-abundance models with diffusion, *ApJ*, 406, 319; and ...IV. Hydrogen and helium mass flows with diffusion, *ApJ*, 572, 636.

Putting It All Together

The modeling discussed here is 1-dimensional and time-independent. We have given the equations for plane-parallel geometry, and without flow velocities, but only a few modifications are needed to convert to spherical coordinates, and to include radial velocities. A complete discussion of the spherical case, including flows, is given by Avrett, E. H. & Loeser, R. 1984, Line transfer in static and expanding spherical atmospheres, in *Methods in Radiative Transfer*, ed. W. Kalkofen, Cambridge Univ. Press, 341. For a review of atmospheric modeling, including references to earlier work, see Avrett, E. H. 1996, Next generation model atmospheres, in *Stellar Surface Structure*, ed K. G. Strassmeier & J. L. Linsky, I.A.U. Symp. 176, (Dordrecht: Kluwer), 503. And see the basic textbook of Mihalas, D. 1978, *Stellar Atmospheres*, 2nd ed. (San Francisco: Freeman).

Different types of model atmospheres can be calculated. The usual input is temperature as a function of some depth variable such as height, radius, column mass, or optical depth at some wavelength. If hydrostatic or pressure equilibrium (including flows) can be assumed (or if pressure is assumed constant, as might be assumed in an interstellar cloud), then the density distribution can be calculated. If energy balance can be imposed, either with radiative equilibrium alone, or including non-radiative heating and energy transfer, then the temperature can be calculated as well, and the model atmosphere and calculated spectrum depend only on parameters such as surface gravity, effective temperature (i.e., the overall energy flux), and the elemental abundances (that control opacities and ionization equilibrium).

Energy-balance models that include the opacities due to large numbers of lines throughout the spectrum are called line blanketed models. LTE line blanketed models for a range of stellar effective temperatures and surface gravities have been given by Kurucz, R. L. 1979, Model atmospheres for G, F, A, B, and O stars, *ApJS*, 40, 1, by Kurucz, R. L. 1992, Model atmospheres for population synthesis, in *The Stellar Populations of Galaxies*, ed. R. Barby & A. Renzini, IAU Symp. 140, 225, and by Castelli, F., & Kurucz, R. L. 2003, New grids of ATLAS9 model atmospheres, in *Modelling of Stellar Atmospheres*, IAU Symp. 210, ed. N. Piskunov, W. W. Weiss, & D. F. Gray, A20, arXiv:astro-ph/04050087v1. See also the extensive models of B. Gustafsson, et al. at <http://www.astro.uu.se>, and those on the Kurucz website.

A solar chromospheric model with non-LTE line blanketing and prescribed non-radiative heating has been calculated by Anderson, L. S., & Athay, R. G. 1989, Line blanketing without local thermodynamic equilibrium. II. A solar-type model in radiative equilibrium, *ApJ*, 339, 558. See also the stellar models with non-LTE line blanketing by Short & Hauschildt 2005 and Fuhrmeister et al. 2006, cited p. 30, Lanz, T. & Hubeny, I. 2007, A grid of NLTE line blanketed model atmospheres of early B-type stars, *ApJS*, 169, 83, and Kudritzki, R. P., Urbaneja, M. A. & Puls, J. 2006, Atmospheres and winds of PN central stars, in *Planetary Nebulae in Our Galaxy and Beyond*, IAU Symp. 234, ed. M. J. Barlow & R. H. Méndez, Cambridge Univ. Press, 119.

It would be remarkable to find that the complete emergent spectrum calculated from such a model of the Sun, star, or another source, matches in detail the spectrum that is observed, due to the many assumptions, approximations, and uncertain data in the calculations. Such a match is the objective, however. Another modeling approach is to try to match the observed spectrum by detailed adjustments of the assumed temperature distribution, and other parameters if necessary, in the model emitting region. This is called semi-empirical modeling, since the results rely on theoretical calculations apart from a minimum of empirical parameter adjustments. Examples are the solar models of Vernazza et al. 1981, cited p.27, and those of Avrett & Loeser 2008, cited p.5.