

Astrophysics

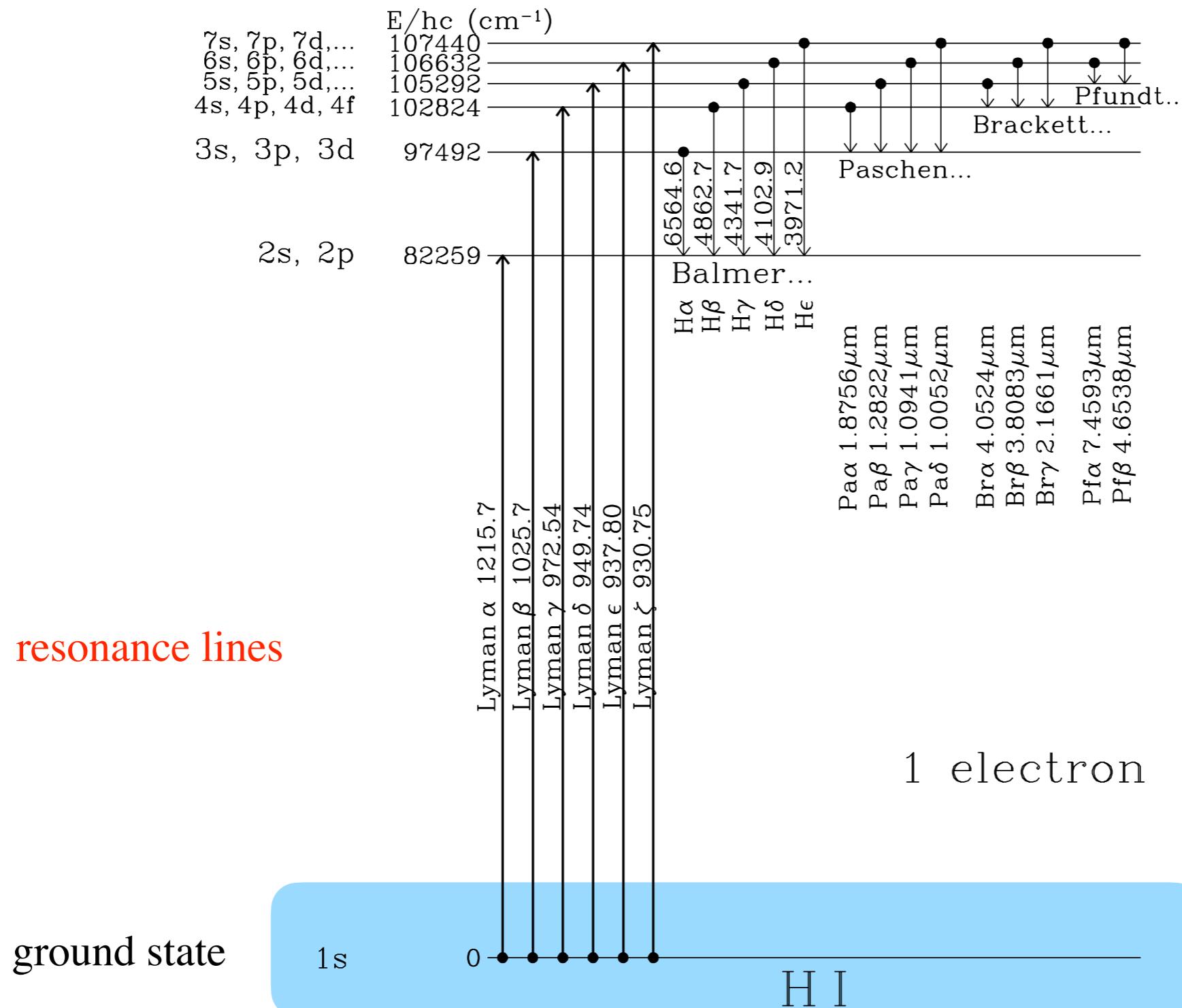
Lecture 14

December 07 (Wed.), 2022

updated 12/03 22:02

선광일 (Kwang-Il Seon)
UST / KASI

Hydrogen Atom Energy Levels

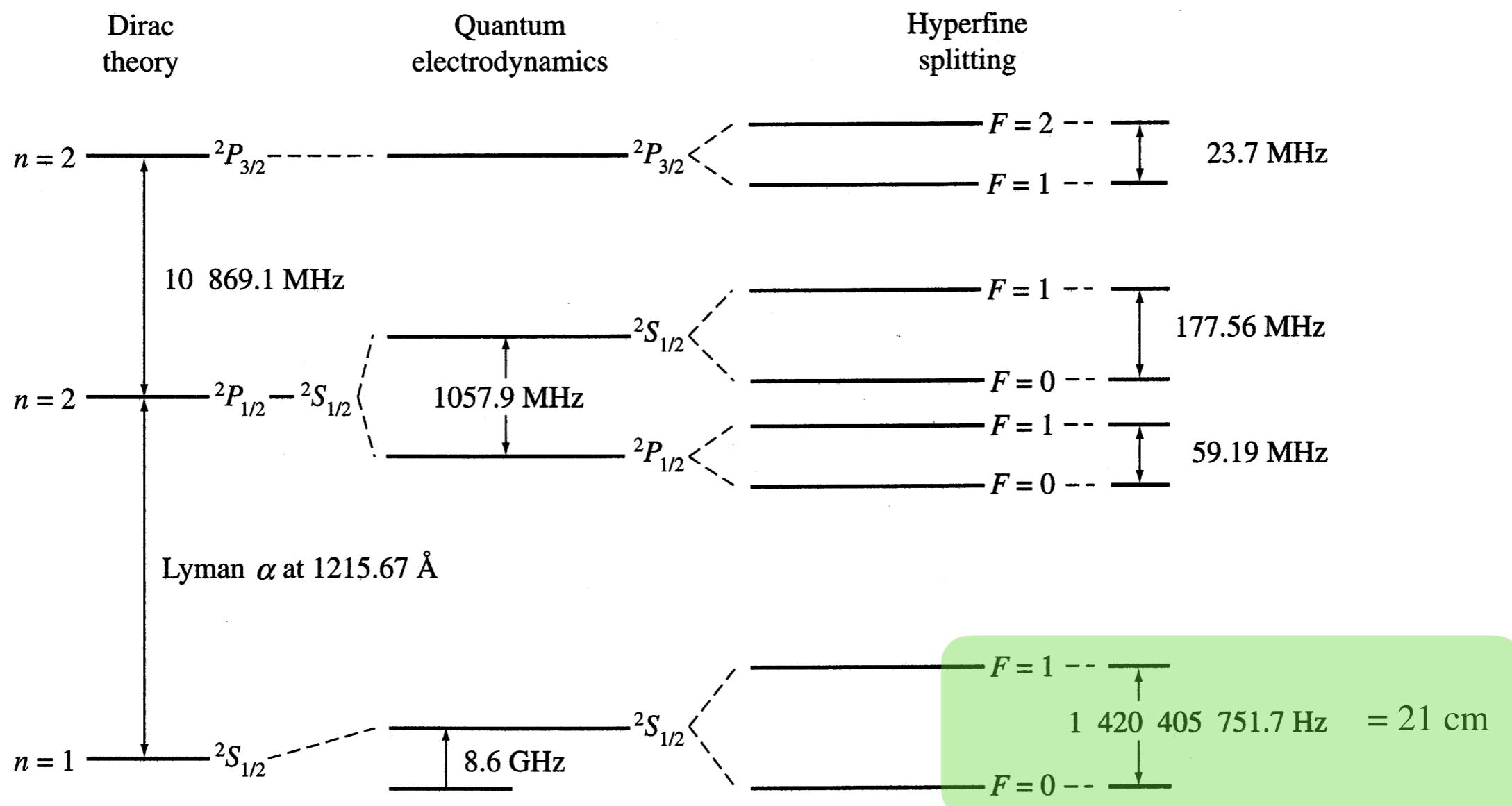


Hydrogen Atom : Hyperfine Structure

- Hyperfine Structure in the H atom

Coupling the nuclear spin I to the total electron angular momentum J gives the final angular momentum F . For hydrogen this means

$$F = J + I = J \pm \frac{1}{2}$$



Hydrogen Atom : Allowed Transitions

- Selection Rules

- Transitions are governed by selection rules which determine whether they can occur.

Δn any  selection rule for configuration

$\Delta l = \pm 1$

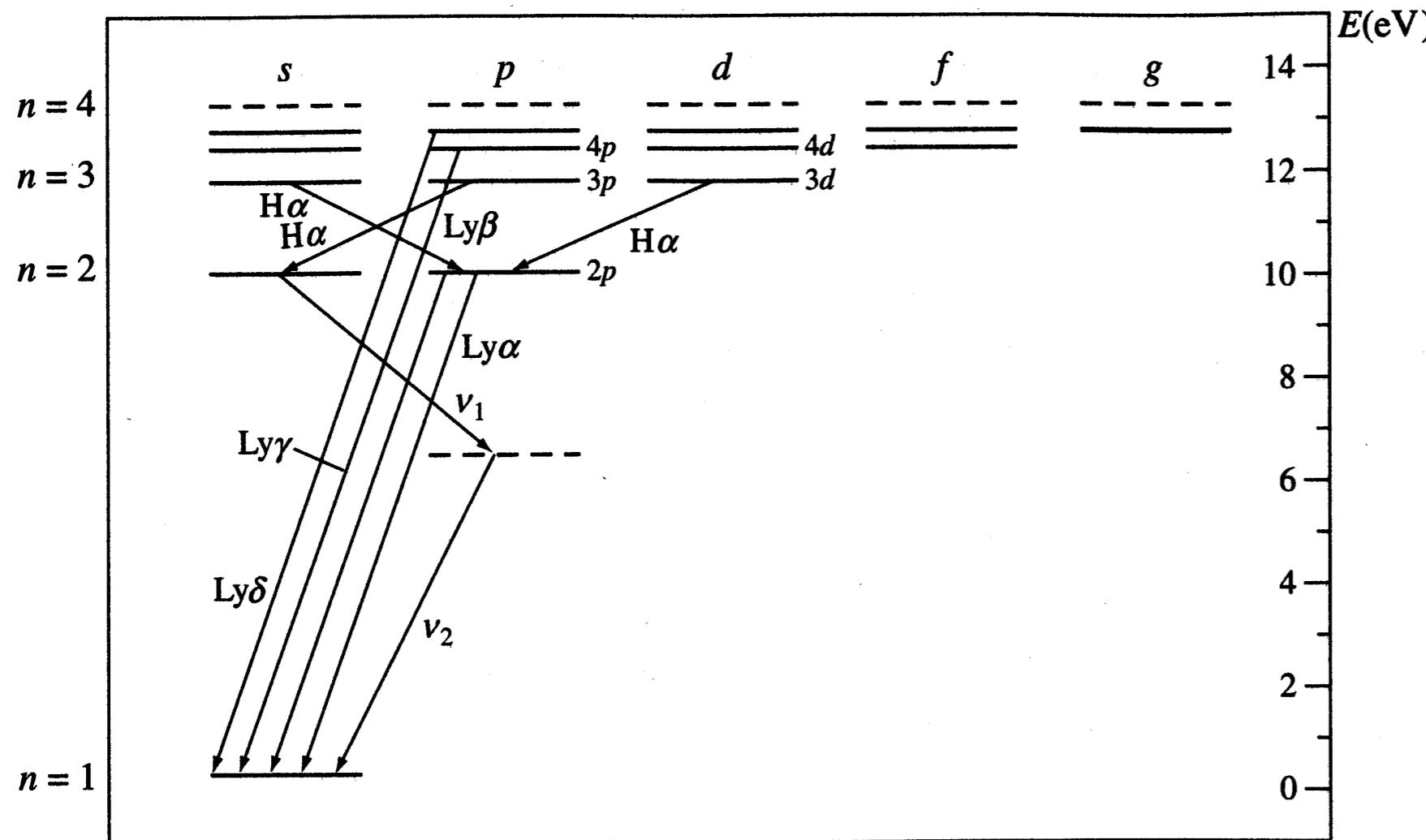
$\Delta S = 0$  For H atom, this is always satisfied as $S = 1/2$ for all states.

$\Delta L = 0, \pm 1$ (not $L = 0 - 0$)

$\Delta J = 0, \pm 1$ (not $J = 0 - 0$)

For H-atom, l and L are equivalent since there is only one electron.

For $H\alpha$ transitions:



Not all $H\alpha$ transitions which correspond to $n = 2 - 3$ are allowed.

$2s_{\frac{1}{2}} - 3p_{\frac{1}{2}}$ is allowed;

$- 3p_{\frac{3}{2}}$ is allowed;

$2p_{\frac{1}{2}} - 3d_{\frac{5}{2}}$ is not allowed; ($\Delta J = 2$)

$- 3s_{\frac{1}{2}}$ is allowed;

$- 3d_{\frac{3}{2}}$ is allowed;

$2p_{\frac{3}{2}} - 3s_{\frac{1}{2}}$ is allowed;

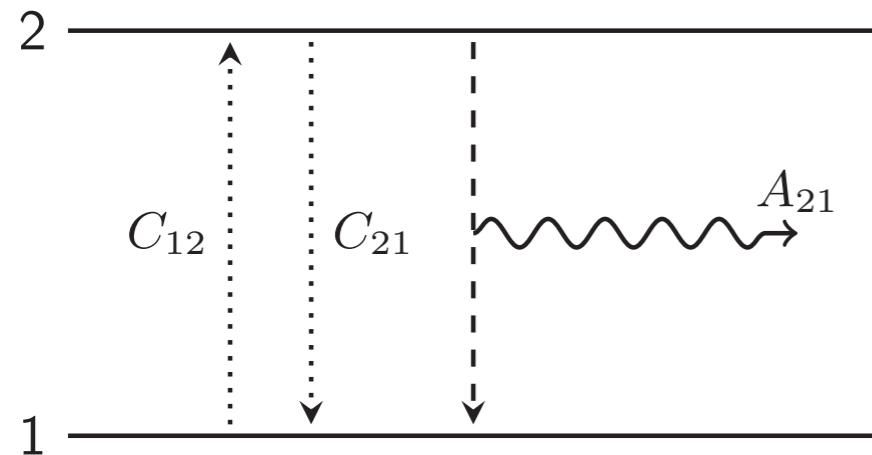
$- 3d_{\frac{3}{2}}$ is allowed;

$- 3d_{\frac{5}{2}}$ is allowed .

The transition between $2s - 1s$ is not allowed ($\Delta l = 0$).

[Atomic Emission Line Mechanisms in ISM]

- **Collisional Line**



Collisions with electrons can excite ions (or atoms), moving it from level 1 to 2, or de-excite it, moving it from level 2 to 1, with rate C_{21} and C_{12} , respectively.

An excited ion can also spontaneously emit radiation at the Einstein A_{21} .

In low density ISM, collisions are rare, so when the occasional collisional excitation happens, the ion(atom) is much more likely to return to level 1 through the emission of a photon than through collisional de-excitation.

- **Recombination Line**

Hot stars produce ultraviolet radiation that can ionize hydrogen and other atoms. Once ionized, recombination back to the neutral state produces recombination continuum and lines. Of course, the recombination requires that the ion encounter an electron, which is a slow process in diffuse gas.

The recombination of a free electron with a proton can occur to any of the energy levels n . For instant, if $n > 1$, the excited hydrogen atom will then decay to lower levels until it reaches the ground state, $n = 1$. This cascade produces a set of photons, the first with an energy corresponding to the potential of the previously unbound electron-proton pair and then the others at fixed values corresponding to the discrete energy jumps between different n .

In most cases, the Lyman alpha and Balmer lines are recombination lines.

[Collisional Excitation]

- Under the conditions of very low density and weak radiation fields,
 - **The vast majority of the atoms reside in the ground state.**
collisional excitation timescale \gg radiative decay time scale
This condition will remain true even if the excited state has a radiative lifetime of several second, which is frequently the case for the forbidden transitions observed in ionized astrophysical plasmas.
 - Flux of an emission line \propto number of collisions \propto product of the number densities of the two colliding species by the probability that a collision will produce a collisional excitation.
 - If the energy gap between the ground state and the excited state E_{12} is much larger than the mean energy of the colliding species ($\sim T$), then, because there are few very energetic collisions, relatively few collisional excitations can occur. Therefore, the resulting emission line will be very much weaker than when $E_{12} < kT$.
This gives us the possibility of measuring temperature from the relative strengths of lines coming from excited levels at different energies above the ground state.

- At high enough densities,
 - The collisional timescales are short.
 - The population in any upper level is set by the balance between collisional excitation, and the collisional de-excitation out of these levels, and are governed by the Boltzmann equilibrium.

Boltzmann equilibrium:
$$\frac{n_2}{n_1} = \frac{g_2}{g_1} \exp\left(-\frac{E_{12}}{k_B T}\right)$$

- At intermediate densities,
 - The collisional rates and the radiative decay rates are compatible.
 - The intensity of an emission line is determined by both the temperature and the density.
 - If the temperature is known, the density can be determined from the intensity ratio of two such lines.

Collisional Excitation & De-excitation

- **Collisional Rate (Two Level Atom)**

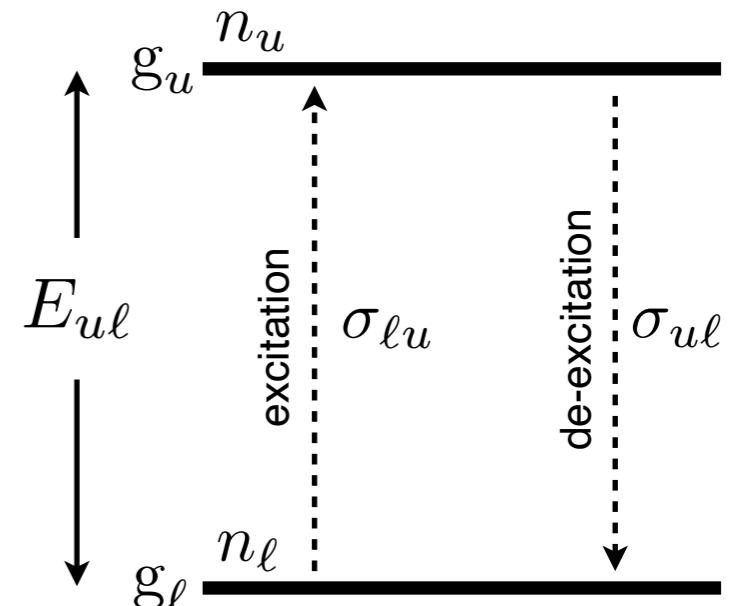
- The cross section $\sigma_{\ell u}$ for collisional excitation from a lower level ℓ to an upper level u is, in general, inversely proportional to the impact energy (or v^2) above the energy threshold $E_{u\ell}$ and is zero below.
- The collisional cross section can be expressed in the following form using a dimensionless quantity called the ***collision strength*** $\Omega_{\ell u}$:

$$\begin{aligned}\sigma_{\ell u}(v) &= (\pi a_0^2) \left(\frac{hR_H}{\frac{1}{2}m_e v^2} \right) \frac{\Omega_{\ell u}}{g_\ell} \text{ cm}^2 \quad \text{for } \frac{1}{2}m_e v^2 > E_{u\ell} \\ &= \frac{h^2}{4\pi m_e^2 v^2} \frac{\Omega_{\ell u}}{g_\ell}\end{aligned}$$

or $\sigma_{\ell u}(E) = \frac{h^2}{8\pi m_e E} \frac{\Omega_{\ell u}}{g_\ell} \quad \left(E = \frac{1}{2}m_e v^2 \right)$

where, $a_0 = \frac{\hbar^2}{m_e e^2} = 5.12 \times 10^{13}$ cm, Bohr radius

$$R_H = \frac{m_e e^4}{4\pi \hbar^3} = 109,737 \text{ cm}^{-1}, \text{ Rydberg constant} \quad \left(\hbar = \frac{h}{2\pi} \right)$$



- The collision strength $\Omega_{\ell u}$ is a function of electron velocity (or energy) but is often approximately constant near the threshold. Here, g_ℓ and g_u are the statistical weights of the lower and upper levels, respectively.

-
- Advantage of using the collision strength is that (1) it removes the primary energy dependence for most atomic transitions and (2) they have the symmetry between the upper and the lower states.

The principle of detailed balance states that ***in thermodynamic equilibrium each microscopic process is balanced by its inverse. Hence, The collisional excitation and de-excitation are balanced in TE.***

$$n_e n_\ell v_\ell \sigma_{\ell u}(v_\ell) f(v_\ell) dv_\ell = n_e n_u v_u \sigma_{u\ell}(v_u) f(v_u) dv_u$$

Here, v_ℓ and v_u are electron velocities before and after the collision, related by $\frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell}$, and $f(v)$ is a Maxwell velocity distribution of electrons. Using the Boltzmann equation of thermodynamic equilibrium,

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

and the Maxwell distribution function in 3D velocity space

$$f(\mathbf{v}) d^3\mathbf{v} = \left(\frac{m_e}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m_e v^2}{2kT}\right) d^3\mathbf{v}$$

or the distribution function of speed

$$f(v) dv = \left(\frac{m_e}{2\pi kT}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{m_e v^2}{2kT}\right) dv$$

we can derive the relation between the cross-sections for excitation and de-excitation

$$\frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell} \quad \rightarrow \quad v_\ell dv_\ell = v_u dv_u$$

$$n_e n_\ell v_\ell \sigma_{\ell u}(v_\ell) f(v_\ell) dv_\ell = n_e n_u v_u \sigma_{u\ell}(v_u) f(v_u) dv_u$$

$$\rightarrow \sigma_{\ell u}(v_\ell) v_\ell^2 \exp\left(-\frac{m_e v_\ell^2/2}{kT}\right) = \sigma_{u\ell}(v_u) v_u^2 \exp\left(-\frac{m_e v_u^2/2}{kT}\right) \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

Relation between the cross-section for excitation and de-excitation

$$g_\ell v_\ell^2 \sigma_{\ell u}(v_\ell) = g_u v_u^2 \sigma_{u\ell}(v_u) \quad \rightarrow \quad g_\ell \cdot (E + E_{u\ell}) \cdot \sigma_{\ell u}(E + E_{u\ell}) = g_u \cdot E \cdot \sigma_{u\ell}(E)$$

where $E = \frac{1}{2}m_e v_u^2$

We also obtain the symmetry of the collision strength between levels are

$$\begin{aligned} \sigma_{\ell u}(v_\ell) &= \frac{h^2}{4\pi m_e^2 v_\ell^2} \frac{\Omega_{\ell u}}{g_\ell} \\ \sigma_{u\ell}(v_u) &= \frac{h^2}{4\pi m_e^2 v_u^2} \frac{\Omega_{u\ell}}{g_u} \end{aligned} \quad \rightarrow \quad \Omega_{\ell u} = \Omega_{u\ell} \quad \text{more precisely } \Omega_{\ell u}(E + E_{u\ell}) = \Omega_{u\ell}(E)$$

These two relations were derived in the TE condition. However, ***the cross-sections are independent on the assumptions, and thus the above relations should be always satisfied.***

- Collisional excitation and de-excitation rates

The ***collisional de-excitation rate per unit volume per unit time, which is thermally averaged,*** is given by

$$\begin{aligned} \left(\frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} &= n_e n_u \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ &= n_e n_u k_{u\ell} \quad [\text{cm}^{-3} \text{ s}^{-1}] \end{aligned}$$

$$k_{u\ell} \equiv \langle \sigma v \rangle_{u \rightarrow \ell}$$

The collisional de-excitation rate can be written as follows:

$$\begin{aligned} k_{u\ell} &= \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ &= \left(\frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \\ &= \frac{\beta}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \quad [\text{cm}^3 \text{ s}^{-1}], \end{aligned}$$

$$\beta \equiv \left(\frac{2\pi\hbar^4}{k m_e^2} \right)^{1/2} = 8.62942 \times 10^{-6}$$

Here, $k_{u\ell}$ is the **collisional rate coefficient for de-excitation** in units of $\text{cm}^3 \text{ s}^{-1}$.

Here, the effective collision strength, averaged over the energy, is given by

$$\text{effective collision strength: } \langle \Omega_{u\ell} \rangle \equiv \int_0^\infty \Omega_{u\ell}(E) e^{-E/k_B T} d(E/k_B T)$$

Its typical values are
 $10^{-2} < \langle \Omega_{u\ell} \rangle < 10$

Similarly, the ***collisional excitation rate per unit volume per unit time, which is thermally averaged,*** is

$$\begin{aligned} \left(\frac{dn_u}{dt} \right)_{\ell \rightarrow u} &= n_e n_\ell \int_{v_{\min}}^{\infty} v \sigma_{\ell u}(v) f(v) dv \\ &= n_e n_\ell k_{\ell u} \quad [\text{cm}^{-3} \text{ s}^{-1}] \end{aligned}$$

Here, $\frac{1}{2} m_e v_{\min}^2 = E_{u\ell}$

$$k_{\ell u} \equiv \langle \sigma v \rangle_{\ell \rightarrow u}$$

Here, $k_{\ell u}$ is the **collisional rate coefficient for excitation** in units of $\text{cm}^3 \text{ s}^{-1}$.

$$\begin{aligned} k_{\ell u} &= \int_{v_{\min}}^{\infty} v \sigma_{\ell u}(v) f(v) dv \\ &= \left(\frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right) \\ &= \frac{\beta}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right) \quad [\text{cm}^3 \text{ s}^{-1}], \end{aligned}$$

$$\beta \equiv \left(\frac{2\pi\hbar^4}{km_e^2} \right)^{1/2} = 8.62942 \times 10^{-6}$$

We note that ***the rate coefficients for collisional excitation and de-excitation are related by***

$$k_{\ell u} = \frac{g_u}{g_\ell} k_{u\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

$$\langle \sigma v \rangle_{\ell \rightarrow u} = \frac{g_u}{g_\ell} \langle \sigma v \rangle_{u \rightarrow \ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

Collisionally-Excited Emission Line

- Emission line flux
 - In the low density limit, the collisional rate between atoms and electrons is much slower than the (spontaneous) radiative de-excitation rate of the excited level. Thus, we can balance the collisional feeding into level u by the rate of radiative transition back down to level ℓ . The level population is determined by

$$n_e n_\ell k_{\ell u} = A_{u\ell} n_u$$

$$\frac{n_u}{n_\ell} = \frac{n_e k_{\ell u}}{A_{u\ell}}$$

$$= \frac{n_e}{A_{u\ell}} \beta \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} T^{-1/2} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

where $A_{u\ell}$ is the Einstein coefficient for spontaneous emission. Then, the line emissivity is given by

$$4\pi j_{u\ell} = E_{u\ell} A_{u\ell} n_u = E_{u\ell} n_e n_\ell k_{\ell u}$$

$$= n_e n_\ell E_{u\ell} \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right) \text{ [erg cm}^{-3} \text{ s}^{-1}\text{]}$$

$$4\pi j_{u\ell} \simeq \beta \chi n_e^2 E_{u\ell} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

proportional to density-square

Here, $\beta = \left(\frac{2\pi\hbar^4}{km_e^2}\right)^{1/2} = 8.62942 \times 10^{-6}$

$$\chi = n_\ell / n_e$$

For low temperature, the exponential term dominates because few electrons have energy above the threshold for collisional excitation, so that the line rapidly fades with decreasing temperature.

At high temperature, the $T^{-1/2}$ term controls the cooling rate, so the line fades slowly with increasing temperature.

- In the high-density limit, the level population are set by the Boltzmann equilibrium, and the line emissivity is

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

$$4\pi j_{u\ell} = E_{\ell u} A_{u\ell} n_u$$

$$= n_\ell E_{\ell u} A_{u\ell} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right)$$

$$4\pi j_{u\ell} \simeq \chi n_e E_{\ell u} A_{u\ell} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right)$$

proportional to density

Here, the line flux scales as n_e rather than n_e^2 , but the line flux tends to a constant value at high temperature.

- Critical density is defined as the density where the radiative depopulation rate matches the collisional de-excitation for the excited state.

$$A_{u\ell} n_u = n_e n_u k_{u\ell}$$

$$n_{\text{crit}} = \frac{A_{u\ell}}{k_{u\ell}}$$

$$\rightarrow n_{\text{crit}} = A_{u\ell} \frac{g_u}{\beta \langle \Omega_{u\ell} \rangle} T^{1/2}$$

$$= 1.2 \times 10^3 \frac{A_{u\ell}}{10^{-4} \text{ s}^{-1}} \frac{g_u}{\langle \Omega_{u\ell} \rangle} \left(\frac{T}{10^4 \text{ K}} \right)^{1/2} [\text{cm}^{-3}]$$

- At densities higher than the critical density, collisional de-excitation becomes significant, and the forbidden lines will be weaker as the density increases.
- At around the critical density, the “line emissivity vs density” plotted in log-log scale changes slope from +2 to +1.

- As can be seen in Tables and the formula, **collisional de-excitation is negligible for resonance and most forbidden lines in the ISM.**

Ion	ℓ	u	E_ℓ/k	E_u/k	$\lambda_{u\ell}$	$n_{H,\text{crit}}(u)$
			(K)	(K)	(μm)	$T = 100 \text{ K}$ (cm^{-3})
C II	$^2\text{P}_{1/2}^o$	$^2\text{P}_{3/2}^o$	0	91.21	157.74	2.0×10^3
CI	$^3\text{P}_0$	$^3\text{P}_1$	0	23.60	609.7	620
	$^3\text{P}_1$	$^3\text{P}_2$	23.60	62.44	370.37	720
O I	$^3\text{P}_2$	$^3\text{P}_1$	0	227.71	63.185	2.5×10^5
	$^3\text{P}_1$	$^3\text{P}_0$	227.71	326.57	145.53	8.4×10^3
Si II	$^2\text{P}_{1/2}^o$	$^2\text{P}_{3/2}^o$	0	413.28	34.814	1.0×10^5
Si I	$^3\text{P}_0$	$^3\text{P}_1$	0	110.95	129.68	4.8×10^4
	$^3\text{P}_1$	$^3\text{P}_2$	110.95	321.07	68.473	9.9×10^4
						1.5×10^3

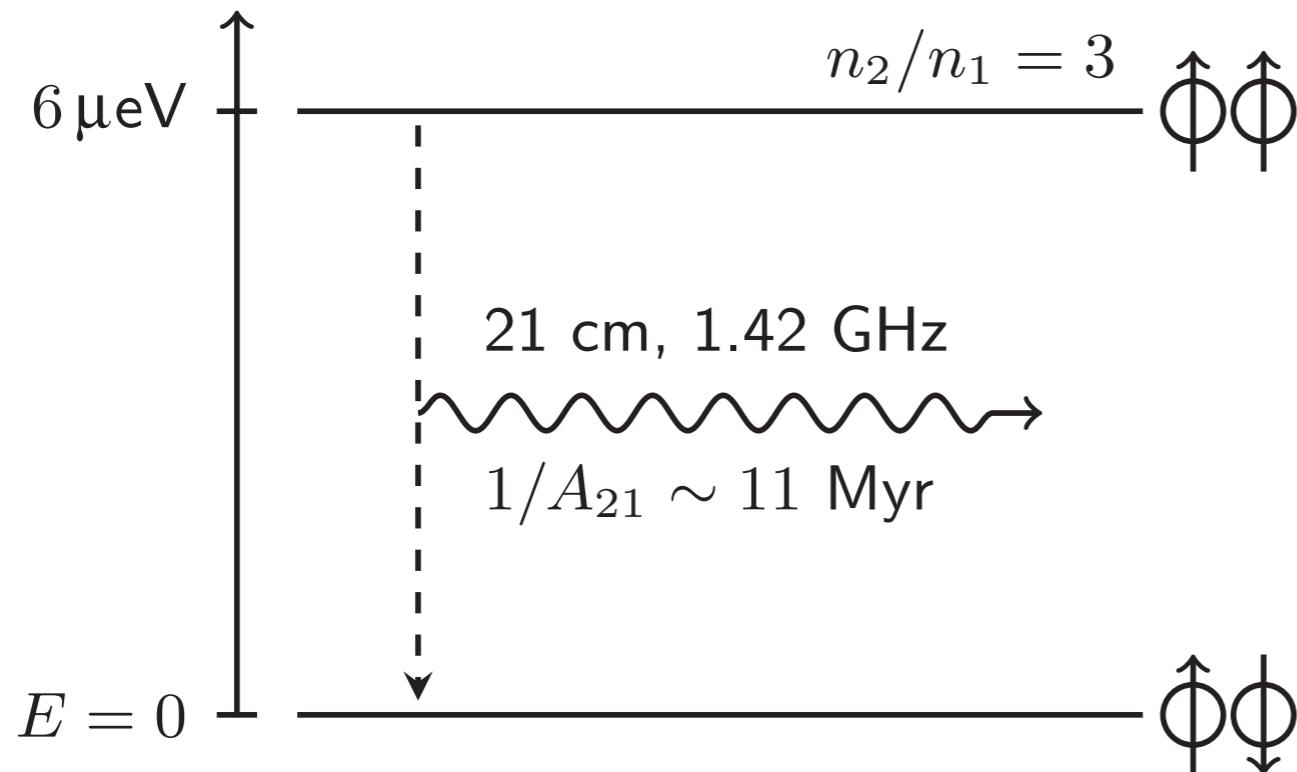
Table 17.1 in [Draine]

- However, it is not true for the 21 cm hyperfine structure line of hydrogen.
 - The critical density for 21cm line is

$$n_{\text{crit}} \sim 10^{-3} (T/100 \text{ K})^{-1/2} [\text{cm}^{-3}]$$
 - $A_{u\ell} = 2.88 \times 10^{-15} [\text{s}^{-1}]$
 - The levels are thus essentially in collisional equilibrium in the cold neutral medium.

Ion	Transition l-u	λ μm	A_{ul} s^{-1}	Ω_{ul}	n_{crit} cm^{-3}
C I	$^3\text{P}_0 - ^3\text{P}_1$	609.1354	7.93×10^{-8}	–	(500)
	$^3\text{P}_1 - ^3\text{P}_2$	370.4151	2.65×10^{-7}	–	(3000)
C II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	157.741	2.4×10^{-6}	1.80	47 (3000)
N II	$^3\text{P}_0 - ^3\text{P}_1$	205.3	2.07×10^{-6}	0.41	41
	$^3\text{P}_1 - ^3\text{P}_2$	121.889	7.46×10^{-6}	1.38	256
	$^3\text{P}_2 - ^1\text{D}_2$	0.65834	2.73×10^{-3}	2.99	7700
	$^3\text{P}_1 - ^1\text{D}_2$	0.65481	9.20×10^{-4}	2.99	7700
N III	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	57.317	4.8×10^{-5}	1.2	1880
O I	$^3\text{P}_2 - ^3\text{P}_1$	63.184	8.95×10^{-5}	–	$2.3 \times 10^4 (5 \times 10^5)$
	$^3\text{P}_1 - ^3\text{P}_0$	145.525	1.7×10^{-5}	–	$3400 (1 \times 10^5)$
	$^3\text{P}_2 - ^1\text{D}_2$	0.63003	6.3×10^{-3}	–	1.8×10^6
O II	$^4\text{S}_{3/2} - ^2\text{D}_{5/2}$	0.37288	3.6×10^{-5}	0.88	1160
	$^4\text{S}_{3/2} - ^2\text{D}_{3/2}$	0.37260	1.8×10^{-4}	0.59	3890
O III	$^3\text{P}_0 - ^3\text{P}_1$	88.356	2.62×10^{-5}	0.39	461
	$^3\text{P}_1 - ^3\text{P}_2$	51.815	9.76×10^{-5}	0.95	3250
	$^3\text{P}_2 - ^1\text{D}_2$	0.50069	1.81×10^{-2}	2.50	6.4×10^5
	$^3\text{P}_1 - ^1\text{D}_2$	0.49589	6.21×10^{-3}	2.50	6.4×10^5
	$^1\text{D}_2 - ^1\text{S}_0$	0.43632	1.70	0.40	2.4×10^7
Ne II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	12.8136	8.6×10^{-3}	0.37	5.9×10^5
Ne III	$^3\text{P}_2 - ^3\text{P}_1$	15.5551	3.1×10^{-2}	0.60	1.27×10^5
	$^3\text{P}_1 - ^3\text{P}_0$	36.0135	5.2×10^{-3}	0.21	1.82×10^4
Si II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	34.8152	2.17×10^{-4}	7.7	(3.4×10^5)
S II	$^4\text{S}_{3/2} - ^2\text{D}_{5/2}$	0.67164	2.60×10^{-4}	4.7	1240
	$^4\text{S}_{3/2} - ^2\text{D}_{3/2}$	0.67308	8.82×10^{-4}	3.1	3270
S III	$^3\text{P}_0 - ^3\text{P}_1$	33.4810	4.72×10^{-4}	4.0	1780
	$^3\text{P}_1 - ^3\text{P}_2$	18.7130	2.07×10^{-3}	7.9	1.4×10^4
S IV	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	10.5105	7.1×10^{-3}	8.5	5.0×10^4
Ar II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	6.9853	5.3×10^{-2}	2.9	1.72×10^6
Ar III	$^3\text{P}_2 - ^3\text{P}_1$	8.9914	3.08×10^{-2}	3.1	2.75×10^5
	$^3\text{P}_1 - ^3\text{P}_0$	21.8293	5.17×10^{-3}	1.3	3.0×10^4
Fe II	$^6\text{D}_{7/2} - ^6\text{D}_{5/2}$	35.3491	1.57×10^{-3}	–	(3.3×10^6)
	$^6\text{D}_{9/2} - ^6\text{D}_{7/2}$	25.9882	2.13×10^{-3}	–	(2.2×10^6)

H I 21 cm



Schematic of the hyperfine transition of the ground electronic state of hydrogen, due to the spin flip from parallel to anti-parallel alignment of the proton-electron pair.

An atom will typically remain in the excited state for about 11 Myr before decaying. This is much greater than the collisional time between atoms in an H I gas. Thus **the two hyperfine states are in collisional equilibrium** and the level populations are in a Boltzmann distribution with excitation temperature equal to the kinetic temperature of the gas, $T_{\text{ex}} = T_{\text{gas}}$

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-E_{21}/kT} \simeq 3$$

Here, $g_1 = 1$ and $g_2 = 3$.

$E_{21}/k = 0.07$ K is much smaller than ISM temperatures (and the temperature of the cosmic background radiation ($T_{\text{CMB}} \simeq 3$ K)).

Therefore, the exponential term is near unity.

[Line diagnostics]

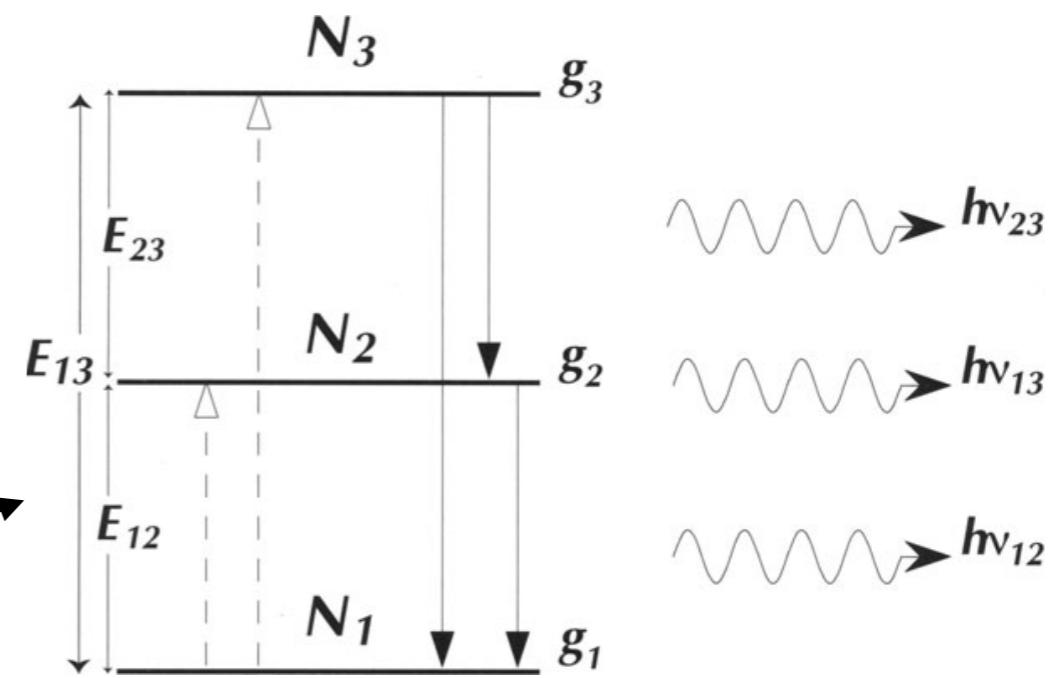
- **The Three-Level Atom (Line diagnostics)**

- Let C_{ij} be the collision rate ($C_{ij} = n_e q_{ij} \text{ s}^{-1}$) between any two levels. The equations of statistical equilibrium for a three level atom are

$$N_1 C_{13} + N_2 C_{23} = N_3 (C_{31} + C_{32} + A_{32} + A_{31})$$

$$N_1 C_{12} + N_3 (C_{32} + A_{32}) = N_2 (C_{23} + C_{21} + A_{21})$$

$$N_1 + N_2 + N_3 = 1$$



- **Electron temperature**

- ◆ Ions in which $E_{12} \sim E_{23}$
- ◆ In the low density limit, collisional de-excitation of the excited levels can be ignored. Therefore,

$$C_{31} \sim C_{32} \sim 0.$$

Also, because of the increasing threshold energies to excite each level, $N_3 \ll N_2 \ll N_1$ so that the equations are reduced to

$$N_3 = \frac{N_1 C_{13}}{(A_{32} + A_{31})}$$

$$N_2 = \frac{N_1 C_{12}}{A_{21}}$$

If we now form the line intensity ratio for the $3 \rightarrow 2$ and $2 \rightarrow 1$ transitions, we have

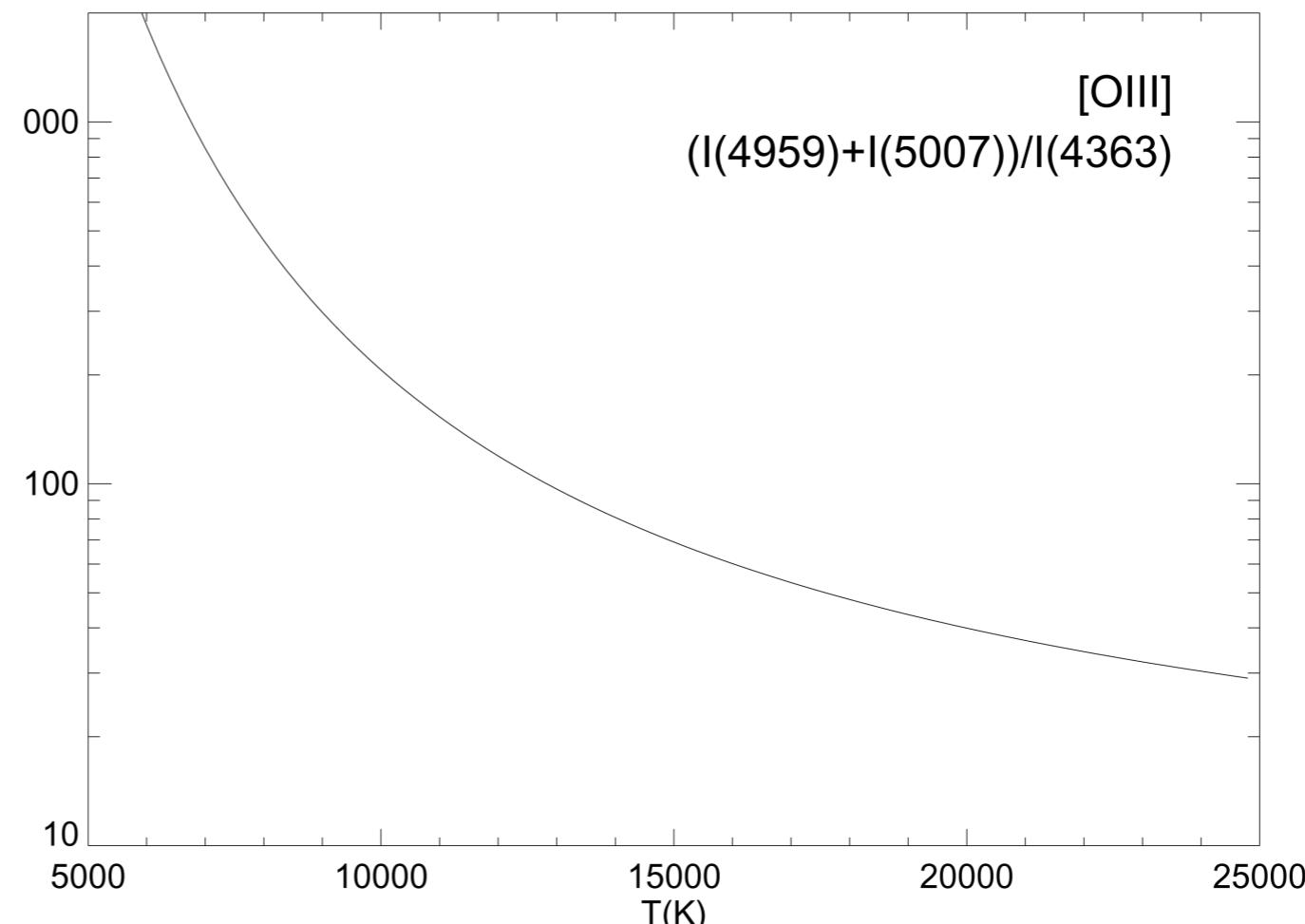
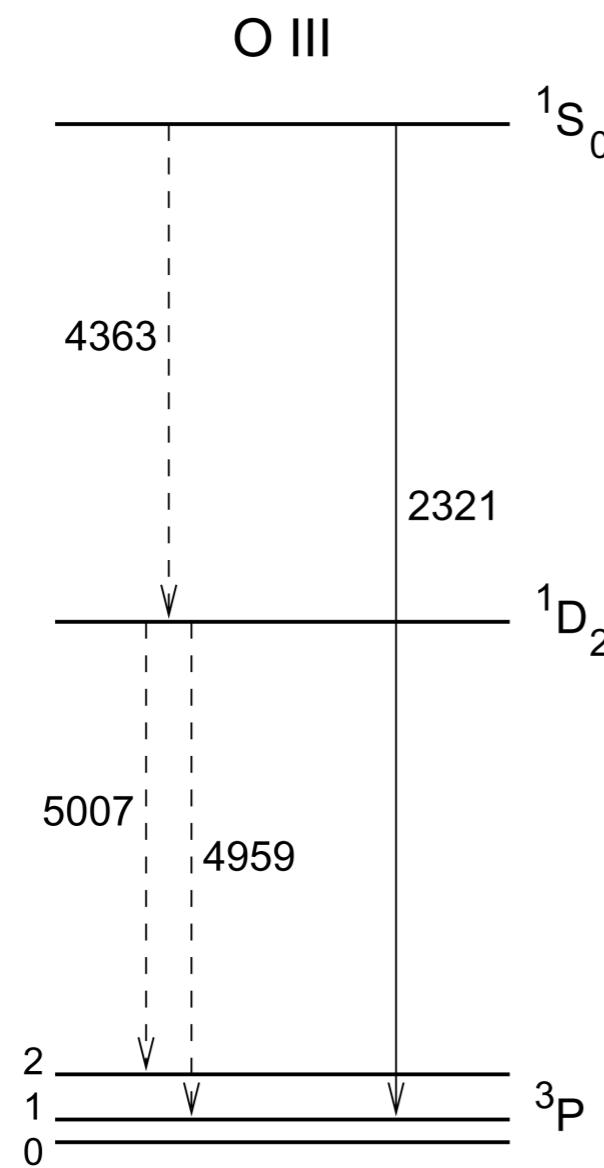
$$\begin{aligned}\frac{F_{32}}{F_{21}} &= \frac{E_{23}N_3A_{32}}{E_{12}N_2A_{21}} \\ &= \frac{E_{23}A_{32}C_{13}}{E_{12}(A_{32} + A_{31})C_{12}} \\ &= \frac{E_{23}A_{32}q_{13}}{E_{12}A_{31}q_{12}} \\ &= \frac{E_{23}A_{32}\Omega_{13}}{E_{12}A_{31}\Omega_{12}} \exp\left(-\frac{E_{23}}{kT}\right)\end{aligned}$$

provided that A_{32} is very much less than A_{31} .

Because this line ratio depends on the temperature, it can be used to measure the electron temperature in the plasma.

Temperature

Use two levels with different excitation energy.



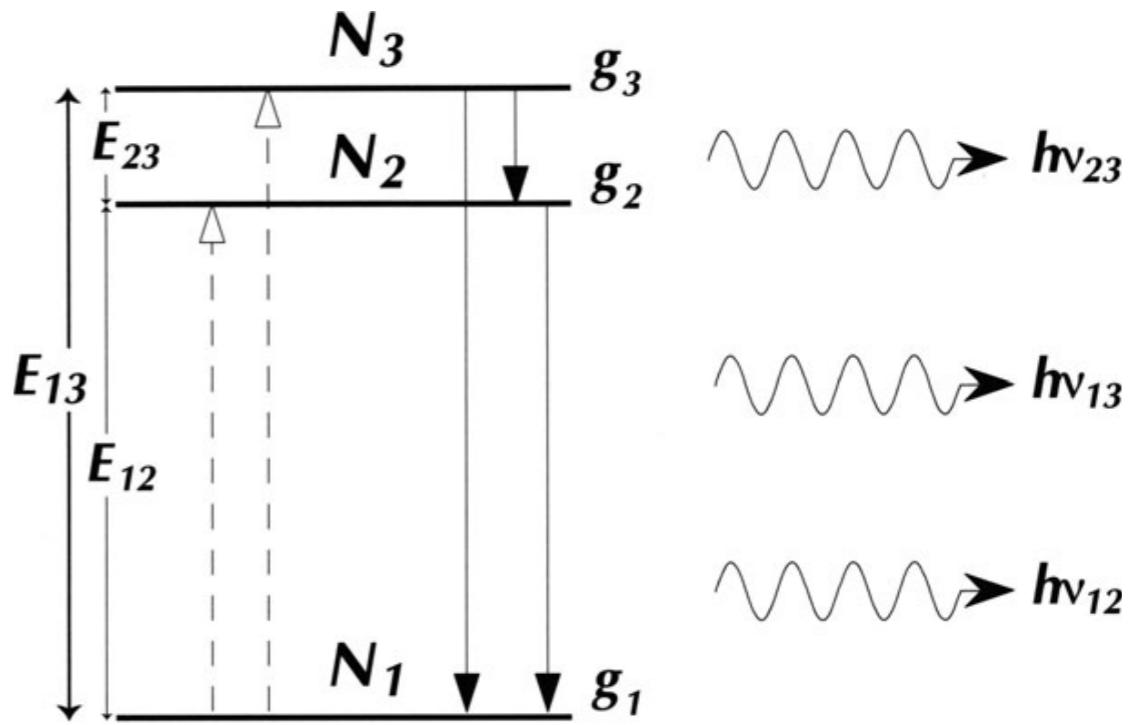
$$\frac{I(4959 + 5007)}{4363} = \frac{7.7 \exp(3.29 \times 10^4 / T)}{1 + 4.5 \times 10^{-4} n_e T^{-1/2}}$$

- **Electron density**

- ♦ Ions in which $E_{23} \ll E_{12}$
- ♦ In low density limit,
we can neglect collisional induced transitions
between the higher levels.

$$N_1 C_{13} = N_3 A_{31}$$

$$N_1 C_{12} = N_2 A_{21}$$



$$\frac{F_{31}}{F_{21}} = \frac{E_{31}A_{31}N_3}{E_{21}A_{21}N_2} = \frac{E_{31}C_{13}}{E_{21}C_{12}} \sim \frac{\Omega_{31}}{\Omega_{21}} \exp\left(-\frac{E_{21}}{kT}\right) \sim \frac{\Omega_{31}}{\Omega_{21}} = \frac{g_3}{g_2}$$

using the quantum-mechanical sum rule for collision strengths.

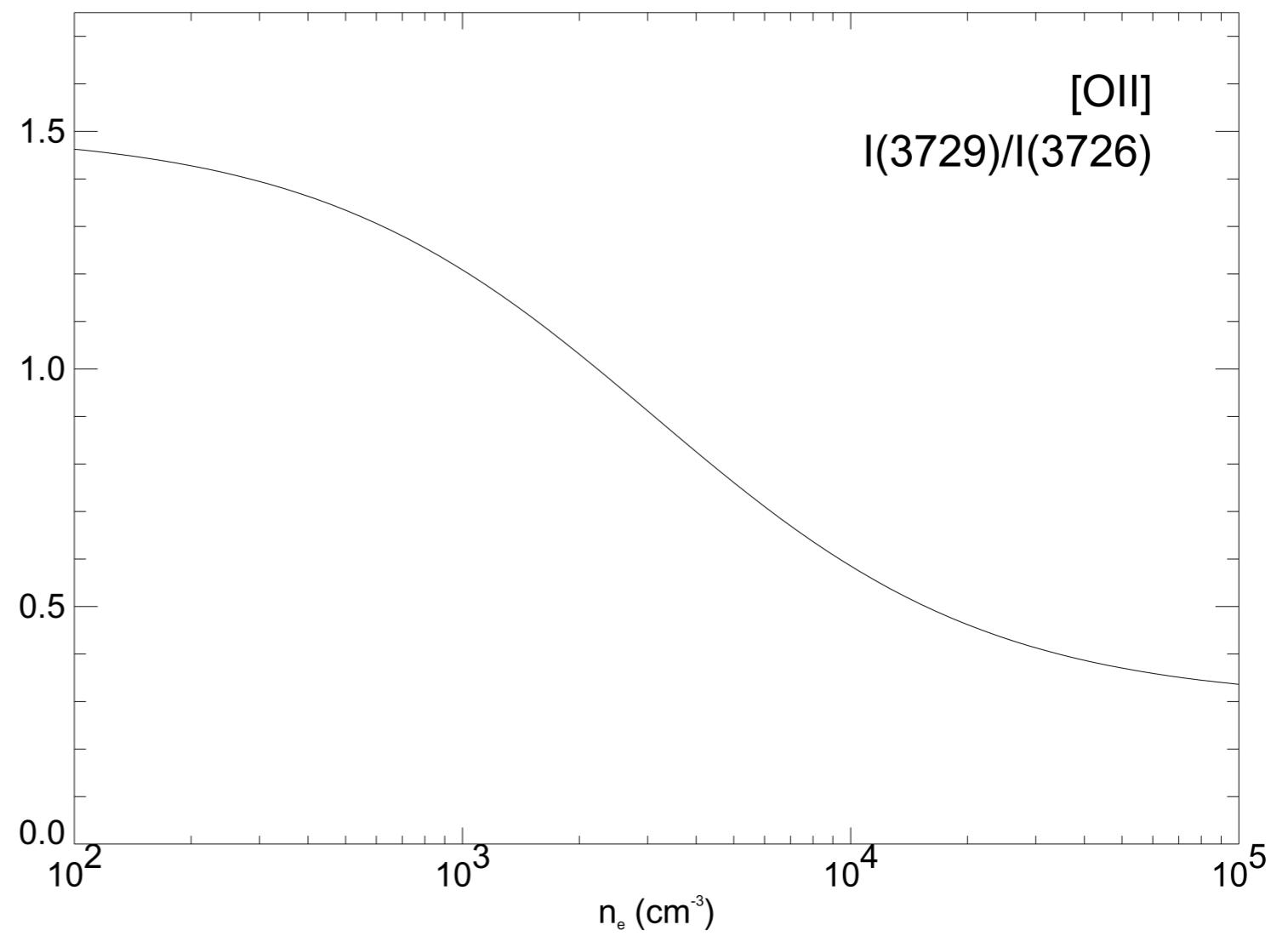
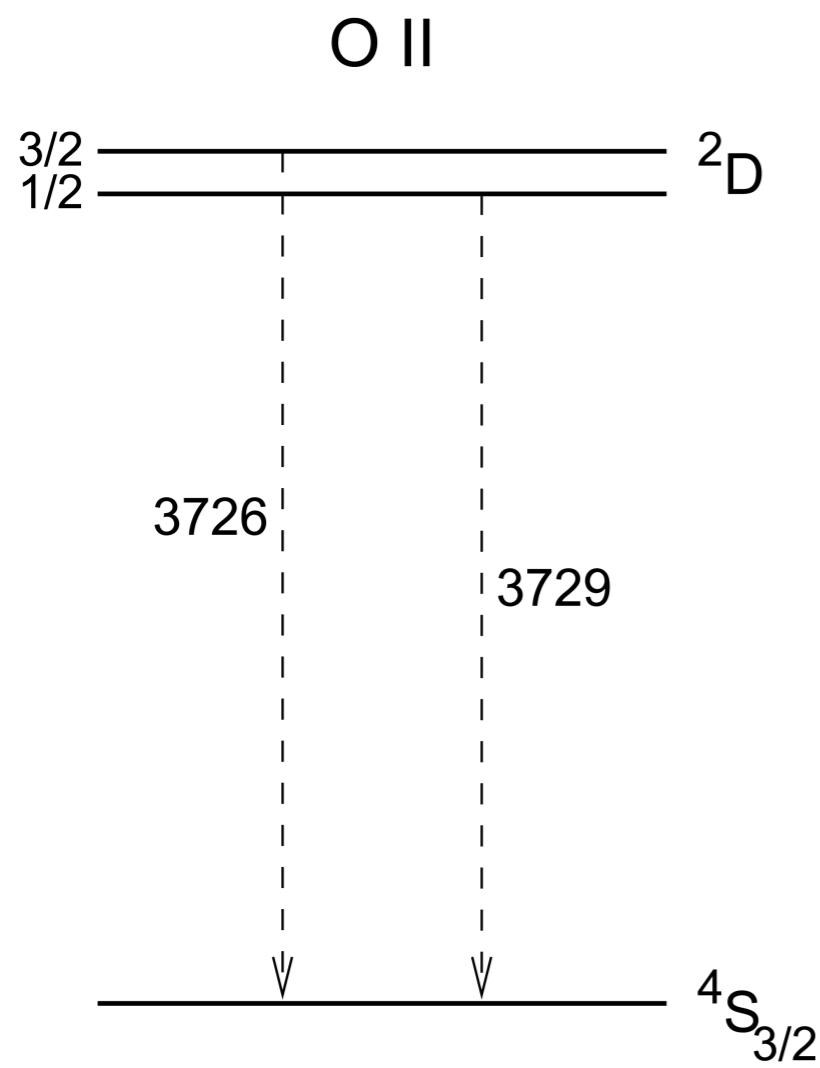
- ♦ In high density limit, the upper levels are populated according to their Boltzmann ratios,

$$\frac{F_{31}}{F_{21}} = \frac{E_{31}A_{31}N_3}{E_{21}A_{21}N_2} \sim \frac{A_{31}g_3}{A_{21}g_2}$$

- ♦ Therefore, the line ratio can be used as density diagnostics in the regime between the critical densities for de-excitation of each of the transitions.

Density

Choose atom with two levels with almost same excitation energy.



[Einstein Coefficients and Oscillator Strengths]

- Recall resonance scattering cross-section and the Einstein relations:

$$\sigma_{lu}(\nu) = \frac{\pi e^2}{mc} \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \quad g_l B_{lu} = g_u B_{ul} \quad A_{ul} = \frac{2h\nu_{lu}^3}{c^2} B_{ul}$$

where $\nu_{lu} \equiv \frac{E_u - E_l}{h} (\nu_0)$

- The Einstein (absorption) B coefficient associated with a classical oscillator can be defined in terms of the total energy extracted from a beam of radiation.

$$\int_0^\infty \sigma_{lu}(\nu) d\nu = \frac{\pi e^2}{mc} \equiv B_{lu}^{\text{classical}} \frac{h\nu_{lu}}{4\pi} \quad \rightarrow \quad B_{lu}^{\text{classical}} = \frac{4\pi}{h\nu_{lu}} \frac{\pi e^2}{mc}$$

It is convenient to define the **absorption and emission oscillator strengths** (f_{lu} and f_{ul}) by the formulae:

$$B_{lu} = B_{lu}^{\text{classical}} f_{lu} = \frac{4\pi^2 e^2}{h\nu_{lu} mc} f_{lu} \quad B_{ul} = \frac{4\pi^2 e^2}{h\nu_{ul}} f_{ul} \quad (\text{note that } \nu_{ul} = -\nu_{lu} < 0 \text{ and } f_{ul} < 0)$$

The oscillator strength (or f value) is the factor which corrects the classical result. The quantum mechanical process can be interpreted as being due to a (fractional) number f of equivalent classical electron oscillators of the same frequency.

-
- In quantum mechanics, the absorption oscillator strength is given by

$$f_{lu} = \frac{2m}{3\hbar^2 g_l e^2} (E_u - E_l) \sum |d_{lu}|^2 \quad d_{lu} \equiv \langle \phi_u | e\mathbf{r} | \phi_l \rangle$$

where the sum is over all substates of the upper and lower levels.

We also have the following relations.

$$\begin{aligned} g_l f_{lu} &= -g_u f_{ul} \\ g_u A_{ul} \equiv -\frac{8\pi^2 e^2 \nu_{ul}^2}{mc^3} g_u f_{ul} &= \frac{8\pi^2 e^2 \nu_{lu}^2}{mc^3} g_l f_{lu} \\ \sigma(\nu) &= \frac{\pi e^2}{mc} f_{lu} \\ &= \frac{\pi e^2}{mc} f_{lu} \phi(\nu) \end{aligned}$$

- *Thomas-Reiche-Kuhn sum rule*

$$\sum_{n'} f_{nn'} = N = \text{ total number of electrons in the atom}$$

Here, the summation is over all states of the atom. Where there is a close shell and a smaller number q of electrons outside the closed shells that are involved in a more limited set of transitions, we also have

$$\sum_{n'} f_{nn'} = q$$

where the sum is now only over those states involve transitions of these outer electrons.

We note that $f \sim 1$ for strong allowed transitions.

[Line Broadening Mechanisms]

- Atomic levels are not infinitely sharp, nor are the lines connecting them.
 - (1) Doppler Broadening
 - (2) Natural Broadening
 - (3) Collisional Broadening
- **Doppler Broadening**

The simplest mechanism for line broadening is the Doppler effect. An atom is in thermal motion, so that the frequency of emission or absorption in its own rest frame corresponds to a different frequency for an observer.

Each atom has its own Doppler shift, so that the net effect is to spread the line out, but not to change its total strength.

The change in frequency associated with an atom with velocity component v_z along the line of sight (say, z axis) is, to lowest order in v/c , given by

$$\nu - \nu_0 = \nu_0 \frac{v_z}{c}$$

Doppler shift: $\left[\frac{\nu}{\nu_0} = \frac{1}{\gamma(1 - \beta \cos \theta)} \rightarrow \nu \approx \nu_0 (1 + \beta \cos \theta) \rightarrow \nu - \nu_0 = \frac{\nu_0 v_z}{c} \right]$

Here, ν_0 is the rest-frame frequency.

The number of atoms having velocities in the range $(v_z, v_z + dv)$ is proportional to

$$f(v_z)dv_z = \exp\left(-\frac{mv_z^2}{2kT}\right)dv_z$$

From the Doppler shift formula, we have

$$v_z = \frac{c(\nu - \nu_0)}{\nu_0} \rightarrow dv_z = \frac{cd\nu}{\nu_0}$$

Therefore, the strength of the emission is proportional to

$$\exp\left(-\frac{mv_z^2}{2kT}\right)dv_z \propto \exp\left[-\frac{mc^2(\nu - \nu_0)^2}{2\nu_0^2 kT}\right]d\nu$$

Then, the normalized profile function is

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-(\nu - \nu_0)^2 / (\Delta\nu_D)^2} \quad \text{where } \Delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}}$$

The line-center cross section for each atom, neglecting stimulated emission, is therefore

$$\begin{aligned}\sigma_{\nu_0} &= B_{12} \frac{h\nu}{4\pi} \phi(\nu_0) = \frac{1}{\Delta\nu_D \sqrt{\pi}} \frac{h\nu_0}{4\pi} B_{12} \\ &= \frac{\pi e^2}{mc} f_{12} \frac{1}{\Delta\nu_D \sqrt{\pi}}\end{aligned}$$

In addition to thermal motions, there can be turbulent velocities associated with macroscopic velocity fields. **When the scale of the turbulence is small in comparison with a mean free path (microturbulence)**, the turbulent motions are accounted for by an effective Doppler width.

$$\Delta\nu_D = \frac{\nu_0}{c} \left(\frac{2kT}{m} + v_{\text{turb}}^2 \right)^{1/2}$$

where v_{turb} is a root-mean-square measure of the turbulent velocities. This assumes that the turbulent velocities also have a Gaussian distribution.

- **Natural Broadening**

A certain width to the atomic level is implied by the uncertainty principle, namely, that the spread in energy ΔE and the duration Δt in the state must satisfy $\Delta E \Delta t \sim \hbar$.

The spontaneous decay of an atomic state n proceeds at a rate

$$\gamma = \sum_{n'} A_{nn'}$$

where the sum is over all states n' of lower energy. The coefficient of the wave function of state n is of the form $e^{-\gamma t/2}$ and then the energy decays proportional to $e^{-\gamma t}$. We then have an emitted spectrum determined by the decaying sinusoid type of electric field. The spectral profile is of the form, which is called a Lorentz (or natural, or Cauchy) profile,

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$

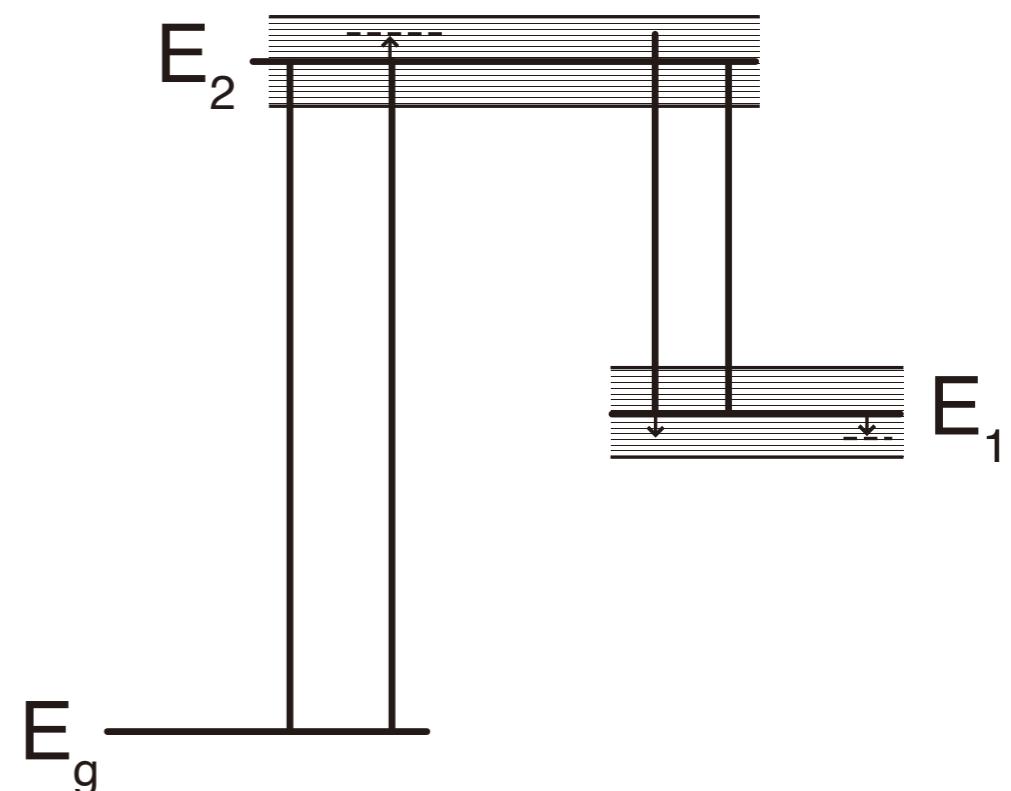
The above profile applies to cases in which only the upper state is broadened.

Semiclassical (Weissokpf-Woolley) Picture of Quantum Levels

- In the semiclassical picture, each level is viewed as a continuous distribution of sublevels with energies close to the energy of the level (E_n).
 - The distribution of sublevels are explained by the Heisenberg Uncertainty Principle. The level has a lifetime $\Delta t = 1/A$ (A = Einstein A coefficient) and a spread in energy about $\Delta E \approx \hbar/\Delta t = \hbar A$.

$$\Delta E \Delta t \approx \hbar$$

- The ground level has no spread in energy because $\Delta t = \infty$.
- The atom is in a definite sublevel of some level.



- A transition in a spectral line is considered to be an instantaneous transition between a definite sublevel of an initial level to a definite sublevel of a final level.
- ***The energy spread of sublevels is described by a Lorentzian profile.***

If both the upper and lower state are broadened, then the appropriate definition for γ is

$$\gamma = \gamma_u + \gamma_l$$

Note that $\gamma_l = 0$ for the ground state.

where γ_u and γ_l are the widths of the upper and lower states involved in the transition.

The longer an excited state exists, the narrower the line width so that metastable states can have very narrow lines (if the thermal Doppler broadening is not important).

- The semiclassical picture postulates that in the process of photon scattering, an atom stays in a given sublevel unless there are elastic collisions that cause a transitions to a different sublevel. Thus if there are no elastic collisions, the next transition starts from the same sublevel where the previous transition ended.

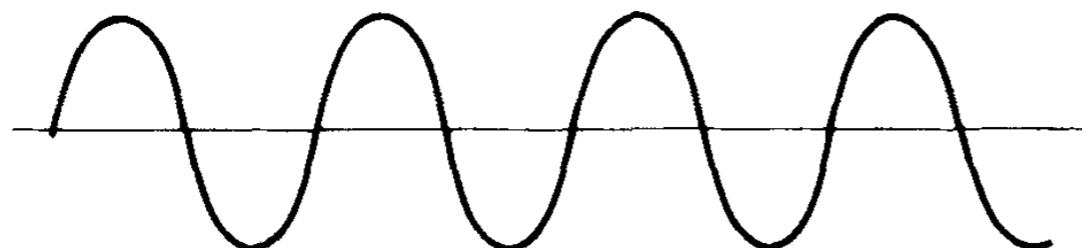
- **Collisional Broadening (by elastic collision)**

The Lorentz profile applies even to certain types of collisional broadening mechanisms.

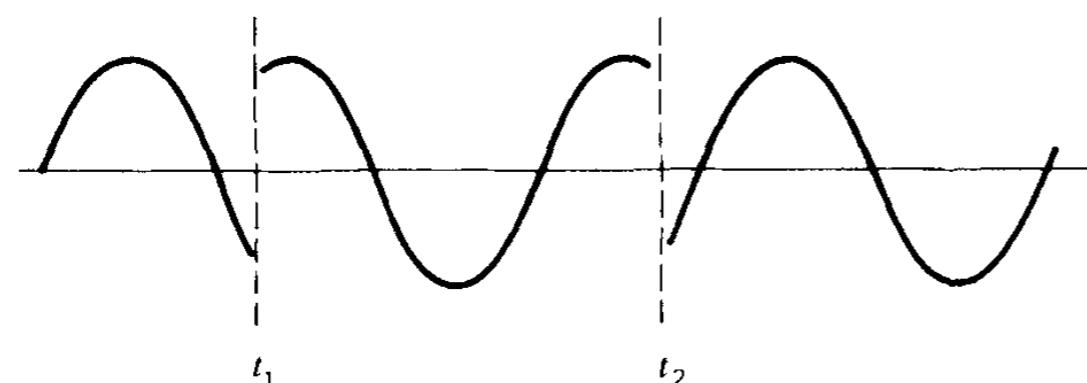
If the atom suffers collisions with other particles while it is emitting, the phase of the emitted radiation can be altered suddenly. If the phase changes completely randomly at the collision times, then information about the emitting frequencies is lost.

If the collisions occur with frequency ν_{col} , that is, each atom experiences ν_{col} collisions per unit time on the average, then the profile is

$$\phi(\nu) = \frac{\Gamma/4\pi^2}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \quad \text{where} \quad \Gamma = \gamma + 2\nu_{\text{col}}$$



purely sinusoidal



random phase interruptions
by atomic collisions

For derivation of the above formula, see Problem 10.7 of Rybiki & Lightman and Chapter 11 of Atomic Spectroscopy and Radiative Processes [Degl'Innocenti].

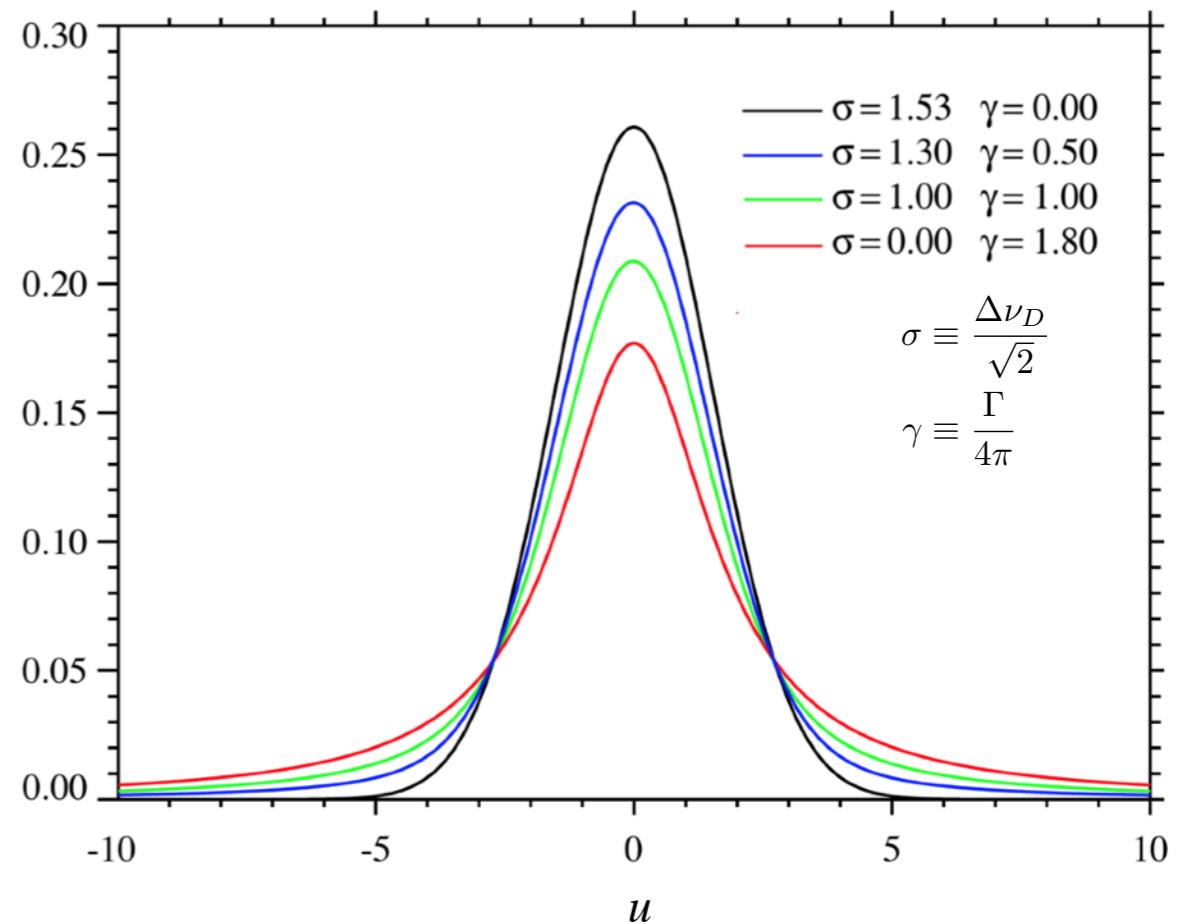
- **Combined Doppler and Lorentz Profiles**

Atoms shows both a Lorentz profile plus the Doppler effect. In this case, we can write the profile as an average of the Lorentz profile over the various velocity states of the atom:

$$\phi(\nu) = \frac{\Gamma}{4\pi^2} \int_{-\infty}^{\infty} \frac{(m/2\pi kT)^{1/2} \exp(-mv_z^2/2kT)}{(\nu - \nu_0(1 + v_z/c))^2 + (\Gamma/4\pi)^2} dv_z$$

The profile can be written using the Voigt function.

$$\begin{aligned}\phi(\nu) &= \frac{1}{\Delta\nu_D \sqrt{\pi}} H(a, u) \\ H(a, u) &\equiv \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{a^2 + (u - y)^2} \\ a &\equiv \frac{\Gamma}{4\pi \Delta\nu_D} \\ u &\equiv \frac{\nu - \nu_0}{\Delta\nu_D} \\ \nu_D &= \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}}\end{aligned}$$



For small a , the center of the line is dominated by the Doppler profile, whereas the “wings” are dominated by the Lorentz profile.