Optical Emission Line Spectra

1. Basics & Nomenclature

Optical (and near ultraviolet and near infrared) emission lines of galaxies are predominantly associated with ionized gas. The emission lines are the result typically of *recombination radiation* or *collisionally excitation*. The physical conditions of ionized gas in galaxies varies by large orders of magnitude in density, from 0.3 to 10^4 cm^{-3} (up to 10^{10} cm^{-3} or more in quasars) but typically has temperatures around 10^4 K.

In astronomical spectroscopy, the ionization state is indicated by Roman numerals. XI indicates neutral "X," XII indicates singly-ionized "X," XIII indicates doubly ionized "X," etc.

The electronic states can be classified by their spin, orbital, and total angular momentum, and is typically labeled $^{2S+1}L_J$, where S is the total spin, $L = S, P, D, F, G, \ldots$ is the total orbital angular momentum (corresponding to $L = 0, 1, \ldots$), and J is the total sum. So $^3P_0$ indicates an atom with $S = 1$, $P = 1$, and $J = 0$.

A critical number for any radiative transition is the transition probability A, sometimes known as the *Einstein A coefficient*, and typically expressed in units of s^{-1}.

1.1. Ionization processes

The ionization state of gas is determined by the balance among effects such as photoionization, collisional ionization, and recombination. In the interstellar medium, the radiation field is generally far from blackbody and statistical mechanical rules like the law of mass action that would otherwise govern the ionization state do not hold.

In many applications in extragalactic astrophysics we are concerned with photoionized gas, in which photons of sufficient energy liberate electrons. The cross-section for photoionization is maximum at the ionization energy; it declines as E^{-3} (or equivalently ν^{-3}) at higher energy, so photoionization for most ionizing spectra is dominated by photons near the threshold.

The degree of ionization of atoms is largely determined by their ionization energy. For hydrogen in the electronic ground state, the *ionization potential* is 13.6 eV, corresponding to a photon of wavelength 912 Å. Helium has an ionization potential of 24.6 eV, and HeII (He^+) has an ionization potential of 54.4 eV. For single ionization, carbon, nitrogen, and oxygen have similar ionization potentials to hydrogen, whereas neon has a slightly deeper potential, and silicon and sulfur have slightly shallower potentials. For more highly ionized species, the ionization potential becomes deeper in general.

The electron temperatures in the interstellar medium ($\sim 10^4$ K) usually correspond to energies

kT far below these ionization potentials (which require temperatures $\sim 10^5$ K). Therefore collisional ionization is usually not important. However, in shock heated gas (for example in supernova remnants) or in some regions of active galactic nuclei these high temperatures can be achieved.

1.2. Recombination

In ionized gas at equilibrium, hydrogen and other elements have electrons recombining at some rate that balances the ionization rate.

The recombination rate for hydrogen can be written:

$$R = n_e n_p \alpha(T) \tag{1}$$

The recombination coefficient α_{nl} (usually in units cm^3 s^{-1}) for a hydrogen atom to some energy level n and orbital angular momentum state l can be expressed in terms of the cross-section to recombination σ_{nl}:

$$\alpha_{nl}(T) = \int_0^\infty \mathrm{d}u \, u f(u) \sigma_{nl}(u) \tag{2}$$

where $f(u)$ is the Maxwell-Boltzmann distribution. Approximately, $\sigma \propto u^{-2}$, so $\alpha \propto \langle 1/u \rangle \propto T^{-1/2}$.

Typically the recombination is to a high energy bound state. The electron will thereafter decay into successively lower states. For hydrogen, two limiting cases exist:

- Case A: optically thin to ionizing photons. The recombination rate is the sum of the recombination rates to each energy level indexed by quantum states n and l:

$$\alpha_A(T) = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \alpha_{nl}(T) \tag{3}$$

- Case B: optically thick to photons at energies just above the H ionization limit (13.6 eV). The recombinations to $n = 1$ virtually always result in an ionizing photon that is immediately reionizes another atom. This means that the effective recombination rate is modified by subtracting the recombinations to $n = 1$:

$$\alpha_B(T) = \alpha_A(T) - \alpha_{1s}(T) \tag{4}$$

For most cases within the interstellar medium, Case B is appropriate because enough neutral H is available, even in HII regions. In such cases, the system is typically also optically thick to all Lyman-series photons; i.e. the neutral atoms are usually in the ground state and the cross-sections for Lyman-series excitation are comparable to the cross-sections for ionization.

The Case A recombination spectrum can be calculated by assuming the levels are populated by recombination according to the individual α_{nl}, and then using the decay probabilities from each state. The Case B recombination spectrum is calculated the same way, but just taking removing all transitions to $n = 1$ from the calculation. The temperature enters the calculation weakly due to its effect on the recombination coefficients α_{nl}. The density enters the calculation because collisions affect the high n levels, but this dependence is weak (until $n > 10^6$ cm^{-3},

In HII regions, where Case B holds, Lyman lines have a special fate. They undergo *resonant scattering*; every Lyman line emitted is very quickly reabsorbed. Since they undergo many scatterings, and also can decay to lower levels between scatterings, eventually they result in a Lyman-α photon. In HII regions, this scattering continues until one of the atoms excited to the $n = 2$ state decays instead in a rare two-photon decay (from the 2s state), or a photon Doppler scattered into the wing of the line where the optical depth is lower.

Helium also contributes recombination radiation. For very hard photoionization sources, He III will predominate. This is a hydrogen-like system with an ionization energy four times as large. The emission lines are shifted in energy by that much, and the overall pattern of transitions in gas at temperature T is the same as hydrogen for a gas with temperature $T/4$.

1.3. Strömgren Spheres

The illustrative case of an HII region is a *Stromgren sphere*, which results from a spherically symmetric, uniform cloud of gas being ionized by such a star. If Q is the number of photons emitted by the star, and assuming Case B recombination (optically thick to photons slightly more energetic that the Lyman limit, but optically thin otherwise), then equilibrium between ionization and recombination dictates:

$$Q = \frac{4\pi}{3} R_S^3 \alpha_B n(H^+) n_e = \frac{4\pi}{3} R_S^3 \alpha_B n_e^2 \tag{5}$$

Typical values are $Q \sim 10^{49}$ s^{-1}, $\alpha_B \sim 4 \times 10^{-13}$ cm^3 s^{-1}, $n_e \sim 10$ cm^{-3}. Solving for R_S yields ~ 10 pc. The size of the sphere is therefore determined by the overall flux.

The above calculation assumes that the hydrogen is fully ionized. We can check this assumption by considering the ionization balance at a point within the sphere, say at 5 pc. The cross-section for photoionization is $a \sim 6 \times 10^{-18}$ cm^2. The balance becomes:

$$n(H_0) a \frac{Q}{4\pi d^2} \approx n_e n_p \alpha_B. \tag{6}$$

Defining the neutral fraction, $n(H_0) = \xi n_H$, so that $n_e = (1 - \xi) n_H$, we find:

$$\xi \frac{aQ}{4\pi d^2} \approx n_H (1 - \xi)^2 \alpha_B \tag{7}$$

For $\xi \ll 1$:

$$\xi \approx \frac{1}{1 + aQ/4\pi d^2 n_H \alpha} \approx \frac{n_H \alpha}{aQ/4\pi d^2} \tag{8}$$

Then $\xi \sim 10^{-5}$, because the recombination rate is much slower than the ionization rate.

At the edge of the system, we must have $\xi \sim 0.5$, and we can check the mean free path at this point, which is:

$$d \sim \frac{1}{\xi n a} \sim 0.01 \text{ pc} \tag{9}$$

The Stromgren sphere has a thin surface relative to its overall size.

In addition to all of the geometrical approximations and neglect of collisional effects and other physics, this basic calculation assumes that the photoionization is dominated by photons right above the photoionization threshold. This approximation is good for O and B stars. However, for harder spectra, such as those from much hotter sources or AGN, the mean photon energy is much larger and therefore the cross-section a is much smaller. This leads to much larger partially ionized regions.

1.4. Collisional excitation

Heavier elements than hydrogen tend to be incompletely ionized in gas nebulae. For such elements, the remaining electrons can be excited by collisions, and then decay radiatively. The excitation potential for He+ is too deep for most nebular temperatures, but O+, O++, N+, and many other species have excited states within reach of collisions in 10^4 K gas. Meanwhile, these excited states can have short enough radiative decay times that at the density of nebular gas they can decay radiatively prior to collisional deexcitation. The resulting lines are called *collisionally excited lines*. Since under terrestrial conditions collisional deexcitation so greatly dominates, they are also called *forbidden lines*.

Among the collisionally excited lines, depending on the radiative decay times, there are both *strong lines* that are bright and easy to measure, and other lines sometimes referred to as *auroral lines* (particularly [OIII] 4363) that tend to be fainter. See the more complete discussion below.

1.5. Measurements of emission lines

We can measure recombination lines and collisionally excited lines in spectra of galaxies. These measurements can constrain properties of the ionized gas, such as its temperature, density, ionization source, and metallicity.

A critical issue for measurement is determination and subtraction of the *continuum* underneath the line, which is primarily due to stars in the galaxies. The stellar continuum is not smooth, which means that subtracting a low order fit near the emission line location is not sufficient. Modern measurements of emission lines use stellar population models to fit the continuum (most often, excluding the wavelengths very close to any emission lines from the fit), or sometimes empirically based models. This process is especially important for Balmer lines, where there is underlying Balmer absorption in the stellar continuum, but affects all lines at some level.

Once the continuum is subtracted, the line can be measured in multiple ways, either by integrating over some fixed wavelength aperture or fitting a Gaussian or other profile to the line. Because lines can vary in their width due to different Doppler shifts, usually the latter route is taken to avoid wavelength aperture effects and to maximize signal-to-noise ratio. The flux of the line can be then inferred from the fit.

The Doppler widths are typically 10–20 km s^{-1} locally within star forming regions, a few hundred km s^{-1} in narrow line regions of AGN, and a few thousaid km s^{-1} in broad line regions. For spectra that integrate over substantial parts of galaxies, the line widths may be larger because they integrate over large scale motions such as rotation.

Emission line strengths can be quantified also by their equivalent width, which is their flux divided by the local flux density of the continuum. The equivalent width is handy in cases that the spectrophotometry is not well understood, but fundamentally it is a combination of the emission line properties and the stellar continuum properties so can be more difficult to interpret in terms of physical parameters.

1.6. Temperature diagnostics

A standard use for emission line measurements is to determine the electron temperature within the ionized gas. The temperature is interesting because it is set by the physical conditions of the nebula and it also is an important parameter to know to interpret the line emission in terms of metallicity and ionization source.

Emission lines from OIII, NII, NeIII, and SIII can used to determine temperature, because they have excited states that are low enough to be well populated in 10^4 K gas but well enough separated to have significantly different Boltzmann factors, and in addition decay through channels that release optical emission lines. The first excited electronic state ${}^1D_2$ can decay to several nearly degenerate ground state levels ${}^3P_0$, ${}^3P_1$, or ${}^3P_2$; the transition to the first requires a quadrupole transition so has a slow rate. The other two correspond to the [OIII] 4959 and 5007 lines and the [NII] 6583 and 6548 lines.

A second excited electronic state ${}^1S_0$ can decay to the ground states ([OIII] 2321 or [NII] 3063) but in the optical also emits the so-called auroral line to ${}^1D_2$ ([OIII] 4363 or [NII] 5755). The name "auroral" is due to the fact that this same transition in [OI] yields the famous 5577 Å sky line, which was first studied and identified in the polar aurorae (McLennan 1928; Kragh 2009). These lines are weak both because the higher state has a larger Boltzmann factor and because the decay probability to the intermediate state is lower.

At low enough densities ($n < 10^5$ cm^{-3}), the populations are not in equilibrium with the electrons; every collision is followed by a radiative transition. The ratio of the collisional excitation rates to the $^1D_2$ and $^1S_0$ populations is equal to:

$$\frac{\Upsilon(^3P, ^1D_2)}{\Upsilon(^3P, ^1S_0)} \exp\left(\Delta E/kT\right) \tag{10}$$

where ΔE is the energy difference between the $^1D_2$ and $^1S_0$ levels, and Υ is the collision strength (which is itself a function of temperature). Therefore, if the ratio of the auroral lines and the strong lines can be measured, and the atomic data on transition probabilities and collision strengths is known, then the temperature can be measured.

At higher densities, collisional deexcitation tends to lower the populations in $^1D_2$ and weaken the pair of strong lines. The collision rate scales as $n_e/T^{1/2}$ and it therefore turns out that the weakening of the line ratio is proportional to:

$$\frac{1}{1 + \alpha n_e/T^{1/2}} \tag{11}$$

where $\alpha \sim 10^{-5}$–10^{-3} cm^3 K$^{1/2}$, depending on the species.

1.7. Density diagnostics

Like temperature, electron density within the ionized gas can be determined from line ratios and knowledge of it helps determine the gas metallicity and ionization source. The line ratios of interest are between lines with nearly the same excitation energy, but different radiative transition probabilities or collisional deexcitation rates.

At low density, every collisional excitation is followed by a radiative transition, so the fluxes of the lines are proportional to the excitation rates (often just the statistical weights of the levels).

At high density, the population levels are in thermal equilibrium so that their relative abundance is just their statistical weight (because their energies are nearly identical). The line strength ratios then are just the statistical weights times the transition probabilities.

The transition between the two regimes is defined by the *critical density*, at which the radiative transition rates are equal to the collisional transition rates. At $T \sim 10^4$ K these critical densities are $\sim 10^3$–10^5 for many of the species of interest. The radiative transition rates are constant, whereas the collisional rates have a dependence of $n_e T^{-1/2}$, so the line ratio dependence on density shifts to higher density as temperature increases.

The relevant lines for this measurement are usually [OII] 3729 and 3726 or SII 6731 and 6716 (from the ^2D levels of each singly-ionized atom).

1.8. Ionization spectrum indicators

The ionization spectrum can also be constrained with line ratios. In the context of galactic observations, indicators exist for both the total flux of ionizing photons, and the hardness of the ionizing spectrum.

The ionizing flux can be quantified by the ionization parameter, usually quantified as:

$$U = \frac{Q_H}{n_H c}, \tag{12}$$

where Q_H is the flux (for example, in units cm^{-2} s^{-1}) of hydrogen-ionizing photons and n_H is the number density of hydrogen atoms. Sometimes the quantity $q = Uc$ is used instead. In addition, there is some ambiguity to the definition in the context of models. For plane-parallel photoionization models, it is evaluated at the point that the ionization flux impinges on the gas, but for spherical models an inner radius of the region must be defined.

An important indicator of ionizing parameter is the [OIII] line. A higher flux of photons will allow the gas to maintain a larger population of doubly-ionized oxygen atoms. The line ratio [OIII]/[OII] is typically used, though it is also somewhat metallicity dependence. The [OIII]/[SII] also can be used, though it too has some sensitivity to metallicity. .

The hardness of the radiation field can be measured, somewhat counterintuitively, by the low-ionization lines of NII and SII. Because the photoionization cross-section declines strongly with frequency above the ionization threshold, the mean free path for these photons are longer. This mean free path sets the size of the partially ionized portion at the edge of the ionized region. These regions contain considerable OI, NII, and SII, and therefore hard radiation fields tend to emit these lines strongly.

1.9. BPT diagrams

Emission line regions can result from several different ionization sources: generally one of star-formation, AGN, hot evolved stars, or shocks. Baldwin et al. (1981) described what is now the classic *BPT classification* which helps to distinguish some of these ionization mechanisms. If the AGN broad-line region is visible, it is unambiguous; however, more commonly only the narrow-line region is visible, and with integrated (as opposed to resolved) spectra.

The BPT diagrams involve the [OIII]/Hβ flux ratio plotted against [NII]/Hα, [OI]/Hα, and [SII]/Hα. The Balmer line normalization accounts for any variation in the overall luminosity of the region due to its size and total energy of the ionization sources. The use of Hβ instead of Hα for [OIII] because this ratio is more stable to reddening and spectrophotometric variations.

[OIII]/Hβ traces the ionization parameter. The other ratios trace the size of the partially ionized region, which increases with the hardness parameter. Stellar ionization sources are limited in their hardness, so generally the higher ratios indicate the present of AGN or post-AGN stars (which reach 10^5 K in temperature).

Thus, to the left and bottom in these plots lie the cases where the emitting flux is dominated by gas ionized from star-formation. In this region, the line ratios are determined mostly by the processes we have described above. To the right and to the right-top of the plot lie the *LINER* (low ionization) and Seyfert regions. In these regions, while the above discussion proves a useful guide, in detail a number of other high energy processes come into play. The Seyfert emission is invariably powered by AGN, but the LINER region can be powered either by low luminosity AGN or other sources, such as post-AGB stars. The extent and line ratio distribution

1.10. Metallicity diagnostics for star-forming galaxies

In the context of understanding galaxy evolution and formation, the metallicity of the interstellar gas is an important parameter, since it traces some combination of the chemical enrichment history and accretion history. Within the star forming region of the BPT diagram, there are a number of established methods of determining the metallicity. In this diagram, the metallicity generally increases with increasing [NII]/Hα; as we will see below, it is an example of a strong-line metallicity indicator.

The first and most reliable metallicity indicator is the *recombination line method*. Within a few individual HII regions, it is possible to measure recombination lines of the metal ions. These recombination lines do depend on the ionization fractions for ions associated with the observed lines, but otherwise have very little dependence on temperature and density, and scale linearly with the ionic abundance. However, because the ions are $< 10^{-4}$ as abundant as hydrogen, the recombination lines are extremely faint and so only a handful of HII regions can be observed with high enough signal-to-noise ratio.

The second most reliable indicator is the *direct method*, which depends on the more strongly emitting collisionally excited lines. This technique makes use of the diagnostics for T_e and n_e described above, which allows one to calculate the emissivity of other indicators, such as [OII] 3726, 3729 or [OIII] 4959, 5008, relative to Hα or Hβ. Then observations of these lines yields the metallicity. However, because it relies on collisionally excited lines, the T_e, n_e, and metallicity indicators all depend on the square of the density, which means that the measurement is biased towards the higher density regions in the presence of density fluctuations in the HII regions. In addition, as described above, the temperature sensitive auroral lines tend to be faint.

Finally, the least reliable, but most commonly applied indicator is the *strong line method*. It is most commonly applied because it relies only on easily measurable lines, which allows it to be used on many more, and more distant, galaxies. These methods take advantage of known correlations within the properties of HII regions, such as between the gas temperature, the N/O abundance ratio and metallicity, etc.). Empirical calibrations of the strong line method use calibrations against the direct method; examples are R23 = ([OII] + [OIII])/Hβ, the similar S23, and O3N2 = [OIII] / N[II]. Theoretical models for HII regions are also available to calibrate these ratios, and they have also also led to the use of the N2O2 = [NII]/[OII] ratio.

2. Commentary

An entire course may be given on the astrophysics of nebulae. This description is extremely simplified. It ignores the detailed derivation of the equilibrium populations as a function of density and temperature in the idealized cases, as well the effects of realistic issues such as fluctuations in density and temperature in the ionized gas. It also ignores many diagnostics, particularly those outside the optical.

Gas metallicity indicators are somewhat famously discrepant with each other in an absolute sense by quite a bit.

3. Key References

- *Physics of the Interstellar and Intergalactic Medium,* **need draine cite**
- *Astrophysics of Gaseous Nebulae and Active Galactic Nuclei, Osterbrock & Ferland (2006)*
- *IZI: Inferring the gas phase metallicity (Z) and ionization parameter (q) of ionized nebulae using Bayesian statistics,* **?**

4. Order-of-magnitude Exercises

1. Estimate the temperature necessary for the typical electron-hydrogen collision to result in an ionization. **finish answer** This condition requires $kT \sim 13.6$ eV.

2. Estimate the typical collisional excitation levels found in 10^4 K gas; i.e. their approximate wavelength of emission were they to decay directly to the ground state. **finish answer**

3. For an HII region with $n_H = 10$ cm^{-3} and of size $s = 10$ pc, at what ionization level $1 - \xi$ is it optically thick to photons just over the threshold for ionizing hydrogen.

   Using the cross-section for ionization in the text, $a \sim 6 \times 10^{-18}$ cm^2, we can write the optical depth as:

   $$\tau \sim n_H a s \xi, \tag{13}$$

   and so it will be optically thick when $\tau \sim 1$, or:

   $$\xi \sim \frac{1}{n_H a s} \sim \frac{1}{(10)(6 \times 10^{-18})(3 \times 10^{19})} \sim \frac{1}{2000} \sim 5 \times 10^{-4}. \tag{14}$$

Thus, even at ionization fractions of $1-\xi=0.9995$, this system will be optically thick to ionizing photons.

does this make sense to calculate? does it show actually most of the photon capture is near the edge of the HII region, since the typical ionization fraction is higher?

5. Analytic Exercises

- **Is there a simple way to calculate ν^{-3}?**
- alpha calculation
- Calculating line ratios vs. temperature
- Ly-alpha scattering

6. Numerics and Data Exercises

1. Download the following five galaxy spectra from the SDSS database, and the following ten stellar spectra. We will concentrate on measuring two particular emission lines in the galaxy spectra, using continuum subtraction based on the stellar spectra.
2. Use of Balmer decrement for dust
3. Running MAPPINGS or other

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