

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, $L = S, P, D, F, G, \dots$ is the total orbital angular momentum (corresponding to $L = 0, 1, \dots$), 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.

For hydrogen in the electronic ground state, the *ionization potential* is 13.6 eV , corresponding to a photon of wavelength 912 \AA . The ionization of other atoms is strongly affected by their ionization energy. 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 ($\sim 10^4 \text{ K}$) 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:

$$R = n_e n_p \alpha(T) \quad (1)$$

The recombination coefficient α_{nl} (usually in units $\text{cm}^3 \text{s}^{-1}$) 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} :

$$\alpha_{nl}(T) = \int_0^\infty du u f(u) \sigma_{nl}(u) \quad (2)$$

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 :

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

- Case B: optically thick to photons at energies just above the H ionization limit (13.6 eV). The recombinations to $n = 1$ do not count, because they just result in an ionizing photon that is immediately recaptured:

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

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 optically thick to all Lyman-series photons.

The Case A recombination spectrum can be calculated by assuming the levels are populated by recombination as above, and then using the decay probabilities from each state. The Case B recombination spectrum is calculated the same way, but just taking all transitions to $n = 1$ out of

the picture. The temperature enters the calculation weakly due to its effect on the recombination coefficients α . The density enters the calculation even more weakly (until $n > 10^6 \text{ cm}^{-3}$), because collisions affect the high n levels.

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, they can escape only through a rare two-photon decay to a continuum (when the state is 2s) or by being Doppler scattered into a wing of the line.

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. 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.

1.4. 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 thousand km s^{−1} in broad line regions. For spectra that integrate over substantial parts of galaxies, the line widths may be larger because of 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.

1.5. 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 be used to determine temperature, because they have excited states that are low enough to be well populated in 10⁴ 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 ¹D₂ can decay to several nearly degenerate ground state levels ³P₀, ³P₁, or ³P₂; 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 ¹S₀ can decay to the ground states ([OIII] 2321 or [NII] 3063) but in the optical also emits the so-called auroral line to ¹D₂ ([OIII] 4363 or [NII] 5755). 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:

$$\frac{\Upsilon(^3P, ^1D_2)}{\Upsilon(^3P, ^1S_0)} \exp(\Delta E/kT) \quad (5)$$

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:

$$\frac{1}{1 + \alpha n_e/T^{1/2}} \quad (6)$$

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

1.6. 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 $T \sim 10^4 \text{ K}$ 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).

1.7. 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:

$$U = \frac{Q_H}{n_H c}, \quad (7)$$

where Q_H is the flux (for example, in units $\text{cm}^{-2} \text{s}^{-1}$) 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.

1.8. BPT diagrams

1.9. Metallicity diagnostics for star-forming galaxies

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.

3. Key References

- *Physics of the Interstellar and Intergalactic Medium*, Draine et al. (2007)
- *Osterbrock Osterbrock & Ferland (2006)*
- *Blanc ?*

4. Order-of-magnitude Exercises

1. Dependence on temperature and resulting metallicity dependence of $H\alpha$
2. Using typical mass-to-light ratios in the i -band, and star formation rate normalizations for $H\alpha$, approximately relate a $H\alpha$ equivalent width to the equivalent specific star formation rate.

5. Analytic Exercises

- Show explicitly from Equation 2 that the recombination coefficients should scale as $\alpha \propto T^{-1/2}$.
- alpha calculation
- Calculating line ratios vs. temperature
- Ly-alpha scattering

6. Numerics and Data Exercises

1. Use of Balmer decrement for dust
2. Running MAPPINGS or other

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REFERENCES

- Draine, B. T., Dale, D. A., Bendo, G., et al. 2007, ApJ, 663, 866
- Osterbrock, D. E., & Ferland, G. J. 2006, *Astrophysics of Gaseous Nebulae and Active Galactic Nuclei* (University Science Books)