ASTR469 Lecture 10: Spectroscopy (Ch. 11–12)
Note: the book covers different types of diffraction gratings in much greater detail than will be discussed in class.

1   Spectroscopy

Generically, spectroscopy is the study of the intensity of light spread out in frequency. This differs from photometry, which is the study of the intensity light at a particular frequency (or measured within a single band/range of frequencies). The spread-out light is called a spectrum, a plot of intensity versus frequency, a word we used before when dealing with blackbodies. You can make spectra at any wavelength in astrophysics, although similarly to photometry the techniques to do so differ.

In UV/optical/IR photometry, we were treating the incoming light as single photons (particles). However, to make spectra for these wavelengths, the detecting apparatuses need to use the wavelike nature of light to spread out the light based on its wavelength.

NOTE that the statistics for detection in spectroscopy still follow the rules that we laid out last lecture. Integrating for longer time will generally raise your signal-to-noise ratio by $\sqrt{t}$ for a given spectral line you're trying to detect.

An individual spectrum can be divided into "continuum" and "line" portions. The continuum is generally smoothly varying, whereas the lines are sharper features in absorption or emission. The difference is that spectral line emission arises from transitions between discrete energy states. We will deal here mostly with spectral lines.

With photometry we talked a lot about what makes light (blackbody radiation; Kirchoff's Laws, etc.). Today we're going to fill in some back-story about what makes spectra interesting, and then we'll briefly discuss UV/optical/IR detection technologies at the end.

2   Physical Origins of Lines

Spectral lines arise from transitions between energy states. There are many ways atoms and molecules can change energy states, but we'll just deal with a few here. If the atom or molecule is gaining energy via absorption of a photon, we see the line in absorption; if it is losing energy by emission of a photon, we see the line in emission.

I should note here that the book Essential Radio Astronomy (search online; the whole book is available there) is an excellent resource for more detailed background physics on these effects.

2.1   Electronic transition lines

You should be familiar with the Bohr model, in which electrons are quantized at fixed separations from the nucleus. These states are quantized by numbers $n = 1, 2, 3, ...$ It takes energy to kick electrons up to higher states. For instance, a Hydrogen atom with $n = 1$ is

in its neutral state, while Hydrogen with an electron at $n = 2$ has been "excited" by some incoming energy.

Each quantized state is characterized by a given amount of energy that has to do with balancing the movement of the electron (kinetic energy), which would naturally carry the electron away from the nucleus, and the Coulomb force (potential energy/centripetal force in this case), which keeps the electron bound in that state. Under the assumption that your nucleus has (relatively) infinite mass compared to the electron, and that the nucleus is stationary (only the electron is moving), this energy is given by

$$E_n = KE + PE = -\frac{m_e e^4}{8h^2 \epsilon_0^2 n^2} \tag{1}$$

where $m_e = 9.109 \times 10^{-31}\,\mathrm{kg}$ is the mass of an electron, $e = 1.602 \times 10^{-16}\,\mathrm{C}$ is the elementary charge, h is the same Planck constant we've seen before, and $\epsilon_0 = 8.854 \times 10^{-12}\,\mathrm{m^{-3}\,kg^{-1}\,s^4\,A^2}$ is the permittivity of free space.

When an electron changes from one state to another (say it decays from a higher n state to a lower n state), it emits some energy. The packet of energy that comes out is the difference between the energies at those two states.

$$\Delta E = E_{n+\Delta n} - E_n = \frac{m_e^4}{8h^2 \epsilon_0^2} \left[\frac{1}{n^2} - \frac{1}{(n + \Delta n)^2} \right] \tag{2}$$

So when an electron jumps between states, a packet of energy ΔE comes out. All of that energy comes out as a single photon!

$$\Delta E = h\nu \tag{3}$$

And you can see, therefore, that the frequency ν of that emitted photon can be uniquely associated with that transition.

OK, so above we made some basic assumptions about the nucleus just to give an idea of how this emission works. But in reality, the derivation is a tad more complicated, and depends on how stationary, and how large the nucleus is. The full expression for the emission frequency of a transition for a particular atom of nuclear mass M is given by

$$\nu_{\mathrm{emit}} = R_M c \left[\frac{1}{n^2} - \frac{1}{(n + \Delta n)^2} \right] \tag{4}$$

$$R_M c \simeq 3.29 \times 10^{15} \left[1 + \frac{m_e}{M} \right]^{-1} \tag{5}$$

Where c is the speed of light. This gives the full expression for the emission frequency (in Hz) of any transition between higher state $n + \Delta n$ and lower state n, for any atom of nuclear mass M.

Notation used to refer to transition lines...

Completely ionized atoms:
These get the atomic symbol with a greek number showing how many atoms are ejected. Greek number "I" refers to a neutral atom, while "II" refers to a singly-ionized atom, and so forth. For example:

HI	Neutral Hydrogen.
HII	One e$^-$ completely removed ($\Delta n = \infty$).
OI	Neutral Oxygen.
OIII	Two electrons removed.

Excited atoms:
These get atomic symbol, then a number indicating the lower energy state, then a greek alpha character representing Δn, the size of the transition. For instance, the greek alphabet goes in order $\alpha, \beta, \gamma, \delta, \epsilon...$, which corresponds to $\Delta n = 1, 2, 3, 4, 5...$ transitions. So for instance:

$$\textbf{H114}\beta$$

H	tells you it's Hydrogen.
114	tells you the transition has $n = 114$.
β	tells you the transition has $\Delta n = 2$.

So this is a transition between the two excited states $n = 116$ and $n = 114$ for the Hydrogen atom.

Balmer and Lyman Series:
There are a few exceptions to this notation for very common Optical-wavelength transitions. Notably...

Lyman Series (base level $n = 1$)

Lyα	$n = 2$ to $n = 1$ transition.
Lyβ	$n = 3$ to $n = 1$ transition.

Balmer Series (base level $n = 2$)

Hα	$n = 3$ to $n = 2$ transition.
Hβ	$n = 4$ to $n = 2$ transition.
Hγ	$n = 5$ to $n = 2$ transition.

Regardless of notation, any of the above transitions can use Equations 4 and 5 to tell the rest emission frequency.

2.2   Spin-flips in Neutral Hydrogen

Our atomic-transition-line notes were somewhat detailed because they are by far the most prevalent type of line you'll see used in astronomical analyses. These last two we will talk about conceptually.

It turns out even neutral atoms can sporadically emit and absorb photons, due to a "spin-flip" of a particle in the atom. Spontaneous emission of these happens relatively rarely, however particularly for neutral (non-ionized) Hydrogen, there is just so much of it in the cosmos that many galaxies are observable in the neutral Hydrogen line.

Electrons and protons have spins, and we can characterize hydrogen as having these spins as aligned or anti-alligned (e.g. both are clockwise: parallel; or one or the other is spinning counter-clockwise: anti-parallel). The The transition from one spin-state to another has a specific transition energy that demarcates the HI line:

$$\Delta E = 5.9 \times 10^{-6} \, \text{eV}$$
$$\nu_{\text{HI}} = 1420.4 \, \text{MHz}$$
$$\lambda_{\text{HI}} = 21 \, \text{cm}$$

2.3   Spinning Molecules

Some molecules have an asymmetric charge distribution; therefore if they spin, they have a dipole moment. It turns out that the atomic quantization of electrons also applies on the macro scale, and that the rotational momentum of molecules is also quantized into specific spin rates. Each spin rate is associated with a given energy, and if the spin rate spontaneously decays to a lower state, a photon with an energy equal to the higher-spin state will be emitted. That outburst of energy (or absorption of energy, if an incoming photon incites a higher spin state in a molecule) is associated with a photon of a specific frequency.

The most abundant molecule is molecular hydrogen (H_2), which unfortunately does not have a dipole moment. Instead, we often use carbon monoxide (CO). More complex molecules are found at higher densities where chemical reactions are faster.

3   Kirchoff's Laws and Observing Spectral Lines

So now we know about what can make photons that are at fixed energy levels, or at a specific frequency/wavelength. How do we actually observe these and what do they look like?

First, to get an observable line you need to have a significant cloud of atoms/molecules all undergoing similar energy transitions. The population of those will lead to observable lines from astronomical distances.

You may see the line in **emission** if you are observing a cloud in local thermal equilibrium, with no hotter background source directly along your line of sight behind it. Most emission lines come from spontaneous decay (higher energy state to lower energy state, thus a photon is emitted). Photons from the same cloud might also be absorbed by the cloud itself, thus sustaining some long-term level of line emission.

You will see a line in **absorption** if you are observing a hot broad-band source with a cooler cloud along your line of sight. Photons from the original target are broad-band, however the
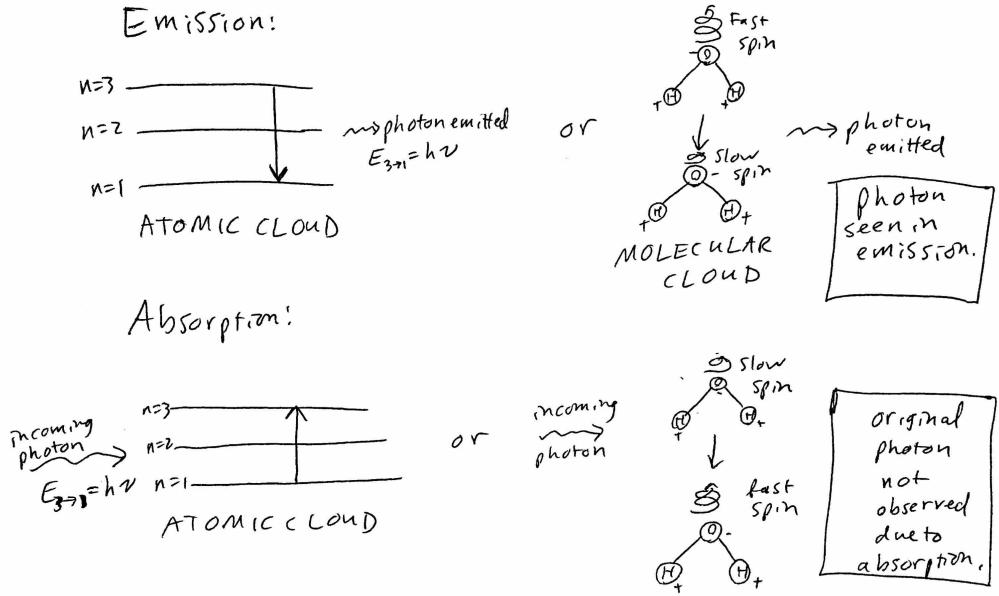
Figure 1: Emission from an atomic transition line and a molecular spin line seen in absorption and emission.

photons entering e. g. a Hydrogen cloud with the right energy to incite a $n = 1$ to 2 jump will go into inciting that jump. Thus, that photon will not be observed by you (it will be absorbed).

See Figure 1 for reference. The same principles apply to any of the processes listed in the previous section.

4 Using Spectral Lines

The basic properties of any line are the height (referred to as peak intensity, flux, or temperature depending on what electromagnetic band you are observing in), the observed peak frequency ν, and the width of the line $\Delta\nu$. These three pieces of information give us a lot of interesting source properties we can infer. Here we'll discuss just a few of these.

4.1 Redshift

You should all be familiar with the Doppler effect. In the case of emission lines, a line observed offset from its emission frequency (e.g. at a shorter or longer wavelength) is experiencing movement compared to you along your line of sight.

In astronomy we think of these in terms of "redshifts" (wavelength gets longer, hence redder) for objects traveling away from us, and "blueshifts" (wavelength gets shorter, hence bluer) for objects traveling towards us. The redshift z is quantified by:

$$z = \frac{v}{c} = \frac{\nu_{\text{emit}}}{\nu_{\text{obs}}} - 1 = \frac{\lambda_{\text{obs}}}{\lambda_{\text{emit}}} - 1 \tag{6}$$

Note that for redshifts, $z > 0$ and the following are true:

- The object (atom or molecule cloud in this case) is traveling away from us.

- Lengths (e.g. λ) appear to grow by $(1 + v/c)$.

- Frequencies (e.g. ν or $\Delta\nu$) appear to shrink by $(1 + v/c)$.

4.2   Line broadening

A number of things can broaden an observed line. This can include, of course, instrumental effects; if you are dividing frequencies into specific sub-bands of frequency, your line can only be as narrow as the narrowest frequency band.

There are intrinsic line widths that arise from quantum-level variations in transitions (no value is exact)! These variations can be related to the Heisenberg uncertainty principle. This is called "natural broadening."

Gas atoms/molecules have a range of velocities (set by the Maxwell-Boltzmann distribution in local thermodynamic equilibrium). Within a given gas cloud some atoms/molecules will be coming towards you and the frequencies of the emitted photons are shifted towards higher values from the Doppler effect. Similarly, some are going away leading to lower frequencies. This is called "thermal broadening."'

There may also be large-scale broadening due to different gas clouds within the same telescope resolution element. This can be called 'turbulent broadening," and has the same physics as seeing. One can learn a lot from the study of spectra.

4.3   Intensity of Spectral Lines

Finally, the intensity of spectral lines (and the relative intensity of several spectral lines in more complex objects like a galaxy) can be used to measure a number of things, including the gas abundance, density, mass, levels of star formation activity, or the presence of an active galactic nucleus. In general, the intensity of spectral lines depends on:

- the amount of material;

- how quickly a transition occurs for a given atom/molecule (some transitions are fast, such as $H\alpha$ and some are slow such as the $21\,cm$ line of HI).

There are other considerations, but these tend to be primary. Of course, if the line is especially broad, it will be at low intensity.

5   UV/Optical/IR Instrumentation

To perform spectroscopy, we need to spread the light out over frequency. In the UV/optical/IR this is done with some sort of dispersive element.
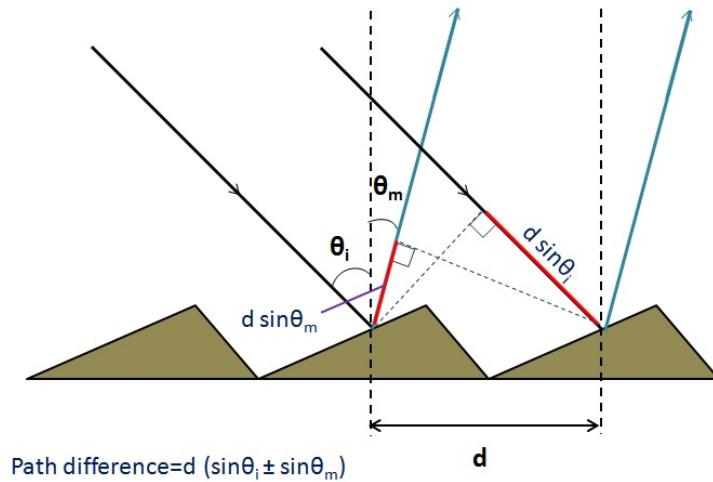
Figure 2: Diffraction Grating.

Your book is quite loquacious on this topic so I will not go into details here. The most common modern technology used is a diffraction grating, rather than a prism.

[Birney Figure 12.1]
We are looking at light passing through a slit of finite width. It gets collimated, dispersed, and focused (at the "camera"), then imaged at the spectrograph (which could be a CCD). The light collected is just an image of the slit, spread out in wavelength.

The collimator and camera are just lenses, so what is the dispersing element? There are a few options:

Prisms [Birney 12.2]
Prisms are the simplest diffraction medium. Snell's law is wavelength dependent (think of chromatic aberration!), so prisms can spread out light. Angular dispersion, the change in diffraction angle with wavelength, $d\theta/d\lambda \propto -\lambda^{-3}$, where θ is deviation angle. The negative sign shows that the angle of deviation is smaller for larger wavelengths: blue light is refracted more than red light. The magnitude of the dispersion much greater at shorter wavelengths - which is the good in some cases, but complicates matters in most applications. For this reason, prisms are not used much any more.

Diffraction Gratings [Birney 12.4]
Diffraction gratings have grooves, and the grooves work to disperse light in a manner similar to that of a prism. This works because light rays diffracted into a given angle will constructively interfere if their path differences are equal to an integer number of wavelengths (see Figure 2).

A few facts about diffraction gratings:
   1. Can be transmission (e.g. holes) or reflection (mirrors with special diffractive proper-

ties)

2. Different from prism in that

    (a) dispersion uniform over small ranges of wavelength,

    (b) shorter wavelengths (blue) dispersed less than longer (red),

    (c) we get several spectra "orders," at once, of decreasing brightness - first, second, third, fourth, etc. order.

3. Can concentrate the light into a single order if dispersing grooves are non-symmetric, a "blaze." To characterize the blaze we have a parameter called the "blaze angle."

The condition for interference is:

$$m\lambda = \sigma(\sin\alpha + \sin\beta) \tag{7}$$

which is known as the "grating equation." α and β have opposite signs [Figure 12.3]. m gives the "order" mentioned earlier. m is an integer, and can be negative. $m = 0$, the grating is a mirror "specular reflection", or zeroth order.

$$\alpha + \beta = 2\theta \tag{8}$$

Let's take an example: 600 grooves/nm, $m = 2$, 500nm, $\alpha = 5°$. This leads to $\beta = 31°$ and $\theta = 18°$

If the orders overlap, the signal is confused and cannot be effectively used. This sets the "free spectral range" where there is no overlap. As m increases, this becomes more and more of a problem. Have to solve it by filtering the light.

Last thing on diffraction gratings, resolving power

$$R = \lambda/\Delta\lambda \tag{9}$$

characterizes the grating. Sometimes high-resolution spectra are desirable (high R), and sometimes low resolution (low R). "Echelle" spectrographs work at very high order, with very high blaze angles, and high resolution.

Assess yourself/study guide after lecture & reading (without peeking at notes)...

1. Remind yourself: what are the primary three fundamental physical ways emission lines might be produced (what produces them, and how)?

2. What is the rest emission frequency of the He87γ transition line?

3. What is the rest emission frequency of the Balmer-series Hβ line?

4. Let's say there's a laser (emission wavelength 430 nm) that is traveling *towards you* at half the speed of light. What is the wavelength you would observe from that laser?

5. What if the previous laser were instead traveling *away from you* at half the speed of light?

6. If you observed a broad-band emitter (like a $T = 7000$ K blackbody star) with a cloud of Hydrogen in front of it, what (qualitatively) would the observed optical spectrum look like? (Would it be a smooth continuum, emission-line spectrum, or absorption-line spectrum, and what lines might be present?)

7. Let's say the cloud in the previous problem is really quite extended, but still in thermal equilibrium (that is, all parts of it are in an equilibrium state of emission/absorption). If you instead observed another part of the same cloud, now not directly observing the part with the hot star behind it, what (qualitatively) would the observed optical spectrum look like? (Would it be a continuum, emission-line spectrum, or absorption-line spectrum, and what lines might be present?)