Lecture 1

1 Basics

1.1 Assessment

1. One problem available from http://www.astro.uvic.ca/˜sara/A503.html. Submision due date (30 %)
2. Computational assignment due (30%)
3. Oral presentation (10%)
4. Essay due (30%)

1.2 Scope of this course

My aim is to provide you with the fundamentals required to understand the physics of the diffuse universe. For the most part, I will avoid lengthy mathematics (you can always get this from a text book) unless I think it provides you with an important computational tool that will be of general use. Beyond the basics of this ISM course, I will try to focus on research relevent materials. As such, the latter part of the semester will focus on current work on the Galactic and extra-galactic ISM (with a heavy inclination towards the latter, reflecting my own bias!). There will be some 'guest' speakers.

1.3 Textbooks

The classic texts are

- Astrophysics of Gaseous Nebulae and Active Galactic Nuclei by Osterbrock
- Physical Processes in the Interstellar Medium by Spitzer

But there are many newer, more user-friendly textbooks e.g.

- The Physics of the Interstellar Medium by Dyson and Williams
- Dust and the Galactic Environment by Whittet
- Astrophysics of the Diffuse Universe by Dopita and Sutherland

No text book is required for this course, but a longish list of relevent texts is available at http://www.astro.uvic.ca/˜sara/A503.html for the interested (dedicated? wealthy?) reader.

2 Notation

Useful website: http://electron6.phys.utk.edu/qm2/modules/m11/Atomic%20Spectra.htm
See aso chapter 2 of Dopita & Sutherland.

Four quantum numbers for an electron of a given energy

- principal quantum number, n= 1,2,3 ...
- orbital angular momentum quantum number, l = 0, 1, 2, ... (n-1)
- magnetic quantum number, m = -l, ... 0 ... +l
- spin quantum number, s = ± 1/2

The orbital angular momentum number, l, is often replaced by a letter.

$l = 0 \longrightarrow s$
$l = 1 \longrightarrow p$
$l = 2 \longrightarrow d$ etc.

Electron orbitals are labelled s (sharp), p (principal), d (diffuse), f (fundamental), g, h, i ... Lower case letters are used when referring to electron configurations in their orbitals (e.g. $1s^2 2s^2$). Upper case letters refer to entire atom, e.g. L = $l_1 + l_2$, S= $s_1 + s_2$ etc (see later). Similarly, the principal quantum number can be replaced by a letter

$n = 1 \longrightarrow K$
$n = 2 \longrightarrow L$
$n = 3 \longrightarrow M$ etc.

There is also the total angular momentum, j, which is $j = \mid l + s \mid$. I.e for an electron $j = \mid l \pm 1/2 \mid$.

For a single electron atom (e.g. neutral hydrogen), when n=1, l=m=0 and s=±1/2, i.e. 2 possible states. When n=3:

n	l	m	s
3	0	0	± 1/2
3	1	-1	± 1/2
3	1	0	± 1/2
3	1	1	± 1/2
3	2	-2	± 1/2
3	2	-1	± 1/2
3	2	0	± 1/2
3	2	1	± 1/2
3	2	2	± 1/2

I.e. 18 states. You can show that the statistical weight $g_n = 2n^2$ for hydrogen (statistical weight = number of states of a given energy). In the general case, the statistical weight, g = 2J+1.

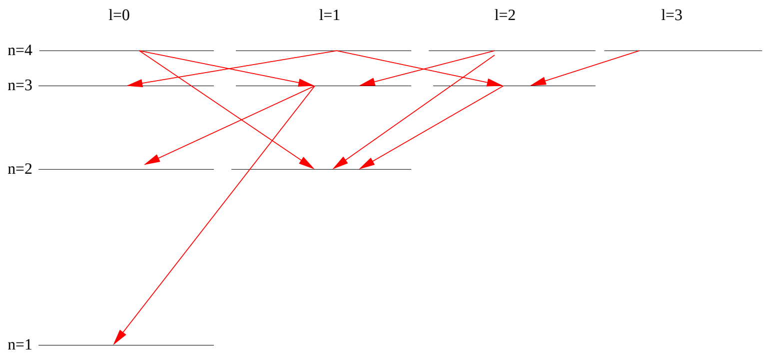

Figure 1: Grotrian diagram for HI

Resonance (permitted) lines require $\Delta l \pm 1$ (one unit of angular momentum carried away by photon). Δn has no restrictions.

The full spectral notation therefore includes the electronic configuration of the orbital, the multiplicity (2S+1), total orbital angular momentum (inner full shells sum to zero) and total angular momentum:

ns^i np^j nd^k ... $^{2S+1}L_J$

This is straightforward for hydrogen-like neutrals (e.g. Li, Na, K) with one optically active electron, or ionized alkali metals.

- For ground state Li: $1s^2\ 2s\ \ ^2S_{1/2}$. Only $s = 1/2$ considered because $s = -1/2$ would mean j is negative (forbidden).
- Mg II (which has 11 electrons) will be written $1s^2\ 2s^2\ 2p^6\ 3s\ \ ^2S_{1/2}$
- Excited Li (still one electron to consider) with $l = 1$. Now $s = \pm 1/2$.

$$s = 1/2 \rightarrow j = 3/2 \rightarrow 1s^2\ 2p\ ^2P_{3/2} \tag{1}$$

$$s = -1/2 \rightarrow j = 1/2 \rightarrow 1s^2\ 2p\ ^2P_{1/2} \tag{2}$$

- Similarly, higher excited states of Li with $l = 2$

$$s = 1/2 \rightarrow j = 5/2 \rightarrow 1s^2\ 2p\ ^2D_{5/2} \tag{3}$$

$$s = -1/2 \rightarrow j = 3/2 \rightarrow 1s^2\ 2p\ ^2D_{3/2} \tag{4}$$

For multiple optically active electrons, we have to define a coupling scheme which considers vector sums. For example LS coupling (Russell-Saunders coupling) or jj coupling. E.g.

L $= l_1 + l_2 = (l_1 + l_2), (l_1 + l_2 - 1)... \mid l_1 - l_2 \mid$
S$= s_1 + s_2 = 1/2 \pm 1/2 = 0, 1.$

In LS coupling the L and S terms combine by magnetic interactions to give the total angular momentum:

J = L + S = (L+S), (L+S−1)...|L−S|

Spins can be either parallel or anti-parallel, i.e. S=0, 1. If S=0 (spins anti-parallel), then multiplicity is 1 $\rightarrow$ singlets (sometimes called 'para'), and if S=1 (spins parallel) then multiplicity is 3 $\rightarrow$ triplets (sometimes called 'ortho'). If $S = 0$ the $J = L$, but if $S = 1$ there are several closely spaced levels. In LS coupling, $\Delta S = 0$ so we can't transition between singlets and triplets.

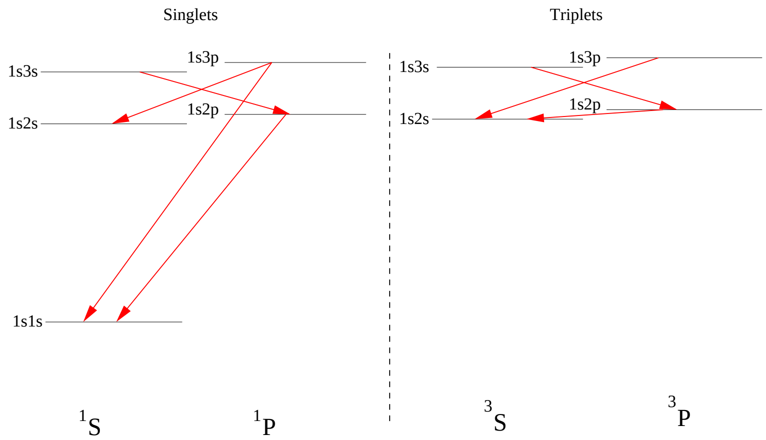

Figure 2: LS coupling in He

Some examples:

- Excited He has two optically active electrons. In an LS coupling scheme we have

$$S = 0 \rightarrow 1s\ 2p\ ^1P_1 \tag{5}$$

$$S = 1 \rightarrow 1s\ 2p\ ^3P_{0,1,2} \tag{6}$$

  In the triplet the values of J can be $J = 1 + 1, 1 + 1 - 1, 1 - 1$

- Mg I is similar in structure to He. Ground state is $1s^2\ 2s^2\ 2p^6\ 3s^2\ \ ^1S_0$ and the excited states are

$$S = 0 \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s3p\ \ ^1P_0 \tag{7}$$

$$S = 1 \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s3p\ \ ^3P_{0,1,2} \tag{8}$$

However, we can get departures from LS coupling. E.g. Mg I has a line at 4571 Å which corresponds to the energy difference between the ground state $3s^2\ 1S_0$ and lowest triplet term $3s\ 3p\ ^3P$, i.e. $\Delta S \neq 0$. This is an intercombination (or intersystem, or semiforbidden) line. This

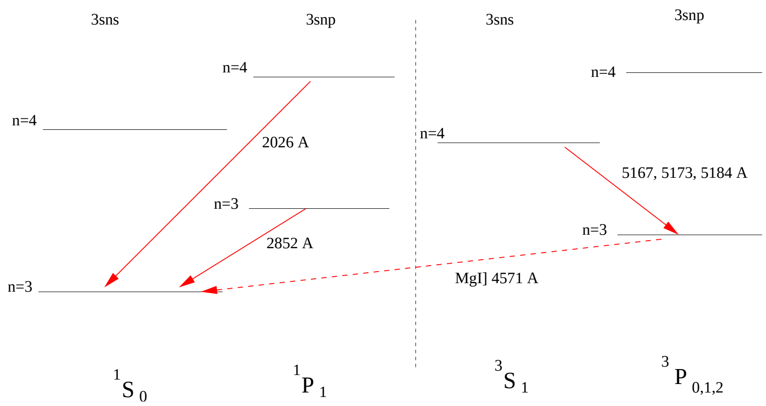

Figure 3: Inter-combination lines for MgI

can happen if the population in lowest triplet level is high (because all other triplet lines decay there).

Forbidden lines violate $\Delta S = 0$ and one of the other selection rules. Only seen in very low density environments when transition time << time between collisions.

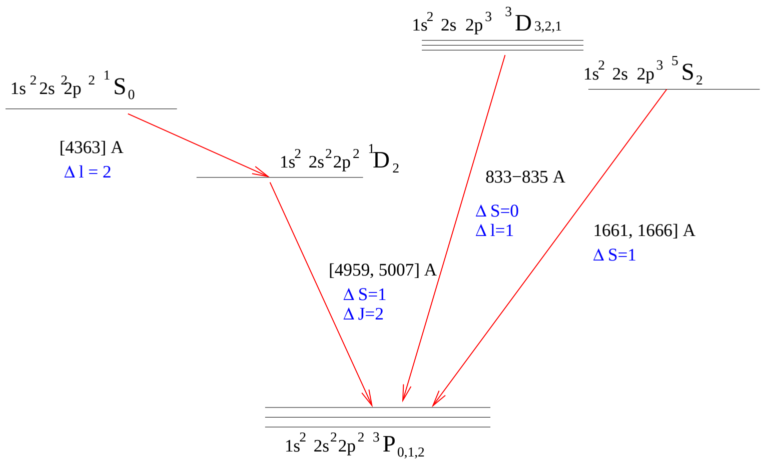

Figure 4: Forbidden lines in OIII

3 Transition Probabilities

Also define Einstein coefficients as probabilities for spontaneous processes (A pertain to emission, B to absorption). The inverse of these coefficients give the radiative lifetimes (i.e. 1/A gives the time for a transition to sponataneously decay).

$$A_{ji} = \frac{8\pi h B_{ij} g_i}{g_j \lambda^3} \tag{9}$$

$$B_{ij} = \frac{f_{ij} e^2 \lambda}{4\epsilon h c m_e} \tag{10}$$

Where f is the oscillator strength. This treats the transition as if it were a bound harmonic oscillator and asks how efficient is the transition at absorbing energy. Often tabulate gf values:

$$g_i f_{ij} = A_{ji} g_j \lambda^2 (\frac{4\epsilon c m_e}{8\pi e^2}) \tag{11}$$

The oscillator strength is a transition probability which can be experimentally or theoretically derived (from QM). Typical A values for permitted resonance transitions ar $10^8 - 10^9$ s^{-1}, $\sim 10^3$ s^{-1} for semi-forbidden lines and $\sim 10^{-3}$ s^{-1} for forbidden lines. The latter are therefore only seen in very diffuse media when the time for collisions is longer than about 1000 seconds.

4 Local Thermodynamic Equilibrium

Distribution of atomic states and energies for LTE given by statistical mechanics. The Boltzmann equilibrium tells us about the relative numbers of atoms in an excited state, j, compared with the ground state (j=1) at a given temperature , T:

$$\frac{N_j}{N_1} = \frac{g_j}{g_1}\ exp(\frac{-\Delta E}{kT}) \tag{12}$$

ΔE is the energy difference between ground and excited states and k is the Boltzmann constant ($k = 1.38 \times 10^{-16} erg K^{-1}$ or 8.62 $\times 10^{-5} eV K^{-1}$). The energies for hydrogen can be approximated with the empirical formula

$$E_n = \frac{-hcR_H}{n^2} = -13.6eV\frac{1}{n^2} \tag{13}$$

The energies of atoms will follow a Maxwell-Boltzmann distribution (this can also be expressed as a function of velocities):

$$n(E) = \frac{2N}{\pi^{1/2}(kT)^{3/2}} E^{1/2}\ exp(\frac{-E}{kT})dE \tag{14}$$

So the most probable energy is kT (alternatively the most probable velocity is $v = \sqrt{(2kT/m)}$).

However, LTE is usully not applicable in the ISM. Low densities mean that Boltzmann equilibrium is rarely achieved because collisions are too rare and radiative processes become important. Nonetheless, species can usually attain a Maxwellian energy distribution.

5 Measuring Absorption/Emission Lines

Lines often measured in terms of equivalent width:

$$EW = \int \frac{I_0 - I_\lambda d\lambda}{I_0} \tag{15}$$

Emission lines have -ve EW and absorption lines are positive. Observed spectra have noise, so there is a detection limit. The nσ detection limit is

$$EW = \frac{n \times d \times \sqrt{M}}{S/N} \tag{16}$$

Where d is the dispersion (pixel width in Angstroms) and M is the number of pixels across the line. For unresolved lines, this can be approximated to

$$EW = \frac{n \times FWHM}{S/N} \tag{17}$$

The width of a line is usually expressed in km/s as either the velocity dispersion (σ) or the FWHM. It can easily be shown from a Gaussian distribution that these quantities are related:

$$FWHM = 2\sqrt{2ln2}\sigma = 2.355\sigma \tag{18}$$

Widths are often also expressed in terms of the Doppler width, b, caused by thermal/turbulent broadening.

$$b = \sqrt{2}\sigma = \frac{FWHM}{2\sqrt{ln2}} \tag{19}$$

For emission lines, more often the flux is quoted. This can be in units of F_ν (ergs s^{-1}cm^{-2}Hz^{-1} or Jy) or F_λ (ergs s^{-1}cm^{-2}Å^{-1}) where

$$F_\lambda = F_\nu c/\lambda^2 \tag{20}$$

Graphs sometimes plotted with λF_λ which is total energy.

6 The Voigt Profile

Lines are broadened by various processes e.g. pressure broadening (more important in stars), thermal, turbulent broadening and natural broadening which occurs due to Heisenberg's uncertainty principle $\Delta E \Delta t \geq \hbar$. Since any transition has a finite lifetime, $\Delta t = 1/A_{ji}$, the natural width in terms of frequency is

$$\Delta\nu_N = A_{ji}/2\pi \tag{21}$$

Often this natural frequency width is replaced by the damping constant, Γ, which is connected to the radiative transfer probability: for a transition from the ground state Γ is the sum over the Einstein coeffficients for spontaneous emission for levels up to the upper level in question.

$$\Gamma = 2\pi\Delta\nu_N \tag{22}$$

The absorption cross section (measure of probability) from natural broadening can then be expressed as

$$\sigma_L(\nu) = (\frac{\pi e^2}{m_e c}) f \frac{\Gamma/4\pi^2}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \tag{23}$$

(this is ignoring the term for stimulated emission).

Thermal and turbulent motions are combined in the Doppler width which is assumed to follow a Gaussian distribution

$$P(v) = \frac{1}{b\sqrt{\pi}} e^{-(v/b)^2} \tag{24}$$

$$b = \sqrt{b^2_{thermal} + b^2_{turbulent}} = \sqrt{\frac{2kT}{m} + +b^2_{turbulent}} \tag{25}$$

If b is dominated by thermal broadening

$$b = 12.8 \text{ km/s}\sqrt{\mathrm{T_4/m}} \tag{26}$$

Combining the effects of Eqns 23 and 24 gives an absorption cross section:

$$\sigma(\nu) = \left(\frac{\pi e^2}{m_e c}\right) f \frac{\Gamma}{4\pi^2} \int_{-\infty}^{+\infty} \frac{1}{b\sqrt{\pi}} \frac{e^{-(v/b)^2} dv}{(\nu - \nu_0(1+v/c))^2 + (\Gamma/4\pi)^2} \tag{27}$$

This expression can be simplified using the Voigt function, $H(a, u)$

$$H(a, u) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2} dy}{(u-y)^2 + a^2} \tag{28}$$

where

$$\Delta\nu = \frac{b\nu_0}{c}; \qquad a = \frac{\Gamma}{4\pi\Delta\nu}; \qquad u = \frac{c(\nu - \nu_0)}{\nu_0 b}; \qquad y = v/b \tag{29}$$

Substituting in equation 27 gives

$$\sigma(\nu) = \frac{\sqrt{\pi}e^2 f}{m_e c} \frac{H(a, u)}{\Delta\nu} \tag{30}$$

We can now write the optical depth ($\tau = N\sigma$) as

$$\tau(\nu) = \frac{\sqrt{\pi}e^2}{m_e} \frac{Nf}{b\nu} H(a, u) \tag{31}$$

or written as a function of wavelength,

$$\tau(\lambda) = \frac{\sqrt{\pi}e^2}{m_e c} \frac{Nf\lambda}{b} H(a, u) = 1.497 \times 10^{-15} \frac{N(\mathrm{cm}^{-2}) f \lambda(\text{Å})}{b(\mathrm{kms}^{-1})} H(a, u) \tag{32}$$

This is the expression for the Voigt profile which simplifies in the line centre to

$$\tau(\lambda_0) = \frac{\sqrt{\pi}e^2}{m_e c} \frac{Nf\lambda_0}{b} = 1.497 \times 10^{-15} \frac{N(\mathrm{cm}^{-2}) f \lambda_0(\text{Å})}{b(\mathrm{kms}^{-1})} \tag{33}$$

Finally, note that

$$\tau_{total} = \tau_1 + \tau_2 \tag{34}$$

7 The Curve of Growth

What is the effect of light incident on absorbing atoms? Optical depth, τ:

$$I(\nu) = I_0(\nu)e^{-\tau} \tag{35}$$

$$\tau(\nu) = N\sigma(\nu) \tag{36}$$

N is the gas column density in units of cm^{-2}. Since EW is *defined* as the normalized net flux removed from the beam:

$$I_0 W = I_0 \int d\nu - \int I(\nu) d\nu \tag{37}$$

$$W = \int (1 - exp[-N\sigma(\nu)]) d\nu \tag{38}$$

When the optical depth of the cloud is small $\tau(\nu) = N\sigma(\nu) << 1$ so

$$W = N \int \sigma(\nu) d\nu \tag{39}$$

$$W(\nu) = \frac{\pi e^2}{m_e \nu} N f \tag{40}$$

$$W(\lambda) = \frac{\pi e^2 \lambda_0}{m_e c^2} N \lambda_0 f \tag{41}$$

and the EW is directly propotional to the number of atoms along the line of sight. This is the linear portion of the curve of growth.

$$\Longrightarrow N = 1.13 \times 10^{20} \frac{W(\lambda)}{\lambda_0^2 f} \tag{42}$$

for wavelength in Å.

As the column density increases, the absorption line will eventually become saturated, see Figure 6b. In this regime,

$$W(\lambda) \sim \frac{2b\lambda_0}{c} \sqrt{\ln\left(\frac{\pi^{0.5} e^2 N \lambda_0 f}{m_e c b}\right)} \tag{43}$$

i.e. $W(\lambda) \propto \sqrt{\ln N}$, this is the flat part of the curve of growth. As can be seen from Figure 5, the precise shape of this flat part of the curve of growth depends heavily on the b-value, causing a degeneracy between N and W. This renders Voigt fitting very uncertain in this regime.

When the column density is high enough ($N \gtrsim 10^{19}$ cm^{-2}) the Lorentzian profile begins to dominate the wings of the absorption line, see Figure 6c. In this regime, $W(\lambda) \propto \sqrt{N}$ and, as for unsaturated lines, this is independent of b-value:-

$$W(\lambda) \sim \frac{\lambda_0^{1.5}}{c} \sqrt{\frac{e^2}{m_e c} N \lambda_0 f \Gamma} \tag{44}$$

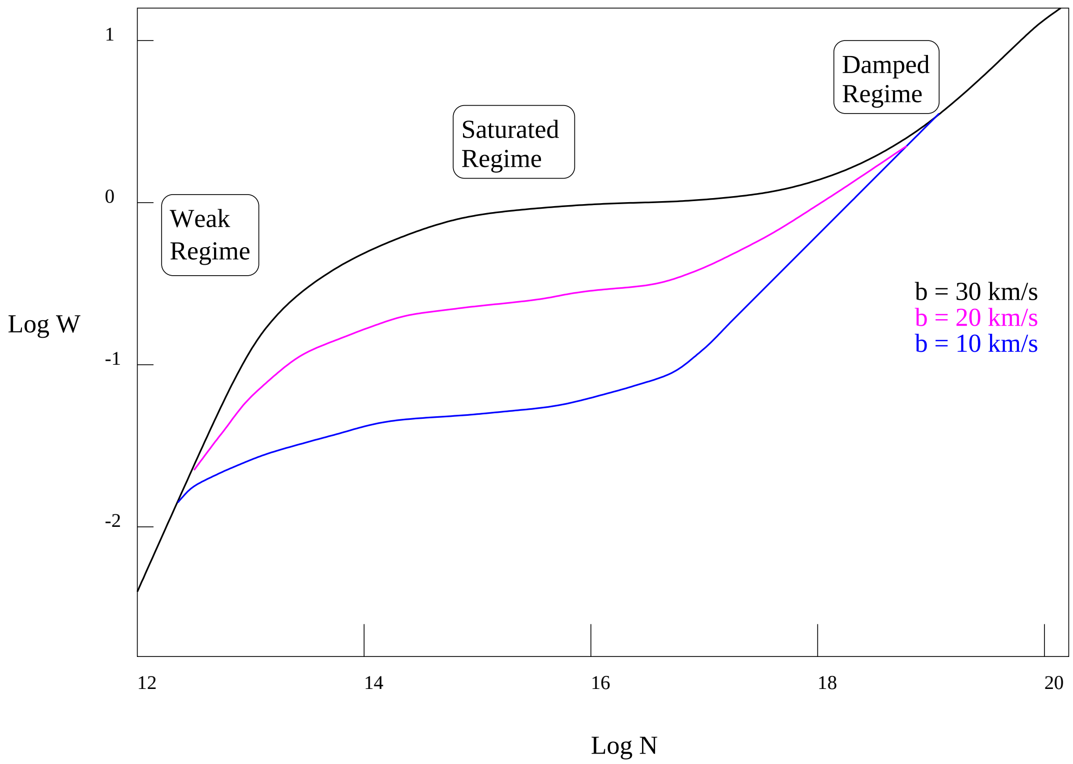

Figure 5: Schematic figure illustrating the curve of growth for Lyα absorption lines for 3 different b-values (Doppler widths).

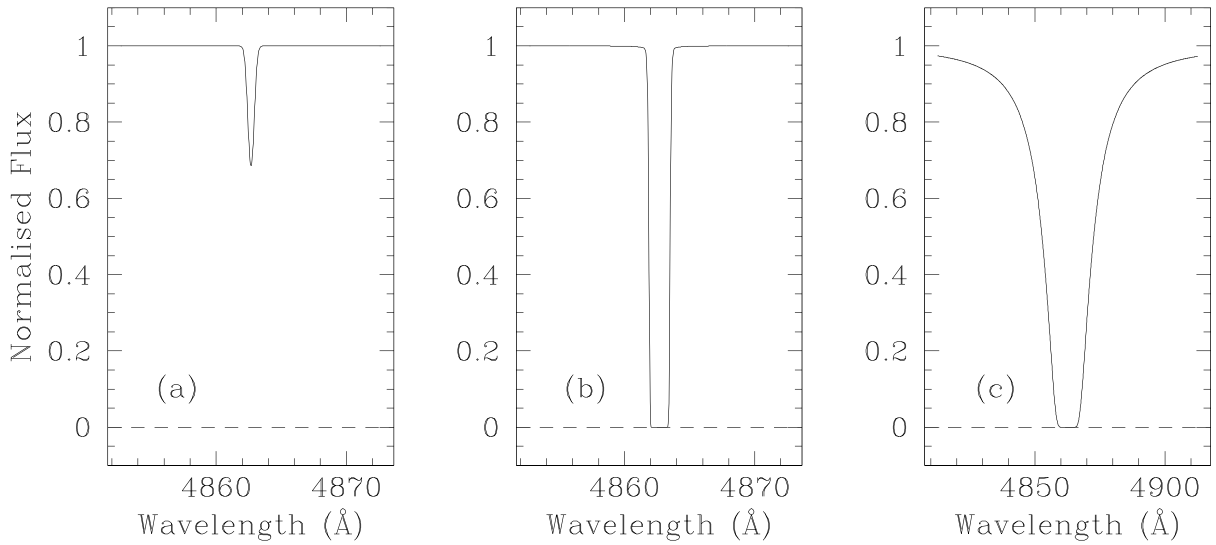

Figure 6: Model Lyα absorption lines for the three regimes illustrated in Figure 5. All profiles are for an absorption redshift of $z_{abs} = 3.0$ and $b = 20$ km/s. Panels (a), (b) and (c) show Lyα lines with log N(H I) = 13, 16 and 20 respectively.

This means that the column density of H I in damped Lyα systems can be reliably determined by fitting a profile to the Lorentzian wings.