Class 6 Notes: Absorption lines

We now come to our second application of what we have learned about radiative transfer: absorption spectroscopy. Before the advent of radio telescopes this was our our only source of knowledge about interstellar gas, and it is still our primary means of studying the ISM and IGM in the high redshift universe, where radio observations are very difficult. Absorption spectroscopy has the disadvantage that it relies on serendipity – we can only observe things that happen to have a bright background source for which we can obtain a spectrum. When that is the case, however, absorption spectroscopy provides the most sensitive measurements available for studying the ISM and IGM.

I. Equivalent width of lines

Consider observing a bright continuum point source, such as a star or quasar that subtends a small solid angle $\Delta\Omega$ on the sky. The source produces an intensity $I_\nu(0)$, and in the absence of any intervening emission of absorption, the flux that we observe from the source is

$$F_\nu = \int I_\nu(0)\, d\Omega = I_\nu(0)\Delta\Omega \equiv F_\nu(0). \tag{1}$$

Now suppose that the light from this source passes through a cloud of foreground gas, which we assume to be uniform over $\Delta\Omega$. The transfer equation for this system is

$$I_\nu = I_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\rm exc})(1 - e^{-\tau_\nu}), \tag{2}$$

where $T_{\rm exc}$ is the excitation temperature of the intervening matter. As a result, the flux that we observe is

$$F_\nu = \int I_\nu\, d\Omega = F_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\rm exc})\Delta\Omega(1 - e^{-\tau_\nu}), \tag{3}$$

where we have used the assumption that τ_ν is constant over the angular extent of the cloud.

For optical frequencies, we usually have $n_u/n_\ell \ll 1$ since most of the ISM is cold, and as a result $B_\nu(T_{\rm exc})\Delta\Omega \ll F_\nu(0)$. Thus, to good approximation we have

$$F_\nu = F_\nu(0)e^{-\tau_\nu}. \tag{4}$$

In general τ_ν has a non-negligible value only over a narrow range in frequency, and outside this narrow range we can directly measure $F_\nu(0)$. By simply interpolating in frequency from one side of a line to the other, we can therefore estimate $F_\nu(0)$ even in the frequency region where a line is absorbed. We therefore define the dimensionless equivalent width of a line by

$$W \equiv \int \left(1 - \frac{F_\nu}{F_\nu(0)}\right)\frac{d\nu}{\nu_0} = \int \left(1 - e^{-\tau_\nu}\right)\frac{d\nu}{\nu_0}, \tag{5}$$

where ν_0 is the frequency of the line centre. The virtue of this definition is that it can be measured even in an observation where the absorption line is not resolved in frequency. It is simply the total power that is missing relative to the unabsorbed continuum.

Note that in the literature you will also sometimes see a dimensional equivalent width, expressed in units of Angstrom. This is simply

$$W_\lambda = W\lambda_0, \tag{6}$$

where $\lambda_0 = c/\nu_0$, i.e., it is just the equivalent width we have defined multiplied by the wavelength of line centre.

The equivalent width is related to the column density of absorbers. To see this, recall that we showed previously that the attenuation coefficient for line absorption is

$$\kappa_\nu = \frac{h\nu}{4\pi} n_\ell B_{\ell u} \left(1 - \frac{g_\ell}{g_u}\frac{n_u}{n_\ell}\right)\phi_\nu, \tag{7}$$

so under our assumption that the cloud is uniform, the optical depth is

$$\tau_\nu = \frac{h\nu}{4\pi} N_\ell B_{\ell u} \left(1 - \frac{g_\ell}{g_u}\frac{n_u}{n_\ell}\right)\phi_\nu, \tag{8}$$

where $N_\ell = \int n_\ell \, ds$ is the column density through the cloud. Note that we are implicitly assuming that the ratio n_u/n_ℓ is constant along the line of sight, which means that we could also write it N_u/N_ℓ.

Also note that instead of an Einstein coefficient, this relation is often written in terms of an oscillator strength, which is related. The dimensionless oscillator strength $f_{\ell u}$ is defined in relation to the cross section, by

$$\sigma_{\ell u}(\nu) = \frac{\pi e^2}{m_e c} f_{\ell u}\phi_\nu. \tag{9}$$

The scaling factor $\pi e^2/m_e c$ is analogous to the one we defined earlier when we introduced the dimensionless collision strength $\Omega_{u\ell}$ – it is the natural order of magnitude for transitions due to leading order terms, and so, for transitions that are not suppressed by some sort of symmetry (i.e., for allowed transitions), we expect $f_{\ell u}$ to be of order unity. For example, the Lyman α line of hydrogen, corresponding to transitions from the $n = 1$ to $n = 2$ state, has $f_{\ell u} = 0.4164$. Additional tabulated values can be found in Draine's book.

We can also relate the dimensionless oscillator strength to the Einstein coefficients, since these are also related to the cross section. Working through the algebra, the relationship is

$$A_{u\ell} = \frac{8\pi^2 e^2 \nu_{u\ell}^2}{m_e c^3}\frac{g_\ell}{g_u} f_{\ell u}, \tag{10}$$

and that upward and downward oscillator strengths obey $f_{\ell u} = -(g_u/g_\ell) f_{u\ell}$. With this definition, the optical depth written in terms of the oscillator strength is

$$\tau_\nu = \frac{\pi e^2}{m_e c} f_{\ell u} N_\ell \left(1 - \frac{g_\ell}{g_u}\frac{n_u}{n_\ell}\right)\phi_\nu. \tag{11}$$

If we have cold interstellar gas, with $g_\ell n_u/g_u n_\ell \ll 1$, then we can approximate the term in parentheses as unity, and we have

$$\tau_\nu = \frac{\pi e^2}{m_e c} f_{\ell u} N_\ell \phi_\nu. \tag{12}$$

The line profile function ϕ_ν is generally a Voigt profile, meaning that it has a Gaussian core and Lorentzian damping wings. If we focus first on the core, we can approximate ϕ_ν by a pure Gaussian,

$$\phi_\nu = \frac{1}{\sqrt{\pi} b} e^{-(1-\nu/\nu_0)^2/(b/c)^2}, \tag{13}$$

where $b = \sqrt{2}\sigma_v$ is the Doppler broadening parameter we introduced earlier, and which is simply $\sqrt{2}$ times the velocity dispersion. This has a maximum value of $1/\sqrt{\pi} b$ at $\nu = \nu_0$, so the maximum optical depth, at $\nu = \nu_0$ is

$$\tau_0 = \sqrt{\pi} \frac{e^2}{m_e c} \frac{f_{\ell u} \lambda_{u\ell} N_\ell}{b} = 0.758 \left(\frac{N_\ell}{10^{13}\ \mathrm{cm}^{-2}}\right) \left(\frac{f_{\ell u}}{0.4164}\right) \left(\frac{\lambda_{u\ell}}{1215.7\ \text{Å}}\right) \left(\frac{10\ \mathrm{km\ s}^{-1}}{b}\right), \tag{14}$$

where $\lambda_{u\ell} = c/\nu_0$, and the normalisation quantities chosen in the second step are those appropriate for the Lyman α line of hydrogen. We refer to τ_0 as the optical depth at line centre. The optical depth in the Gaussian part of the line profile is then

$$\tau_\nu = \tau_0 e^{-u^2/b^2}, \tag{15}$$

where $u = c(\nu_0 - \nu)/\nu_0$ is the velocity shift required to produce a frequency shift ν.

II. The curve of growth

Clearly the equivalent width W of the line is an increasing function of τ_0, with a subsidiary dependence on the Doppler broadening parameter b and the oscillator strength and wavelength $f_{\ell u}\lambda_{u\ell}$. The function $W(\tau_0)$ is referred to as the curve of growth and, we can compute it numerically simply by numerically evaluating the Voigt profile. However, it is useful to understand how W behaves in limiting cases, to gain physical insight.

A. Optically thin lines

First consider the case when $\tau_0 \ll 1$, so that even at line centre the line is optically thin. In this case we can series expand the factor $1 - e^{-\tau_\nu}$ that appears in the definition of the equivalent width:

$$W = \int \left(1 - e^{-\tau_\nu}\right) \frac{d\nu}{\nu_0} \approx \int \left(\tau_\nu - \frac{\tau_\nu^2}{2}\right) \frac{d\nu}{\nu_0}. \tag{16}$$

For small τ_0 almost all of the absorption occurs in the Gaussian core of the line, so we can approximate τ_ν by the Gaussian form we just derived, and this makes the integral trivial to evaluate. Doing so, we obtain

$$W \approx \sqrt{\pi} \frac{b}{c} \tau_0 \left(1 - \frac{\tau_0}{2\sqrt{2}}\right). \tag{17}$$

Draine recommends replacing this with a formula that is equivalent to first order in τ_0 but behaves sensibly as τ_0 increases, rather than going to zero for large enough τ_0:

$$W \approx \sqrt{\pi}\frac{b}{c}\left[\frac{\tau_0}{1+\tau_0/(2\sqrt{2})}\right]. \tag{18}$$

Numerically this formula is accurate for any $\tau_0 \lesssim 1$. For small τ_0 the second term in the denominator is negligible compared to 1, and we simply have

$$W = \sqrt{\pi}\frac{b}{c}\tau_0 = \pi\frac{e^2}{m_e c^2} f_{\ell u}\lambda_{u\ell}N_\ell \tag{19}$$

Note that b drops out, which makes sense: since we're only absorbing a small amount of power at each frequency, the total power absorbed over the entire line doesn't depend on the distribution of the absorption in frequency. This implies that W is simply proportional to N_ℓ, with a constant of proportionality that depends only on known atomic constants for the line. This is very useful, because it means that, given a measurement of W, we immediately know N_ℓ.

B. Saturated lines

As τ_0 increases, all the photons near line centre are absorbed, and it is no longer the case that W increases linearly with N_ℓ. This is easy to understand: if we add more absorbers, most of these will have velocities such that they can only absorb near line centre. Since there are no more photons near line centre to absorb, they do not contribute to the equivalent width. Only that small fraction of particles that have velocities away from line centre contribute. Thus W increases sub-linearly with N_ℓ. In this case we say that the line centre has become saturated.

We can approximate this by continuing to use the Gaussian-only core of τ_ν, but treating the $1 - e^{\tau_\nu}$ as simply an inverted top-hat function, which is 0 for frequencies near ν_0, and is 1 otherwise. We take the width of the top-hat to be the full width at half maximum. Thus we have

$$\exp\left(-\tau_0 e^{-[(\Delta u)_{\mathrm{FWMH}}/2)^2/b^2}\right) = \frac{1}{2}. \tag{20}$$

Solving, we have

$$W = \frac{(\Delta u)_{\mathrm{FWHM}}}{c} = \frac{(\Delta \nu)_{\mathrm{FWHM}}}{\nu_0} = \frac{2b}{c}\sqrt{\ln(\tau_0/\ln 2)}. \tag{21}$$

As we can see, the equivalent width increases only vary slowly with τ_0 in this regime – as the square root of the log. We refer to this as the flat part of the curve of growth. In this regime it is not easy to determine the column density from an observation of W, because W is far more sensitive to variations in b, or to any non-Gaussianity in the velocity distribution, than it is to changes in N_ℓ.

C. Damped lines

As τ_0 continues to increase, the saturation region around line centre continues to grow up to the point where it extends beyond the Doppler core of the line, and we must consider the Lorentzian damping wings. In this limit we can ignore the Gaussian part of the line profile, and instead treat the line profile as a pure Lorentzian, so that

$$\tau_\nu = \frac{\pi e^2}{m_e c} N_\ell f_{\ell u} \frac{4\gamma_{\ell u}}{16\pi^2(\nu-\nu_0)^2 + \gamma_{\ell u}^2}. \tag{22}$$

Inserting this into the formula for the equivalent width, we have

$$W = \int \left(1 - \exp\left[-\frac{\pi e^2}{m_e c} N_\ell f_{\ell u} \frac{4\gamma_{\ell u}}{16\pi^2(\nu-\nu_0)^2 + \gamma_{\ell u}^2}\right]\right) \frac{d\nu}{\nu_0}. \tag{23}$$

The integrand is of the form $1 - e^{-a/x^2}$, and integrals of this form may be evaluated exactly to give $\sqrt{\pi a}/2$ (at least in the approximation where the range of integration goes from $-\infty$ to ∞). Thus the equivalent width is

$$W = \sqrt{\frac{e^2}{m_e c^2} N_\ell f_{\ell u} \lambda_{\ell u} \left(\frac{\gamma_{\ell u}\lambda_{\ell u}}{c}\right)} = \sqrt{\frac{b}{c}\frac{\tau_0}{\sqrt{\pi}}\frac{\gamma_{\ell u}\lambda_{\ell u}}{c}}. \tag{24}$$

Inverting this to solve for N_ℓ, we have

$$N_\ell = \frac{m_e c^3}{e^2} \frac{W^2}{f_{\ell u}\gamma_{\ell u}\lambda_{\ell u}^2}. \tag{25}$$

Thus in this regime $N_\ell \propto W^2$, and we can again measure the column density reasonably well. As in the case of optically thin lines, we don't need to know b – this time because Doppler broadening is weaker than natural broadening.

The transition between the damped and flat parts of the curve of growth occurs roughly where the two formulae for W in those two regimes are equal. Solving, this gives

$$\tau_0 \approx 4\sqrt{\pi}\frac{b}{\gamma_{\ell u}\lambda_{\ell u}} \ln\left(\frac{\tau_0}{\ln 2}\right). \tag{26}$$

This transcendental equation cannot be solved analytically, but when $b \gg \gamma_{\ell u}\lambda_{\ell u}$, as is almost always the case (if it were not, there wouldn't be a Doppler core), the solution is well-approximated by

$$\tau_0 = 4\sqrt{\pi}\frac{b}{\gamma_{\ell u}\lambda_{\ell u}} \ln\left(\frac{4\sqrt{\pi}}{\ln 2}\frac{b}{\gamma_{\ell u}\lambda_{\ell u}}\right). \tag{27}$$

This gives the characteristic line centre optical depth for which the damping wings begin to dominate. As an example, consider a typical Lyman α absorption system. For Lyman α, $\gamma_{\ell u}\lambda_{\ell u} = 7616$ cm s^{-1}, and typical Doppler parameters are $b \approx 100$

km s^{-1}, so damping begins to dominate at $\tau_0 \approx 10^5$. Looking back to our earlier formula for τ_0, this corresponds to a column density N_ℓ of a few times 10^{19} cm^{-2}. This is the reason that one traditionally defines damped Lyman α systems as those with column densities above about 10^{20} cm^{-2}.

D. Doublet ratios

Curve of growth gives us a way to directly measure the column density of a given species. However, there are some limitations. If we cannot directly measure the line shape and only have the equivalent width, we don't know b, and thus we don't know the line centre optical depth, and we don't know what part of the curve of growth we're on. This is a significant problem, because we could be on the flat part, in which case we cannot reliably measure the column density. Fortunately, for certain cases nature has provided us with a natural detector for this condition.

Often the upper state u into which transitions occurs is a doublet. Thus an absorbing state ℓ will be able to transition to two different excited states u_1 and u_2 that are separated slightly in energy due to fine structure. An example from the IGM is C IV, which has transitions at 1548 and 1551 Å; an example from stars and the ISM is the Ca II H and K lines at 3970 and 3935 Å. If we have sufficient spectral resolution we can measure the equivalent width of each of these two lines, and the resolution required to do that is generally a lot lower than the resolution required to resolve the individual lines.

The advantage of this technique is that the ratio of the two lines then provides a sensitive indicator for whether or not we're on the flat part of the curve of growth. To see why, let $f_{\ell u_1}$ and $f_{\ell u_2}$ be the oscillator strengths of the two lines, and λ_1 and λ_2 be their wavelengths. We adopt the convention that $f_{\ell u_2}\lambda_{\ell u_2} > f_{\ell u_1}\lambda_{\ell u_1}$, i.e. line 2 is the stronger one.

In the optically thin limit, the equivalent width is proportional to $f_{\ell u}\lambda_{\ell u}N_\ell$, and N_ℓ is the same for both lines, so the ratio of equivalent widths is simply

$$\frac{W_2}{W_1} = \frac{f_{\ell u_2}\lambda_{\ell u_2}}{f_{\ell u_1}\lambda_{\ell u_1}}, \tag{28}$$

i.e. it depends only on atomic constants.

Now suppose that we increase N_ℓ. The stronger line saturates at its centre and enters the flat part of the curve of growth first, and eventually both lines reach this regime. When they do, the line ratio becomes

$$\frac{W_2}{W_1} = \left[1 + \frac{\ln(f_{\ell u_2}\lambda_{\ell u_2}/f_{\ell u_1}\lambda_{\ell u_1})}{\ln(\tau_{0,1}/\ln 2)}\right]^{1/2}, \tag{29}$$

where $\tau_{0,1}$ is the line centre optical depth for the transition to state u_1. Similarly, in the damping limit, the line ratio is

$$\frac{W_2}{W_1} = \frac{\lambda_{\ell u_2}}{\lambda_{\ell u_1}}\sqrt{\frac{f_{\ell u_2}\gamma_{\ell u_2}}{f_{\ell u_1}\gamma_{\ell u_1}}}. \tag{30}$$

Thus the line ratio changes as column density and optical depth increase, and in each of the three regimes it takes on a value that is determined solely or almost solely (discounting the logarithmic dependence on τ_0 in the flat regime) by atomic constants. By measuring the line ratio we therefore learn what part of the curve of growth we're on, and which formula we should use to compute the column density.

III. The Lyman Series

One important application of curve of growth analysis is to the Lyman series of hydrogen transitions, which provides one of our primary means of studying the ISM and IGM beyond the local universe. The Lyman series consist of allowed transitions between a lower $1s$ state (the ground state) and an upper np state, where $n = 2$ is Lyman α, $n = 3$ is Lyman β, etc. Note that it must be a p state for the transition to be allowed, since one of the selection rules is that change in the angular momentum of the single-electron wavefunction must be $\Delta\ell = \pm 1$, so transitions between two s states, or between and s and a state with $\ell > 1$, are forbidden and much weaker.

For Lyman α, the upper state is a doublet of a ${}^2\mathrm{P}^{\mathrm{o}}_{3/2}$ and ${}^2\mathrm{P}^{\mathrm{o}}_{1/2}$, and the ground state is a singlet ${}^2\mathrm{S}_{1/2}$. Both transitions have $A_{u\ell} = 6.265 \times 10^8$ s^{-1}, so the transition is very strong. The transitions have wavelengths of 1215.674 and 1215.668 Å, and the difference between those two, corresponding to a velocity shift of 1.33 km s^{-1}, is so small that in astrophysical environments we essentially never see the line split. It is always blended by thermal or non-thermal motions. For this reason, we regard it as a single line in practice.

Many other Lyman lines can be observed as well, up to what is called the Lyman limit. This is limit is that, as n increases, the lines become more and more closely spaced in energy, until such time as they blend together due to thermal broadening and simply form a smooth continuum. The condition for this to happen is

$$\frac{d\lambda_n}{dn} < \frac{(\Delta v)_{\mathrm{FWHM}}}{c}\lambda_n \qquad \Longrightarrow \qquad n > \left[\frac{2c}{(\Delta v)_{\mathrm{FWHM}}}\right]^{-1/3} = 67\left[\frac{(\Delta v)_{\mathrm{FWMH}}}{2\ \mathrm{km\ s}^{-1}}\right]^{-1/3}. \tag{31}$$

Higher n lines than this are not individually distinguishable.

IV. Abundance measurements

Beyond measuring hydrogen column densities, the next most important application of abundance spectroscopy is measuring abundances of other elements relative to hydrogen. This is the main technique used to study chemical evolution of the universe. Measuring the column density of an element in practice requires two conditions. First, we must either know the dominant ionization state of the element (since different ionization states have different lines) or we must be able to measure the abundances over a range of ionization states. Second, the element must have an absorption line that is below the ionization potential of hydrogen (13.6 eV), since photons above this energy tend not to get very far in the ISM. Fortunately many elements meet these requirements.

We usually describe the abundance of an element X in terms of the log of its ratio to hydrogen or some other element, normalized to the solar value. The notation is

$$[X/Y] \equiv \log_{10}(N_{\mathrm{X}}/N_{\mathrm{Y}}) - \log_{10}(M_{\mathrm{X}}/M_{\mathrm{Y}})_{\odot}, \tag{32}$$

where M_{X} is the mass of element X in the Sun.