Excitations



Principle of detailed balance

Consider a 2-level system, excitation occurs if the incoming free electrons have kinetic energy $\frac{1}{2}mv^2 > \chi$



Define the excitation rate coefficient γ_{01} so that # of excitation s⁻¹ cm⁻³(= $n_e n_0 v \sigma$) $\equiv n_e n_0 \gamma_{01}$ where both n_e and n_0 have units of [cm⁻³].

$$\gamma_{01} \equiv \langle \sigma v \rangle = \int_{\chi = \frac{1}{2}mv^2}^{\infty} v \sigma_{01}(v) f(\vec{v}) d^3 \vec{v}$$

Here σ_{01} is the excitation cross section, and $f(\vec{v})$ is the Maxellian distribution function

$$f(v;T) dv = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}} dv$$

So

$$\gamma_{01} = \frac{4}{\sqrt{\pi}} \left(\frac{1}{2kT}\right)^{1/2} \int_{\chi = \frac{1}{2}mv^2}^{\infty} v^3 \sigma_{01}(v) \ e^{-\frac{mv^2}{2kT}} \ dv \quad \text{(A)}$$

This is the upward transition.

Downward transition:

• spontaneous emission, rate = $n_1 A_{10}$

• deexcitation by collisions, rate = $n_1 n_e \gamma_{10}$, where $\gamma_{10} = \int_0^\infty v \sigma_{10}(v) f(v) dv = \gamma_{10}(T)$

Detailed balancing

In steady state, [upwards] = [downwards]

$$n_0 n_e \gamma_{01}(T) = n1 [A_{10} + n_e \gamma_{10}(T)]$$

$$\frac{n_1}{n_0} = \frac{n_e \gamma_{01}}{A_{10} + n_e \gamma_{10}} = \frac{\gamma_{01}}{\gamma_{10}} \frac{1}{1 + \frac{A_{10}}{n_e \gamma_{10}}} \tag{B}$$

(i) At <u>high</u> densities, i.e., $n_e \rightarrow \infty$, (i.e., collisional excitation and deexcitation dominate \rightarrow in TE)

$$\frac{n_1}{n_0} = \frac{\gamma_{01}}{\gamma_{10}}$$

But since $\frac{n_1}{n_0} = \frac{g_1}{g_0} e^{-\chi/kT}$,
$$\frac{\gamma_{01}}{\gamma_{10}} = \frac{g_1}{g_0} e^{-\chi/kT} \text{ for } n_e >> 1$$

When collision dominates, recall (A),

$$n_e n_0 v_0^3 \sigma_{01}(v_0) \exp(-\mu v_0^2/2kT) dv_0$$

= $n_e n_1 v_1^3 \sigma_{10}(v_1) \exp(-\mu v_1^2/2kT) dv_1$,

where μ is the reduced mass, and v_0 , and v_1 are relative velocities of the colliding particles.

Energy:
$$(1/2)\mu v_0^2 = (1/2)\mu v_1^2 + \chi$$
,
so $v_0 dv_0 = v_1 dv_1$

Plugging back, we get

$$n_0 v_0^2 \sigma_{01} \exp(-\frac{\mu v_0^2}{2kT}) = n_1 v_1^2 \sigma_{10} \exp(-\frac{\mu v_1^2}{2kT})$$
$$= \frac{n_0 g_1}{g_0} e^{-\chi/kT} v_1^2 \sigma_{10} e^{-\frac{\mu v_1^2}{2kT}}$$

The exponential parts cancel out from the energy conservation.

$$g_0 v_0^2 \sigma_{01} = g_1 v_1^2 \sigma_{10}$$

(ii) At low densities, i.e.,
$$n_e \rightarrow 0$$
 upward by collision

$$\frac{n_1}{n_0} \rightarrow \frac{\gamma_{01}}{\gamma_{10}} \frac{n_e \gamma_{10}}{A_{10}} = \frac{n_e \gamma_{01}}{A_{10}} \overset{\checkmark}{\longrightarrow} \frac{1}{A_{10}} \overset{\land}{\longrightarrow} \frac{1}{A$$

This means every collisional excitation is followed by the emission of a photon.

<u>Note</u>: The cooling rate [cm⁻³ s⁻¹] is $n_1 A_{10} hv_{10}$ = $n_e n_0 \gamma_{01} hv_{10}$ Consider the radiative transition $1 \rightarrow 0$, the rate of emission of line photons [s⁻¹ atom⁻¹] ... recall eq. (B)

$$\frac{n_1}{n_0} A_{10} = A_{10} \frac{\gamma_{01}(T)}{\gamma_{10}(T)} \frac{1}{1 + \frac{A_{10}}{n_e \gamma_{10}(T)}}$$

(i) At <u>high</u> densities

(ii) At <u>low</u> densities

$$\frac{n_1 A_{10}}{n_0} = A_{10} \frac{\gamma_{01}}{\gamma_{10}} \frac{n_e \gamma_{10}}{A_{10}} = n_e \gamma_{01} \quad \checkmark \quad T$$

This is what we had earlier ; i.e., every collisional excitation \rightarrow emission of a line photon.

Consider a 2-level system, for which the electron collides with an ion in the lower level. The collisional cross section, $\sigma_{01} = \sigma_{01}(v)$ Collisions between electrons and ions in a lower level



This is for the electron velocity. Ions are neglected.

$$\begin{cases} \sigma_{01} = 0 & \text{if } (1/2)mv^2 < \chi \\ \sigma_{01}(v) \propto 1/v^2 & \text{if } (1/2)mv^2 > \chi \end{cases}$$

Usually express σ in terms of **collisional strength** $\Omega(0,1)$

$$\sigma_{01}(v) = \frac{\pi \hbar^2}{m_e^2 v_0^2} \frac{\Omega(0,1)}{g_0}$$

 Ω is on the order of unity Recall that $g_0 v_0^2 \sigma_{01} = g_1 v_1^2 \sigma_{10}$, $\Omega(0,1) \equiv \Omega(1,0)$ So the deexcitation rate coefficient is

$$\gamma_{10} = \int_{0}^{\infty} v \,\sigma_{10}(v) \,f(v) \,dv$$
$$= \sqrt{\frac{2\pi}{kT}} \frac{\hbar^2}{m^{3/2}} \frac{\Omega(0,1)}{g_1}$$
$$= \frac{8.629 \times 10^{-6} \,\Omega(0,1)}{g_1 T^{1/2}}$$

Excitation per volume per time is $n_e n_0 \gamma_{01}$ where $\gamma_{01} = (g_1/g_0) \gamma_{10} \exp(-\chi/kT)$

 Ω 's must be calculated quantum mechanically and can be found tabulated with specific temperature values.

Forbidden Lines

Allowed (= electric dipole) transitions that satisfy the selection rules:

- 1. Parity much change.
- 2. $\Delta L = 0, 1.$
- 3. $\Delta J=0, 1, but J = 0 \rightarrow 0$ is forbidden.
- 4. Only one single-electron wave function $n\ell$ changes, with $\Delta \ell = 1$.
- 5. Δ S=0: Spin does not change.

Spectroscopic Notation...

Ionization State

I ---- neutral atom, e.g., $H I \rightarrow H^0$

- II --- singly ionized atom, e.g., H II \rightarrow H⁺
- III doubly ionized atom, e.g., O III \rightarrow O⁺⁺
- and so on....e.g., Fe IIIXX

Peculiar Spectra

e (emission lines), p (peculiar, affected by magnetic fields), m (anomalous metal abundances) e.g., B5 Ve

Allowed (regular) Line: due to electric dipole; $A \sim 10^{+8} \text{ s}^{-1}$; denoted by no bracket, e.g., C IV, O I

- **Forbidden Line:** fails to fulfill at least one of the selection rules 1 to 4. It may be a magnetic dipole or an electric quadrupole transition; $A \sim 10^{0}$ -- 10^{-4} ; denoted by with a pair of square brackets, e.g., [O III], [N II]; the H 21 cm line A=2.88 x 10^{-15} s⁻¹, or 1/[11 Myr].
- Semi-forbidden (intercombination or intersystem) Line: all electric dipole selection rules except $\Delta S \neq 0$, $A \sim 10^{+2}$ s, denoted by a single bracket, e.g., [OII

- Normally an atom stays in the excited state for 10⁻⁸ s.
- A forbidden transition occurs for excitation levels < a few eV, and stays in the excited state for seconds or longer before returning to the ground state.
- In the lab n ↑↑↑, both excitation and de-excitation take place frequently, so radiative transition (emitting a photon) is unlikely.
- In ISM, the electrons are not energetic enough to excite the atoms to normal levels (10-20 eV), but enough to excite to metastable levels.
- Once (collisionally) excited (kinetic energy) → emission
 → escaped → efficient cooling



An example -----Ring Nebula (M57), a planetary nebula

Slit = 8' x 1"





 $\frac{1}{1} \frac{1}{1} \frac{1}$

1-D spectrum shows
little continuum, and a
few emission lines
→ A line spectrum

4959Å and 5007Å doublet from twiceionized oxygen, O++, or OIII in spectroscopic notation → (oxygen) gas is ionized, with T > a few thousand K and density < 100/cm³

Excitation Theory --- Applications

Consider a 3-level system, with the two **upper** levels close together.

$\frac{j_{\lambda 3729}}{2}$ _	_ <u>j21</u> _	$- \frac{n_2 A_{21} h \nu_{21}}{n_2 A_{21} h \nu_{21}}$
$j_{\lambda 3726}$ -	- <u>j</u> 31 -	$-\frac{1}{n_3A_{31}h\nu_{31}}$



Recall that $n_e \rightarrow \infty$, collisional excitation and deexcitation $n_e \rightarrow 0$, every collisional excitation is followed by emission





$$n_e \rightarrow \infty$$

$$\frac{j_{21}}{j_{31}} = \frac{g_2}{g_3} \frac{A_{21}}{A_{31}} \frac{\nu_{21}}{\nu_{31}} e^{-E^{23}/kT} \approx \frac{g_2}{g_3} \frac{A_{21}}{A_{31}} = \frac{6}{4} \frac{3.6 \times 10^{-5}}{1.8 \times 10^{-4}} = 0.3$$

Note: $\Delta\lambda=0.3 \text{ nm} \rightarrow \text{needs high-resolution spectrograph}$

 $n_e \rightarrow 0$ $\frac{j_{21}}{j_{31}} = \frac{\gamma_{12}}{\gamma_{13}} = \frac{g_1}{g_3} e^{-E_{23}/kT} \approx \frac{g_2}{g_3} = \frac{6}{4} = 1.5$ $\gamma_{21} \approx \gamma_{12} \text{ and } E_{23} << kT$ Statistical weight = 2 J+1, so $g_2 = 2 \ge (5/2) + 1 = 6$ So with this level configuration ([O II] or [S II]), the line ratio is sensitive to the electron number density.



Osterbrock

Some examples of density determinations ...

TABLE 5.6Electron densities in H II regions

Object	$rac{I(\lambda 3729)}{I(\lambda 3726)}$	$N_e(\mathrm{cm}^{-3})$
NGC 1976 A	0.50	3.0×10^{3}
NGC 1976 M	1.26	1.4×10^2
M 8 Hourglass	0.65	1.5×10^{3}
M 8 outer	1.26	1.5×10^2
NGC 281	1.37	7×10
NGC 7000	1.38	6×10

	[O II]		[S II]	
Nebula	$\frac{\lambda 3729}{\lambda 3726}$	N_e a (cm ⁻³)	$rac{\lambda 6716}{\lambda 6731}$ $N_e^{-a} \ ({\rm cm}^{-3})$	
NGC 40	0.78	1.1×10^{3}	$0.69 2.1 \ \times \ 10^3$	
NGC 650/1	1.23	2.1×10^{2}	$1.08 4.0 \ \times \ 10^2$	
NGC 2392	0.78	1.1×10^{3}	$0.88 9.1 \ imes 10^2$	
NGC 2440	0.64	1.9×10^{3}	$0.62 3.2 \ imes 10^3$	
NGC 3242	0.62	2.2×10^{3}	$0.64 2.8 \ imes 10^3$	
NGC 3587	1.30	1.4×10^{2}	$1.25 1.8 \ imes 10^2$	
NGC 6210	0.47	5.8×10^{3}	$0.66 2.5 \ imes 10^3$	
NGC 6543	0.44	7.9×10^{3}	$0.54 5.9 \ imes 10^3$	
NGC 6572	0.38	2.1×10^{4}	$0.51 8.9 \ \times \ 10^{3}$	
NGC 6720	1.04	4.7×10^{2}	$1.14 3.2 \ imes 10^2$	
NGC 6803	0.57	2.8×10^{3}		
NGC 6853	1.16	2.9×10^{2}		
NGC 7009	0.50	4.6×10^{3}	$0.61 3.3 \ imes 10^3$	
NGC 7027	0.48	5.2×10^{3}	$0.59 4.0 \ \times \ 10^3$	
NGC 7293	1.32	1.3×10^2	1.28 1.6 $\times 10^2$	
NGC 7662	0.56	3.0×10^{3}	$0.64 2.8 \ imes 10^3$	
IC 418	0.37	3.2×10^{5}	$0.49 9.5 \ \times \ 10^{3}$	
IC 2149	0.56	3.0×10^{3}	$0.57 4.6 \times 10^3$	
IC 4593	0.63	2.0×10^{3}		
IC 4997	0.34	1.0×10^{6}	$0.45 1.0 \ imes 10^5$	

TABLE 5.7Electron densities in planetary nebulae

^a N_e given for assumed $T = 10^4$ ° K; for any other T divide listed value by $(T/10^4)^{1/2}$.

Osterbrock

Now consider a different level configuration with [O III] or [N II], for which the two **lower** levels are close together.



Osterbrock

Note: Rate of excitation to ¹S and ¹D levels $\leftarrow \rightarrow T$

When $n \rightarrow 0$, i.e., collisional deexcitation is negligible

- Every excitation to ${}^{1}D \rightarrow \lambda 5007$ or $\lambda 4959$ (probability 3:1)
- Every excitation to ${}^{1}S \rightarrow \lambda 4363$ or $\lambda 2321$ $\longrightarrow \lambda 5007$ or $\lambda 4959$

It is left for homework to show that

$$\begin{split} I_{4959} \propto \gamma_{(^{3}P,^{1}D)} \frac{A_{(^{1}D,^{3}P_{1})}}{A_{(^{1}D,^{3}P_{2})} + A_{(^{1}D,^{3}P_{1})}} h\nu_{4959} \\ I_{5007} \propto \gamma_{(^{3}P,^{1}D)} \frac{A_{(^{1}D,^{3}P_{2})}}{A_{(^{1}D,^{3}P_{2})} + A_{(^{1}D,^{3}P_{1})}} h\nu_{5007} \\ I_{4363} \propto \gamma_{(^{3}P,^{1}S)} \frac{A_{(^{1}S,^{1}D)}}{A_{(^{1}S,^{1}D)} + A_{(^{1}S,^{3}P)}} h\nu_{4363} \end{split}$$

$$\frac{\underline{j_{4959} + j_{5007}}}{\underline{j_{4363}}} = \frac{\Omega_{(^{3}P,^{1}D)}}{\Omega_{(^{3}P,^{1}S)}} [\frac{A_{(^{1}S,^{1}D)} + A_{(^{1}S,^{3}P)}}{A_{(^{1}S,^{1}D)}}] \frac{\overline{\nu}_{(^{3}P,^{1}D)}}{\nu_{4363}} \exp(\Delta E/kT)$$

$$\approx \frac{7.73 \exp[(3.29 \times 10^{4})/T]}{1 + 4.5 \times 10^{-4} (N_{e}/T^{1/2})}$$

where

$$\bar{\nu} = \frac{A_{(1D,^{3}P_{2})} \nu_{5007} + A_{(1D,^{3}P_{1})} \nu_{4959}}{A_{(1D,^{3}P_{2})} + A_{(1D,^{3}P_{1})}}$$

and ΔE is the energy difference between ${}^{1}D$ and ${}^{1}S$.

This holds up to $n_e \approx 10^5 \text{ cm}^{-3}$.

At higher densities, collisionalde-excitation begins to play a role.

Similarly, for [N II],

$$\frac{j_{6548} + j_{6583}}{j_{5755}} \approx \frac{6.91 \exp[(2.50 \times 10^4)/T]}{1 + 2.5 \times 10^{-3} (N_e/T^{1/2})}.$$

So with this kind of level configuration ([O III] or [N II]), the line ratio is sensitive to the temperature.



1. I_{4959} and I_{5007} are strong but I_{4363} is weak

2. I_{4363} is close to Hg I λ 4358

Osterbrock

Some examples of temperature determinations ...

TABLE 5.1

Temperature determinations in H II regions

[N II]				[O III]	
Nebula	$\frac{I(\lambda 6548) + I(\lambda 6583)}{I(\lambda 5755)}$	<i>T</i> (° K)	$N_e/T^{1/2}$	$\frac{I(\lambda 4959) + I(\lambda 5007)}{I(\lambda 4363)}$	<i>T</i> (° K)
NGC 1976 2b	81	10.000	51	338	8.700
NGC 1976 1a	102	9,100	68	371	8,500
NGC 1976 5b	111	8,900	21	310	8,900
NGC 1976 5a	189	7,500	12	263	9,300
M 8 I	162	7,900	(10)	445	8,100
M 17 I	257	6,900	(10)	330	8,700
NGC 2467 la	46	13,000	(1)	129	11,600
NGC 2467 1b	53	12,200	(1)	137	11,400
NGC 2359 av			(1)	90	13,200

Typically T~10,000 K

TABLE 5.2Temperature determinationsfor planetary nebulae

Nebula	T[N II] (° K)	T[O III] (° K)	
NGC 650	9,500	10,700	
NGC 4342 NGC 6210	10,100	9,700	
NGC 6543 NGC 6572	9,000	$8,100 \\ 10,300$	
NGC 6720 NGC 6853	$10,600 \\ 10.000$	$11,100 \\ 11.000$	
NGC 7027	 	12,400	
NGC 7293 NGC 7662	10,600	12,800	
IC 418 IC 5217	_	9,700 11,600	
BB 1 Haro 4-1	10,500	$12,900 \\ 12,000$	T~10 000 V
K 648	_	13,100	1 ⁻ 10,000 K

Gum Nebula



41 deg wide