# Modern Astronomy

## Part 1. Interstellar Medium (ISM)

Week 2

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# Brief Introduction to Atomic Spectroscopy

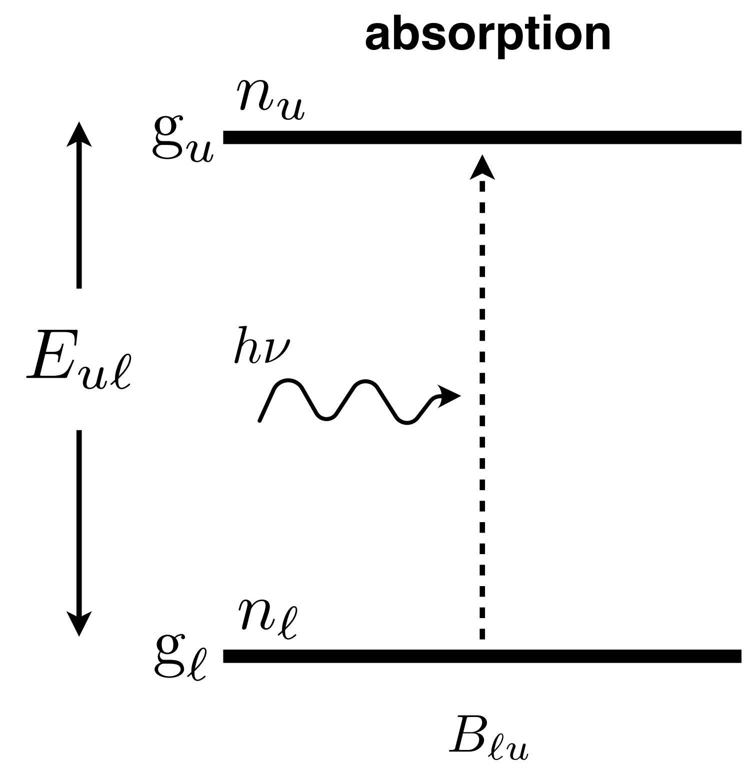
# Atomic Processes

- In order for an atom in the ISM to radiate, it has to be first excited to a higher state.
- **Excitation and de-excitation (Transition)**
  - Radiative excitation (photoexcitation; photoabsorption)
  - Radiative de-excitation (spontaneous emission and stimulated emission)
  - Collisional excitation
  - Collisional de-excitation
- **Emission Line**
  - Collisionally-excited emission lines
  - Recombination lines (recombination following photoionization or collisional ionization)
- **Ionization**
  - Photoionization and Auger-ionization
  - Collisional Ionization (Direct ionization and Excitation-autoionization)
- **Recombination**
  - Radiative recombination <=> Photoionization
  - Dielectronic Recombination (not dielectric!)
  - Three-body recombination <=> Direct collisional ionization
- **Charge exchange**

# Radiative Excitation and De-excitation (Absorption and Emission)

- **Three Radiative Transitions and Einstein Coefficients**
  - *Absorption*:
    - If an absorber (atom, ion, molecule, or dust grain) X is in a lower level $\ell$ and there is radiation present with photons having an energy equal to $E_{u\ell}$ . The absorber can absorb a photon and undergo an upward transition.

$$\text{absorption}: \quad X_\ell + h\nu \;\rightarrow\; X_u \;(h\nu = E_{u\ell})$$




    - The rate per volume at which the absorbers absorb photons will be proportional to both the energy density $u_\nu$ of photons of the appropriate energy and the number density $n_\ell$ of absorbers in the lower level $\ell$.

$$\left(\frac{dn_u}{dt}\right)_{\ell\rightarrow u} = -\left(\frac{dn_\ell}{dt}\right)_{\ell\rightarrow u} = n_\ell B_{\ell u} u_\nu$$

    - The proportionality constant $B_{\ell u}$ is the ***Einstein B coefficient*** for the upward transition $\ell \rightarrow u$.

energy density & mean intensity

$$u_\nu = \frac{4\pi}{c} J_\nu$$

$$J_\nu = \frac{1}{4\pi}\int I_\nu d\Omega$$

- ***Emission***:
  - An absorber X in an excited level $u$ can decay to a lower level $\ell$ with emission of a photon. There are two ways this can happen:

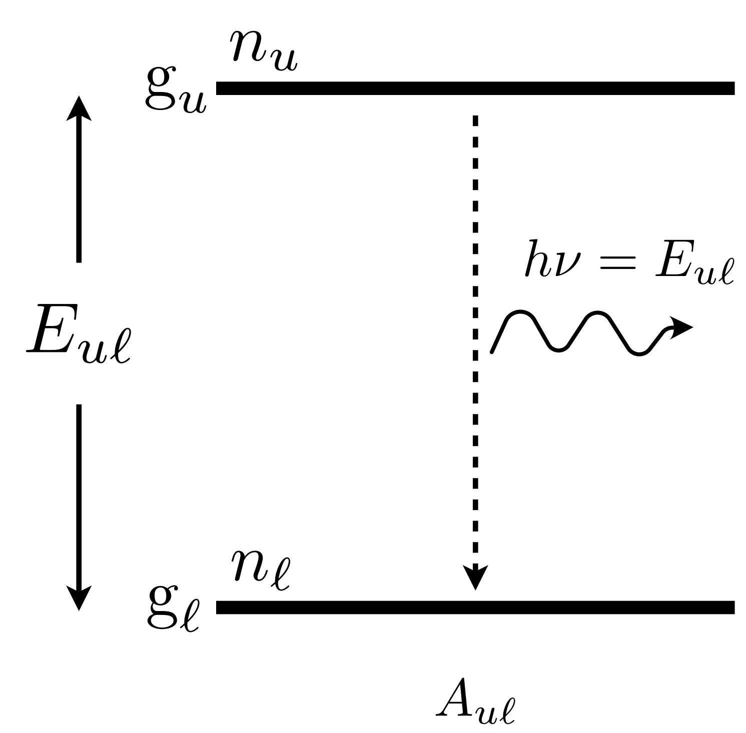
$$\text{spontaneous emission}: \quad X_u \;\rightarrow\; X_\ell + h\nu \quad (h\nu = E_{u\ell})$$
$$\text{stimulated emission}: \quad X_u + h\nu \;\rightarrow\; X_\ell + 2h\nu \quad (h\nu = E_{u\ell})$$

  - ***Spontaneous emission*** is a random process, independent of the presence of a radiation field.
  - ***Stimulated emission*** occurs if photons of the identical frequency, polarization, and direction of propagation are already present, and the rate of stimulated emission is proportional to the energy density $u_\nu$ of these photons.

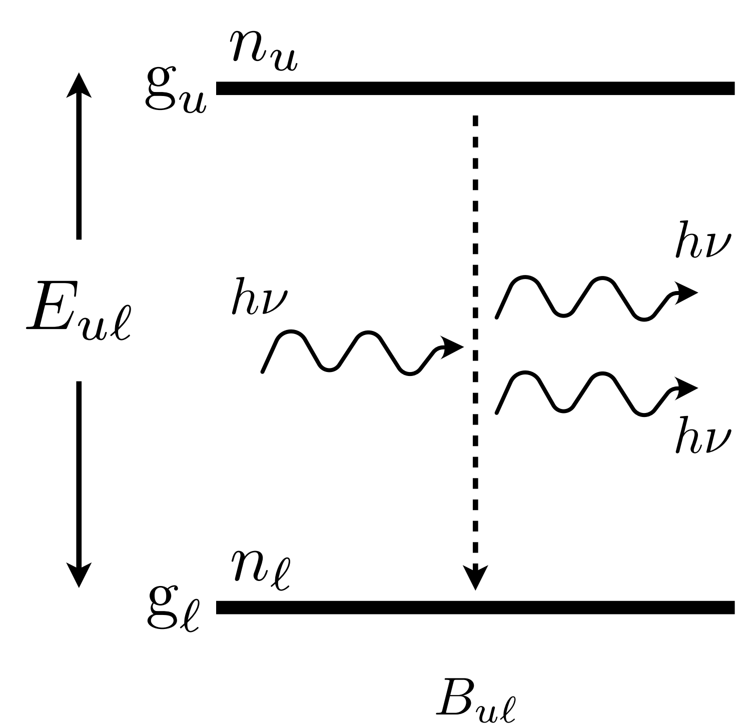
$$\left(\frac{dn_\ell}{dt}\right)_{u\rightarrow\ell} = -\left(\frac{dn_u}{dt}\right)_{u\rightarrow\ell} = n_u\left(A_{u\ell} + B_{u\ell}u_\nu\right)$$

  - The probability per unit time $A_{u\ell}$ is the ***Einstein A coefficient*** for spontaneous transition. The coefficient $B_{u\ell}$ is the ***Einstein B coefficient*** for the downward transition $u \rightarrow \ell$.

**spontaneous emission**




**stimulated emission**



# Relations between the Einstein coefficients

- The three Einstein coefficients are not mutually independent.
- ***In thermal equilibrium***, the radiation field becomes the “blackbody” radiation field and the two levels must be populated according to the Boltzmann distribution.

$$(u_\nu)_{\rm TE} = \frac{4\pi}{c} B_\nu(T) = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/k_{\rm B}T} - 1}$$

$$\left(\frac{n_u}{n_\ell}\right)_{\rm TE} = \frac{g_u}{g_\ell} e^{-E_{u\ell}/k_{\rm B}T} \quad \text{Here, } E_{u\ell} = h\nu.$$

- The net rate of change of level $u$ should be equal to zero, in TE.

$$\begin{aligned}\frac{dn_u}{dt} &= \left(\frac{dn_u}{dt}\right)_{\ell\to u} + \left(\frac{dn_u}{dt}\right)_{u\to\ell} \\ &= n_\ell B_{\ell u} u_\nu - n_u \left(A_{u\ell} + B_{u\ell} u_\nu\right) \\ &= 0\end{aligned}$$

$$n_\ell B_{\ell u} u_\nu - n_u \left(A_{u\ell} + B_{u\ell} u_\nu\right) = 0$$

$$\left(n_\ell B_{\ell u} - n_u B_{u\ell}\right) u_\nu = n_u A_{u\ell}$$

$$\begin{aligned} u_\nu &= \frac{n_u A_{u\ell}}{n_\ell B_{\ell u} - n_u B_{u\ell}} \\ &= \frac{\left(n_u A_{u\ell}\right) / \left(n_\ell B_{\ell u}\right)}{1 - \left(n_u B_{u\ell}\right) / \left(n_\ell B_{\ell u}\right)} \\ &= \frac{\left(\mathrm{g}_u/\mathrm{g}_\ell\right) e^{-h\nu/kT} \left(A_{u\ell}/B_{\ell u}\right)}{1 - \left(\mathrm{g}_u/\mathrm{g}_\ell\right) e^{-h\nu/kT} \left(B_{u\ell}/B_{\ell u}\right)} \quad \leftarrow \quad \frac{n_u}{n_\ell} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} e^{-h\nu_{u\ell}/kT_{\mathrm{exc}}} \\ &= \frac{\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(A_{u\ell}/B_{\ell u}\right)}{e^{h\nu/kT} - \left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(B_{u\ell}/B_{\ell u}\right)} \end{aligned}$$

[Note] If there is no stimulated emission $(B_{u\ell} = 0)$, the only way to make the left eq. consistent with the Planck function is to assume $h\nu/kT \gg 1$ (Wien's regime). Therefore, the stimulated emission is negligible in the Wien's regime. In other words, the stimulated emission term is required in the Rayleigh-Jean regime.

Comparing the above eq. with Planck function,

$$u_\nu = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1}$$

we can immediately recognize that the following relations should be satisfied.

$$\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(A_{u\ell}/B_{\ell u}\right) = \frac{8\pi h \nu^3}{c^3}$$

$$\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(B_{u\ell}/B_{\ell u}\right) = 1$$

In summary, we obtained the following relations between the Einstein coefficients.

$$A_{u\ell} = \frac{8\pi h \nu^3}{c^3} B_{u\ell} \qquad B_{u\ell} = \frac{c^3}{8\pi h \nu^3} A_{u\ell}$$

$$B_{\ell u} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} B_{u\ell} \qquad B_{\ell u} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} \frac{c^3}{8\pi h \nu^3} A_{u\ell}$$

# Quantum Numbers / H-atom

- Each bound state of the hydrogen atom is characterized by a set of four quantum numbers $(n, l, m, m_s)$
  - $n = 1, 2, 3, \cdots$ : principal quantum number
  - $l = 0, 1, 2, \cdots, n-1$ : orbital angular momentum quantum number
    - By convention, the values of $l$ are usually designated by letters.

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | ... |
| s | p | d | f | g | h | i | k | l | ... |

  - $m = -l, \ -l+1, \cdots, 0, \cdots, l-1, l$ : magnetic quantum number.
    - It determines the behavior of the energy levels in the presence of a magnetic field.
    - This is the projection of the electron orbital angular momentum along the $z$-axis of the system.

- Spin
  - The electron possesses an intrinsic angular momentum with the magnitude of $|s| = \frac{1}{2}$.
  - There are two states, $m_s = \pm\frac{1}{2}$, for the spin.

- Degeneracy for a given *n*: $2 \times \sum_{l=0}^{n-1} (2l+1) = 2n^2$

# H-atom Spectra

- The spectrum of the hydrogen atom comes from electrons jumping between different levels in the atom.

- Spectral series of the H atom
  - The spectrum of H is divided into a number of series linking different upper levels $n_2$ with a single lower level $n_1$ value. ***Each series is denoted according to its $n_1$ value and is named after its discoverer.***
  - Within a given series, ***individual transitions are labelled by Greek letters.***

| $n_1$ | Name | $n_2 \longleftrightarrow n_1$ Symbol | Spectral region |
|---|---|---|---|
| 1 | Lyman | Ly | ultraviolet |
| 2 | Balmer | H | visible |
| 3 | Paschen | P | infrared |
| 4 | Brackett | Br | infrared |
| 5 | Pfund | Pf | infrared |
| 6 | Humphreys | Hu | infrared |

$\Delta n \equiv n_2 - n_1$

$\Delta n = 1$ is $\alpha$,

$\Delta n = 2$ is $\beta$,

$\Delta n = 3$ is $\gamma$,

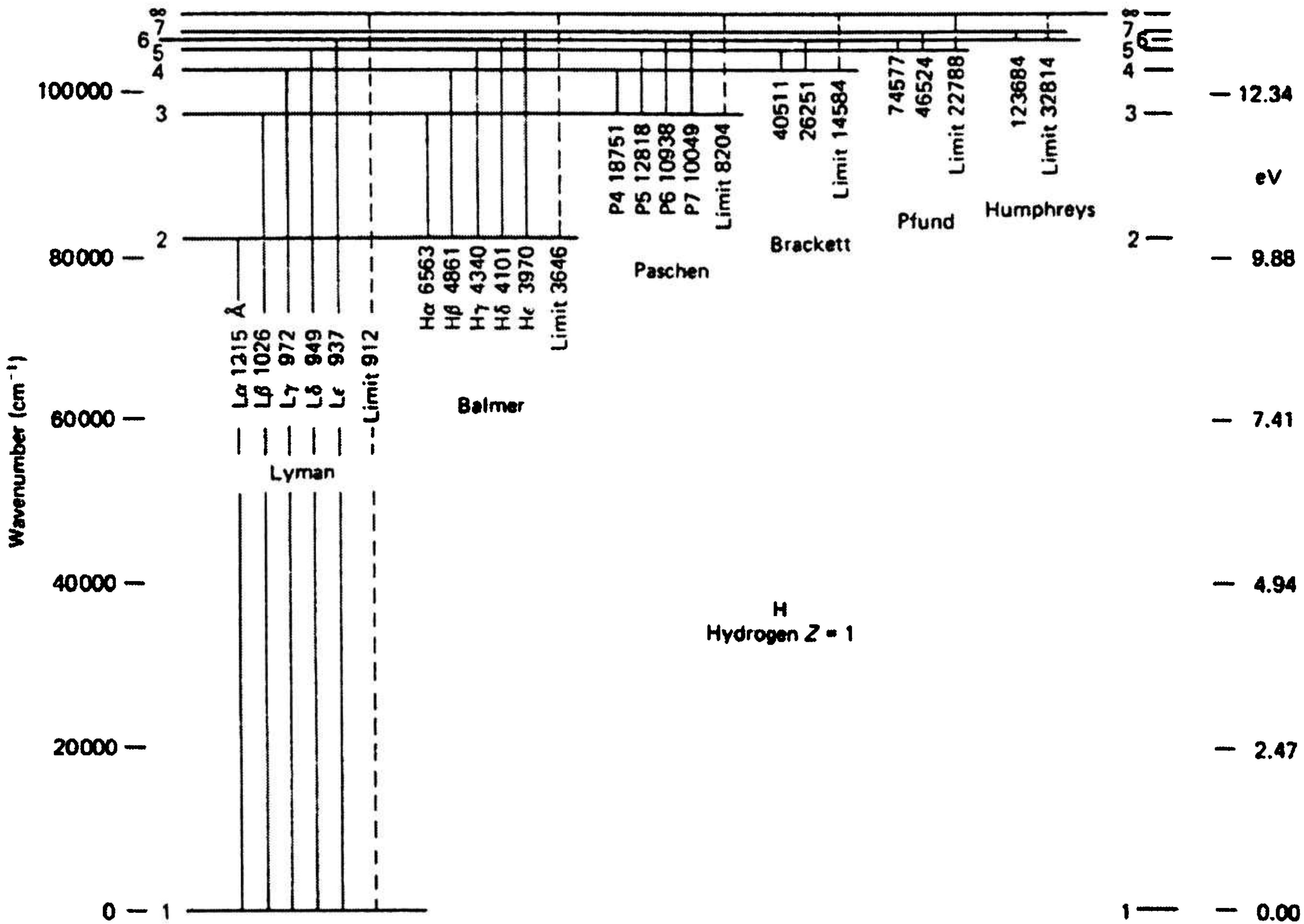
$\Delta n = 4$ is $\delta$,

$\Delta n = 5$ is $\epsilon$.

Lyman series : $\mathrm{Ly}\alpha, \mathrm{Ly}\beta, \mathrm{Ly}\gamma, \cdots$
Balmer series : $\mathrm{H}\alpha, \mathrm{H}\beta, \mathrm{H}\gamma, \cdots$
Paschen series: $\mathrm{P}\alpha, \mathrm{P}\beta, \mathrm{P}\gamma, \cdots$
Brackett series : $\mathrm{Br}\alpha, \mathrm{Br}\beta, \mathrm{Br}\gamma, \cdots$

Transitions with high $\Delta n$ are labelled by the $n_2$. Thus, $H15$ is the Balmer series transition between $n_1 = 2$ and $n_2 = 15$.

Schematic energy levels of the hydrogen atom with various spectral series identified.
The vertical numbers are wavelengths in Å.



# Complex Atoms : Electron Configuration

- <u>**The configuration** is the distribution of electrons of an atom in atomic **orbitals**.</u>
  - The configuration of an atomic system is defined by specifying the $nl$ values of all the electron orbitals: $nl^x$ means $x$ electrons in the orbital defined by $n$ and $l$.
  - Each orbital labelled $nl$ actually consists of orbitals with $2l+1$ different $m$ values, each with two possible values of $m_s$. Thus <u>the $nl$ orbital can hold a maximum $2(2l+1)$ electrons.</u>

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \cdots$$

- <u>**shells, subshells**</u>**:**
  - ***Principal quantum number = shell***: Shells correspond with the principal quantum numbers (1, 2, 3, ...). They are labeled alphabetically with letters used in the X-ray notation (K, L, M, ...).
  - ***Orbital angular momentum quantum number = subshell***: Each shell is composed of one or more subshells. The first (K) shell has one subshell, called “1s”; The second (L) shell has two subshells, called “2s” and “2p”.

- **open shell configuration, closed shell configuration:**
  - open shell = shell that is not completely filled with electrons: For instance, the ground state configuration of carbon, which has six electrons:

$$1s^2 2s^2 2p^2$$

  - closed shell = shell of which orbitals are fully occupied: For example, the ground state configuration of neon atom, which has ten electrons:

$$1s^2 2s^2 2p^6$$

- **Active electrons:** As a result of the Pauli Principle, closed shells and sub-shells have both $L = 0$ and $S = 0$. This means that ***it is only necessary to consider 'active' electrons, those in open or partially-filled shells.***

# Angular Momentum Coupling

- Atoms contain several sources of angular momentum.
  - electron orbital angular momentum $L$
  - electron spin angular momentum $S$
  - nuclear spin angular momentum $I$
  - The nuclear spin arises from the spins of nucleons. Protons and neutrons both have an intrinsic spin of a half.

- As in classical mechanics, only the total angular momentum is a conserved quantity.
  - It is therefore necessary to combine angular momenta together.

- Addition of two angular momenta:
  - The orbital and spin angular momenta are added vectorially as $\mathbf{J} = \mathbf{L} + \mathbf{S}$. This gives the total electron angular momentum.
  - One then combines the total electron and nuclear spin angular momenta to give the final angular momentum $\mathbf{F} = \mathbf{J} + \mathbf{I}$.

# Lifting Degeneracy in Configuration: Angular Momentum Coupling, Terms

- There are two coupling schemes or ways of summing the individual electron angular momentum to give the total angular momentum.
- ***L-S coupling (Russell-Saunders coupling):***
  - The orbital and spin angular momenta are added separately to give the total angular momentum $\boldsymbol{L}$ and the total spin angular momentum $\boldsymbol{S}$. These are then added to give $\boldsymbol{J}$.

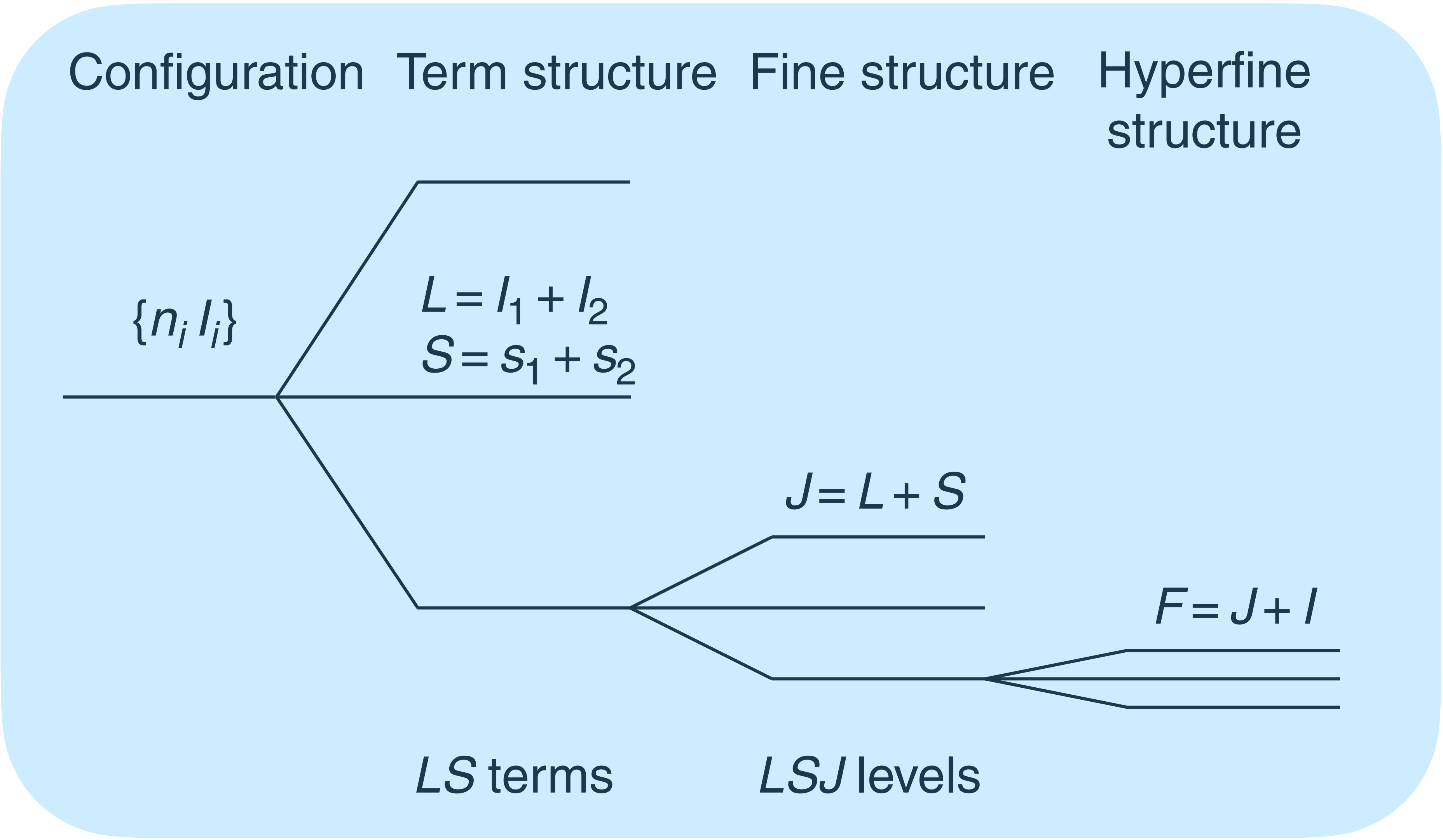
$$\boldsymbol{L} = \sum_i \boldsymbol{l}_i, \quad \boldsymbol{S} = \sum_i \boldsymbol{s}_i \quad \rightarrow \quad \boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$$

  - The configurations split into **terms** with particular values of $L$ and $S$.
- ***j-j coupling***
  - An alternative scheme is to consider the total angular momentum $\boldsymbol{j}_i$ for each electron by combining $\boldsymbol{l}_i$ and $\boldsymbol{s}_i$ and then coupling these $\boldsymbol{j}$'s together to give the total angular momentum.

$$\boldsymbol{j}_i = \boldsymbol{l}_i + \boldsymbol{s}_i \quad \rightarrow \quad \boldsymbol{J} = \sum_i \boldsymbol{j}_i$$

- Why two coupling schemes?
  - They give the same results for *J*.
  - For light atoms (lighter than iron), the values of *L* and *S* are approximately conserved quantities, and the *L-S* coupling scheme is the most appropriate.
  - For heavy atoms (beyond iron), *L* and *S* are no longer conserved quantities and *j-j* coupling is more appropriate.

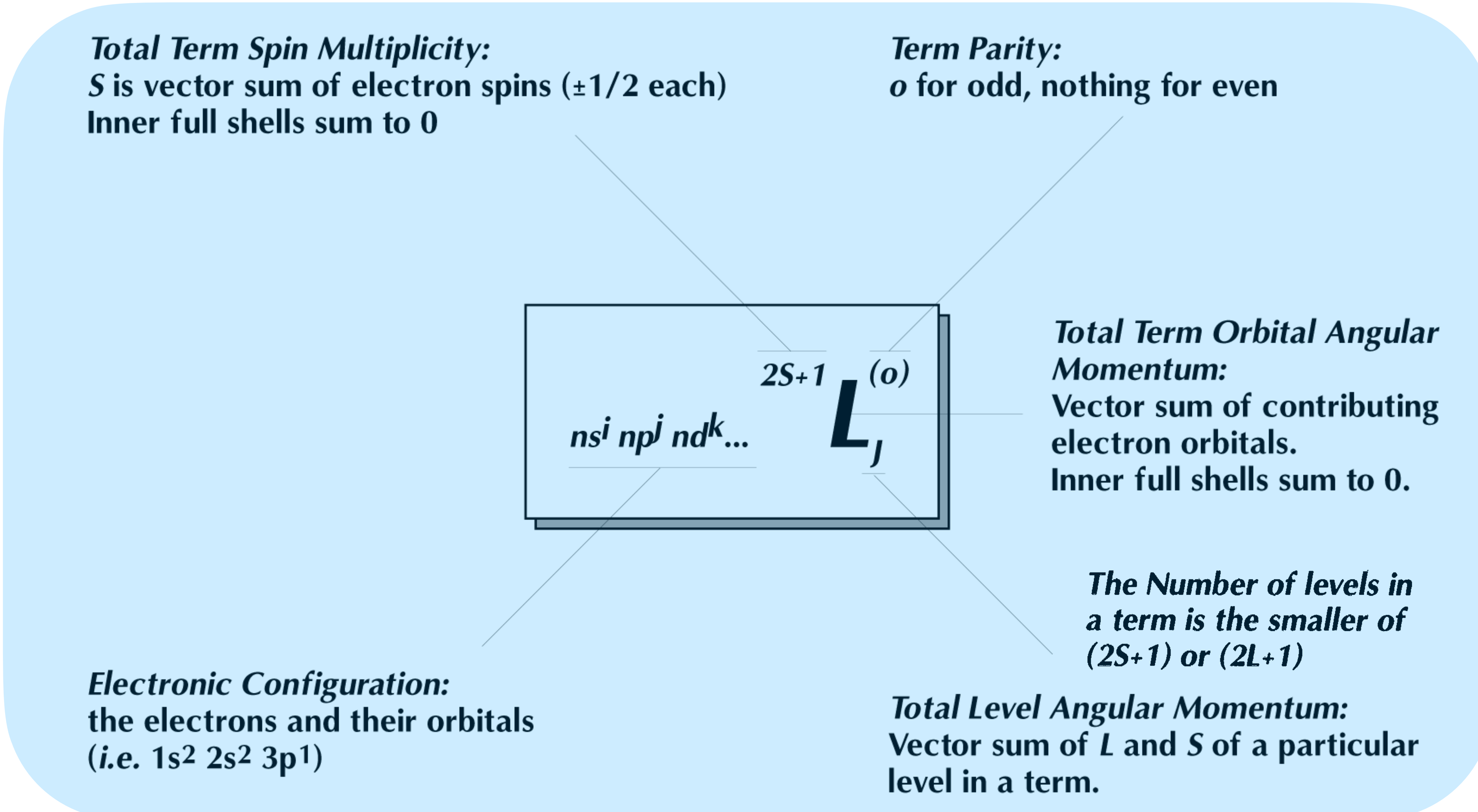
- Electronic configuration and energy level splitting
  - Configurations ⇒ Terms ⇒ Fine Structure (Spin-Orbit Interaction) ⇒ Hyperfine Structure (Interaction with Nuclear Spin)




[Pradhan & Nahar] Atomic Astrophysics and Spectroscopy

# Spectroscopic Notation

- **Spectroscopic Notation**




- A state with S = 0 is a ‘singlet’ as 2S+1 = 1.
  - $J = L$ (singlet)
- A state with S = 1/2 is a ‘doublet’ as 2S+1 = 2
  - $J = L - 1/2, L + 1/2$ (doublet if $L \geq 1$)
- One with S = 1 is a ‘triplet’ as 2S+1 = 3
  - $J = L - 1, L, L + 1$ (triplet $L \geq 1$)

$$n = 1, 2, 3, 4, 5 \cdots \quad \rightarrow \quad K, L, M, N, O, \cdots$$
$$\ell = 0, 1, 2, 3, 4 \cdots \quad \rightarrow \quad s, p, d, f, g, \cdots$$
$$L = 0, 1, 2, 3, 4 \cdots \quad \rightarrow \quad S, P, D, F, G, \cdots$$

sharp, principal, diffuse, fundamental,…

# Selection Rules

- **Selection Rules**

(1) one electron jumps
(2) $\Delta n$ any
(3) $\Delta l = \pm 1$
(4) parity change

selection rule for configuration

(5) $\Delta S = 0$

***intercombination*** line if only this rule is violated.

(6) $\Delta L = 0, \ \pm 1$ (except $L = 0 - 0$)
(7) $\Delta J = 0, \ \pm 1$ (except $J = 0 - 0$)
(8) $\Delta F = 0, \ \pm 1$ (except $F = 0 - 0$)

It is only rarely necessary to consider this.

- ***Allowed = Electric Dipole*** : Transitions which satisfy all the above selection rules are referred to as ***allowed transitions***. These transitions are strong and have a typical lifetime of $\sim 10^{-8}$ s. Allowed transitions are denoted without square brackets.

$$\text{e.g., C IV } 1548, 1550 \text{ Å}$$

- Photons do not change spin, so transitions usually occur between terms with the same spin state ($\Delta S = 0$). However, relativistic effects mix spin states, particularly for high *Z* atoms and ions. As a result, one can get (weak) spin changing transitions. These are called ***intercombination (semi-forbidden or intersystem) transitions*** or lines. They have a typical lifetime of $\sim 10^{-3}$ s. An intercombination transition is denoted with a single right bracket.

$$\text{C III] } 2\text{s}^2\ ^1\text{S} - 2\text{s}2\text{p}\ ^3\text{P}^\text{o} \text{ at } 1908.7\,\text{Å}. \quad (\Delta S = 1)$$

- If any one of the rules 1-4, 6-8 are violated, they are called ***forbidden transitions*** or lines. They have a typical lifetime of $\sim 1 - 10^3$ s. A forbidden transition is denoted with two square brackets.

$$1906.7\,\text{Å [C III] } 2\text{s}^2\ ^1\text{S}_0 - 2\text{s}2\text{p}\ ^3\text{P}^\text{o}_2, \quad (\Delta S = 1, \Delta J = 2)$$

- ***Resonance line*** denotes a dipole-allowed transition arising from the ground state of a particular atom or ion.

# Forbidden Lines

- Forbidden lines are often difficult to study in the laboratory as collision-free conditions are needed to observe metastable states.
  - In this context, it must be remembered that laboratory ultrahigh vacuums are significantly denser than so-called dense interstellar molecular clouds.
  - ***Even in the best vacuum on Earth, frequent collisions knock the electrons out of these orbits (metastable states) before they have a chance to emit the forbidden lines.***
  - In astrophysics, low density environments are common. In these environments, the time between collisions is very long and an atom in an excited state has enough time to radiate even when it is metastable.
  - Forbidden lines of nitrogen ([N II] at 654.8 and 658.4 nm), sulfur ([S II] at 671.6 and 673.1 nm), and oxygen ([O II] at 372.7 nm, and [O III] at 495.9 and 500.7 nm) are commonly observed in astrophysical plasmas. ***These lines are important to the energy balance of planetary nebulae and H II regions.***
  - ***The forbidden 21-cm hydrogen line is particularly important for radio astronomy as it allows very cold neutral hydrogen gas to be seen.***
  - Since metastable states are rather common, forbidden transitions account for a significant percentage of the photons emitted by the ultra-low density gas in Universe.
  - ***Forbidden lines can account for up to 90% of the total visual brightness of objects such as emission nebulae.***

# Notations

- Notations for Spectral Emission Lines and for Ions
  - There is a considerable confusion about the difference between these two ways of referring to a spectrum or ion, for example, C III or $C^{+2}$. These have very definite different physical meanings. However, in many cases, they are used interchangeably.
  - $C^{+2}$ is a baryon and C III is a set of photons.
  - **$C^{+2}$ refers to carbon with two electrons removed**, so that is doubly ionized, with a net charge of +2.
  - **C III is the spectrum produced by carbon with two electrons removed.** The C III spectrum will be produced by impact excitation of $C^{+2}$ or by recombination of $C^{+3}$. So, depending on how the spectrum is formed. C III may be emitted by $C^{+2}$ or $C^{+3}$.

    collisional excitation: $C^{+2} + e^- \rightarrow C^{+2*} + e^- \rightarrow C^{+2} + e^- + h\nu$

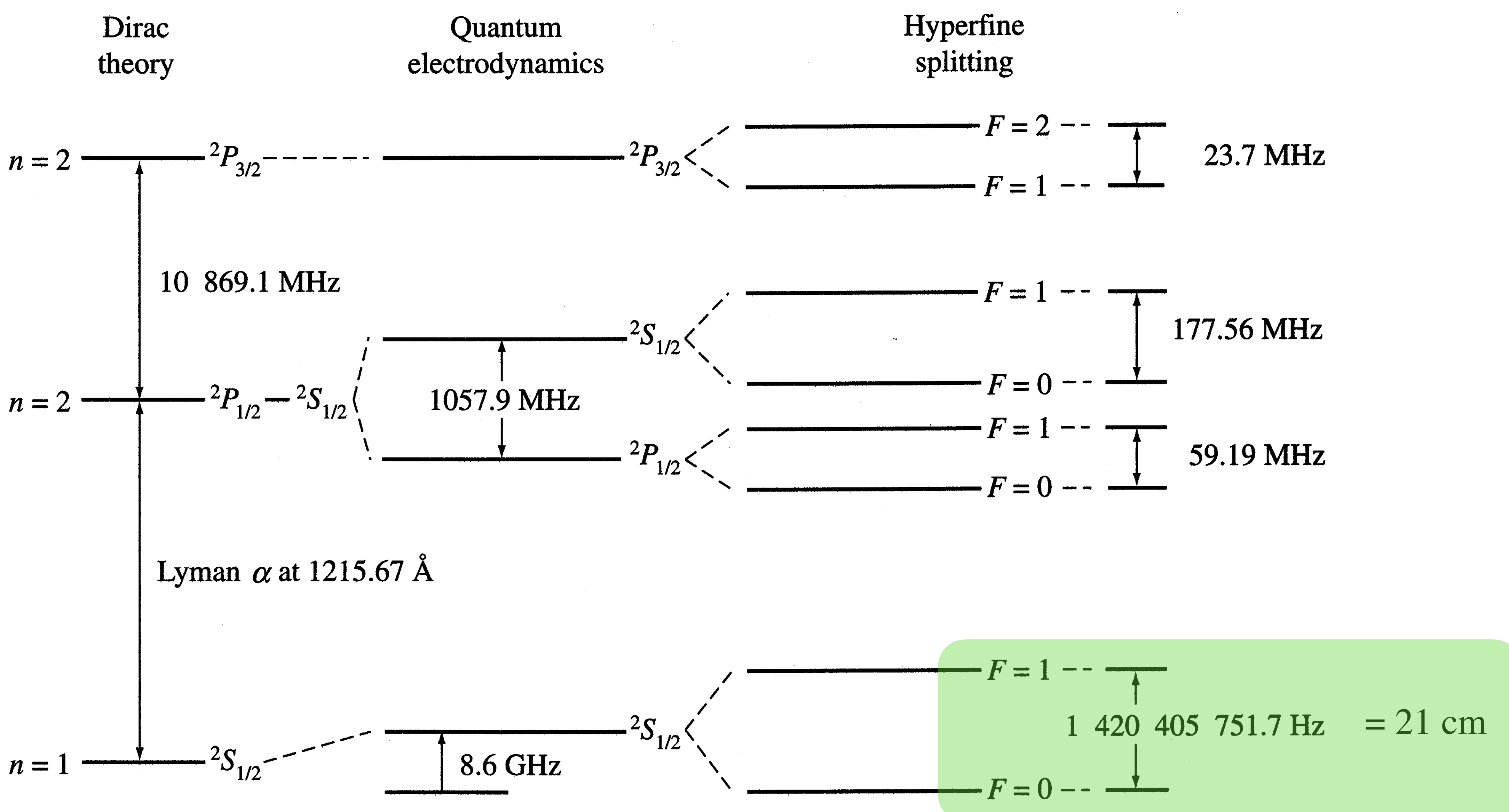
    recombination: $C^{+3} + e^- \rightarrow C^{+2} + h\nu$

  - There is no ambiguity in absorption line studies - only $C^{+2}$ can produce a C III absorption line. This had caused many people to think that C III refers to the matter rather than the spectrum.
  - But this notation is ambiguous in the case of emission lines.

# Hydrogen Atom : Fine & Hyperfine Structures

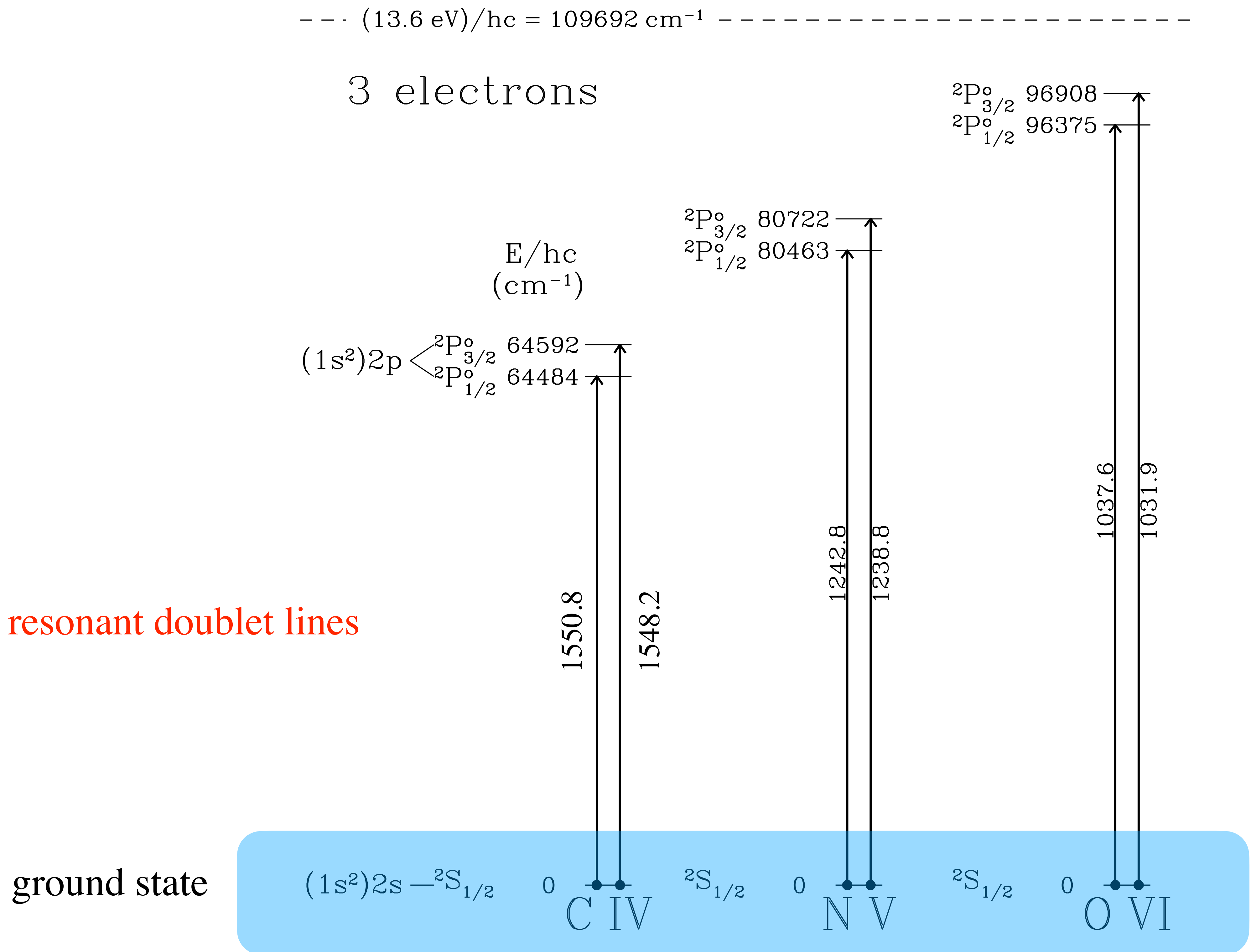
- ***Hyperfine Structure in the H atom***
  - Coupling the nuclear spin $I$ to the total electron angular momentum $J$ gives the final angular momentum $F$. For hydrogen this means

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




[Kwok] Physics and Chemistry of the ISM, [Bernath] Spectra of atoms and Molecules

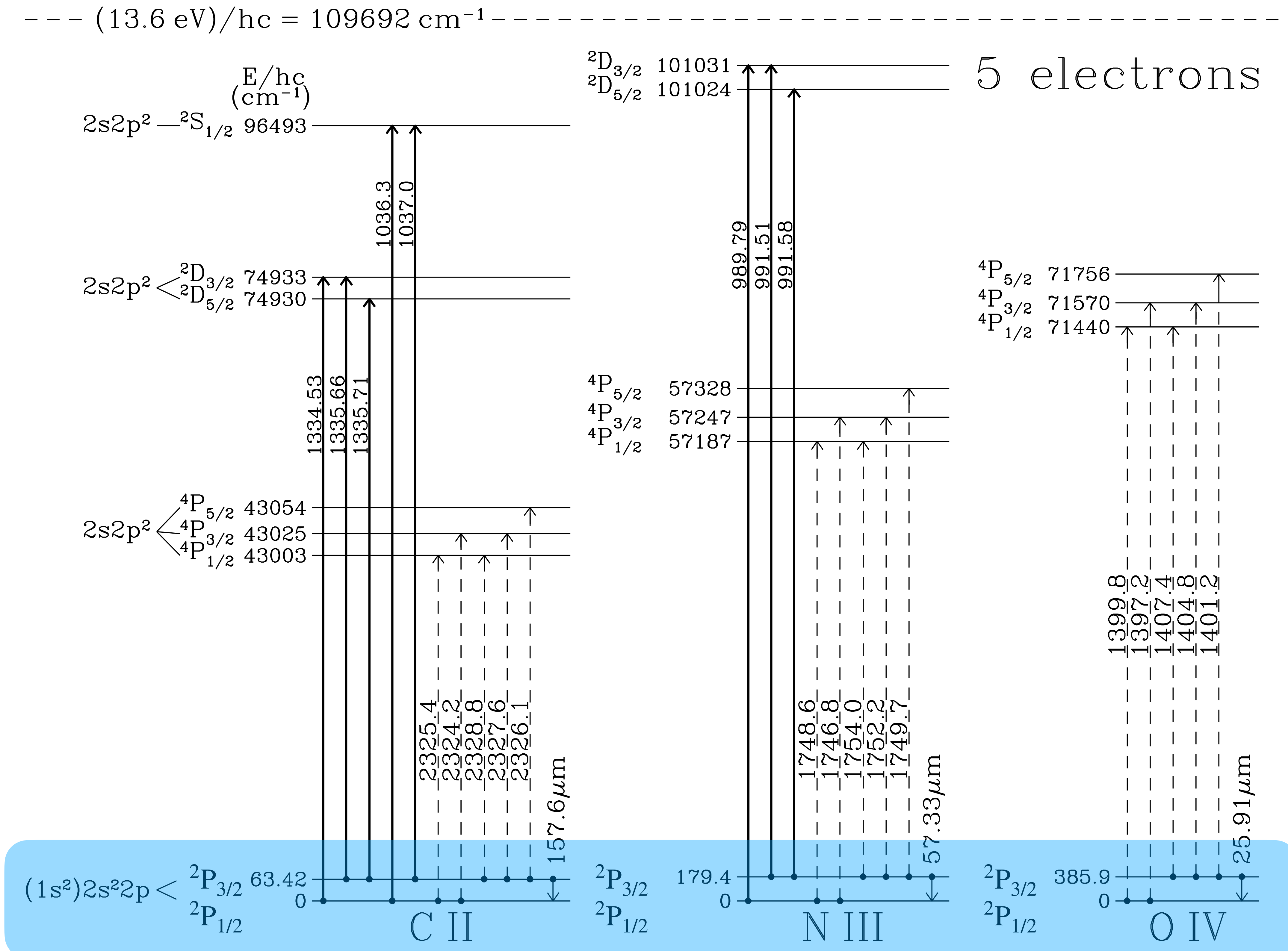
- 3 electrons (Lithium-like ions)




[Draine] Physics of the Interstellar and Intergalactic Medium

- 5 electrons

Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden

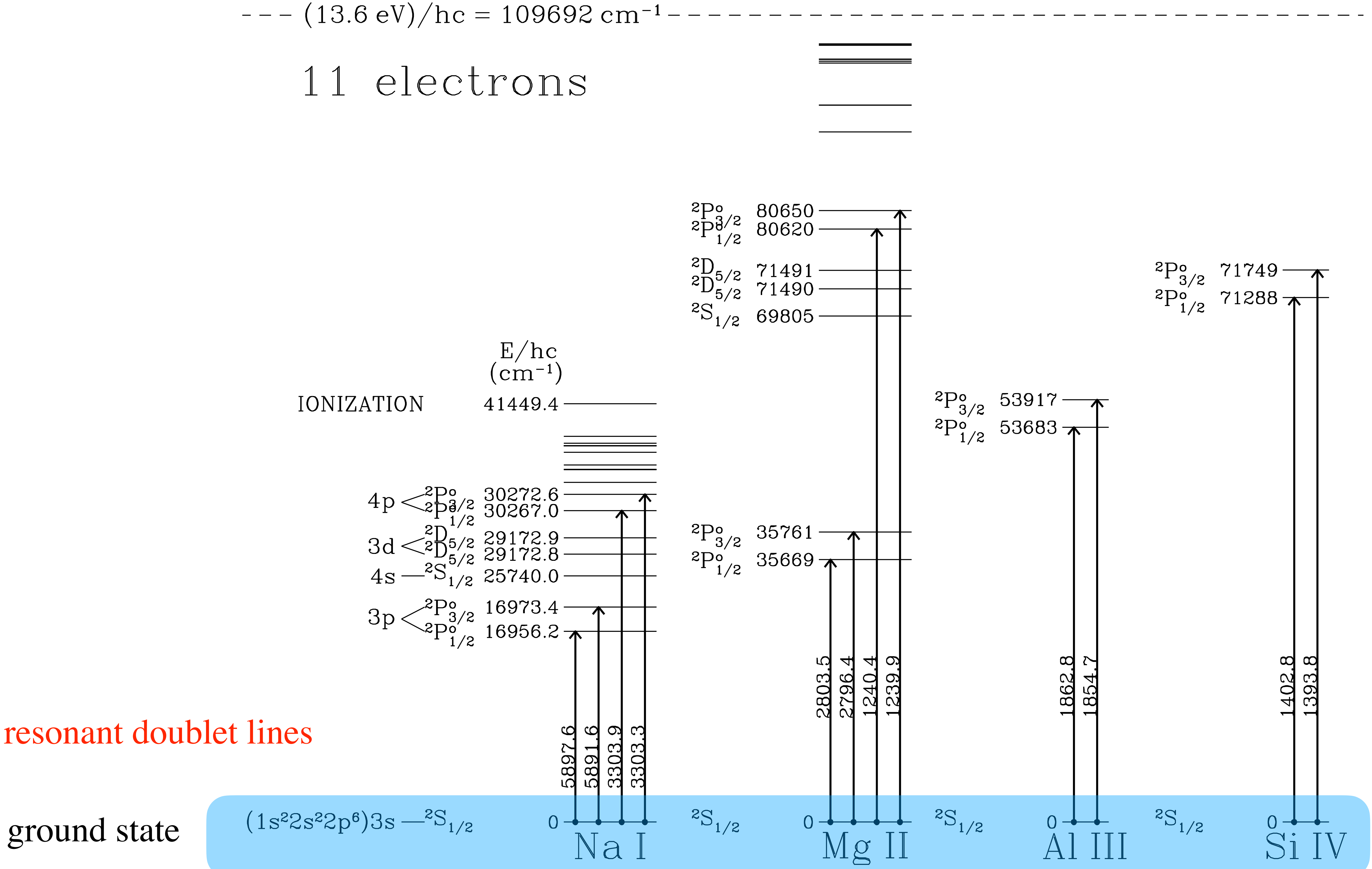



forbidden lines

[Draine] Physics of the Interstellar and Intergalactic Medium

- 11 electrons

Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden




[Draine] Physics of the Interstellar and Intergalactic Medium

# Absorption & Emission Line Profile

- ***In the classical / quantum theory of spectral lines,***

we obtain a Lorentzian line profile:

$$\sigma_\nu = f_{nn'} \frac{\pi e^2}{mc} \frac{\gamma/4\pi^2}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2}$$

$$\int_0^\infty \sigma_\nu d\nu = f_{nn'} \frac{\pi e^2}{mc}$$

where $f_{nn'}$ is called the ***oscillator strength*** or ***f-value*** for the transition between states $n$ and $n'$.

$\gamma = A$ is the ***damping constant (or Einstein A-coefficient)***.

Selected Resonance Lines[a] with $\lambda < 3000$ Å

| | Configurations | $\ell$ | $u$ | $E_\ell/hc(\mathrm{cm}^{-1})$ | $\lambda_{\mathrm{vac}}(\text{Å})$ | $f_{\ell u}$ |
|---|---|---|---|---|---|---|
| C IV | $1s^22s-1s^22p$ | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | 0 | 1550.772 | 0.0962 |
| | | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | 0 | 1548.202 | 0.190 |
| N V | $1s^22s-1s^22p$ | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | 0 | 1242.804 | 0.0780 |
| | | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | 0 | 1242.821 | 0.156 |
| O VI | $1s^22s-1s^22p$ | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | 0 | 1037.613 | 0.066 |
| | | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | 0 | 1037.921 | 0.133 |
| C III | $2s^2-2s2p$ | $^1\mathrm{S}_0$ | $^1\mathrm{P}^\mathrm{o}_1$ | 0 | 977.02 | 0.7586 |
| C II | $2s^22p-2s2p^2$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | $^2\mathrm{D}^\mathrm{o}_{3/2}$ | 0 | 1334.532 | 0.127 |
| | | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | $^2\mathrm{D}^\mathrm{o}_{5/2}$ | 63.42 | 1335.708 | 0.114 |
| N III | $2s^22p-2s2p^2$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | $^2\mathrm{D}^\mathrm{o}_{3/2}$ | 0 | 989.790 | 0.123 |
| | | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | $^2\mathrm{D}^\mathrm{o}_{5/2}$ | 174.4 | 991.577 | 0.110 |
| C I | $2s^22p^2-2s^22p3s$ | $^3\mathrm{P}_0$ | $^3\mathrm{P}^\mathrm{o}_1$ | 0 | 1656.928 | 0.140 |
| | | $^3\mathrm{P}_1$ | $^3\mathrm{P}^\mathrm{o}_2$ | 16.40 | 1656.267 | 0.0588 |
| | | $^3\mathrm{P}_2$ | $^3\mathrm{P}^\mathrm{o}_2$ | 43.40 | 1657.008 | 0.104 |
| N II | $2s^22p^2-2s2p^3$ | $^3\mathrm{P}_0$ | $^3\mathrm{D}^\mathrm{o}_1$ | 0 | 1083.990 | 0.115 |
| | | $^3\mathrm{P}_1$ | $^3\mathrm{D}^\mathrm{o}_2$ | 48.7 | 1084.580 | 0.0861 |
| | | $^3\mathrm{P}_2$ | $^3\mathrm{D}^\mathrm{o}_3$ | 130.8 | 1085.701 | 0.0957 |
| N I | $2s^22p^3-2s^22p^23s$ | $^4\mathrm{S}^\mathrm{o}_{3/2}$ | $^4\mathrm{P}_{5/2}$ | 0 | 1199.550 | 0.130 |
| | | $^4\mathrm{S}^\mathrm{o}_{3/2}$ | $^4\mathrm{P}_{3/2}$ | 0 | 1200.223 | 0.0862 |
| O I | $2s^22p^4-2s^22p^33s$ | $^3\mathrm{P}_2$ | $^3\mathrm{S}^\mathrm{o}_1$ | 0 | 1302.168 | 0.0520 |
| | | $^3\mathrm{P}_1$ | $^3\mathrm{S}^\mathrm{o}_1$ | 158.265 | 1304.858 | 0.0518 |
| | | $^3\mathrm{P}_0$ | $^3\mathrm{S}^\mathrm{o}_1$ | 226.977 | 1306.029 | 0.0519 |
| Mg II | $2p^63s-2p^63p$ | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | 0 | 2803.531 | 0.303 |
| | | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | 0 | 2796.352 | 0.608 |
| Al III | $2p^63s-2p^63p$ | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{1/2}$ | 0 | 1862.790 | 0.277 |
| | | $^2\mathrm{S}_{1/2}$ | $^2\mathrm{P}^\mathrm{o}_{3/2}$ | 0 | 1854.716 | 0.557 |

Table 9.4 in [Draine]
See also Table 9.3

# Line Broadening Mechanisms

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

- **Voigt profile : Thermal + Natural broadening**
  - 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:
  - Voigt profile = convolution of a Lorentz function (natural broadening) and Gaussian function (thermal broadening).

- The profile can be written using the Voigt function.

$$\phi(\nu) = \frac{1}{\Delta\nu_{\rm D}\sqrt{\pi}} H(u,a)$$

Here, $a$ is a ratio of the intrinsic broadening to the thermal broadening.

$u$ is a measure of how far you are from the line center, in units of thermal broadening parameter.
In terms of Doppler velocity, $u$ can be expressed as

$$u = \frac{\nu-\nu_0}{\Delta\nu_{\rm D}} = \frac{\nu-\nu_0}{\nu_0}\frac{c}{v_{\rm th}}$$

In the velocity term,

$$u = \frac{v}{v_{\rm th}}, \ \ \text{where } v = \frac{\nu-\nu_0}{\nu_0}c$$

Voigt-Hjerting function:

$$H(u,a) \equiv \frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}dy}{(u-y)^2+a^2}$$

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_{\rm D}}$$

$$u \equiv \frac{\nu-\nu_0}{\Delta\nu_{\rm D}}$$

$$\Delta\nu_{\rm D} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$$

Including the turbulent motion

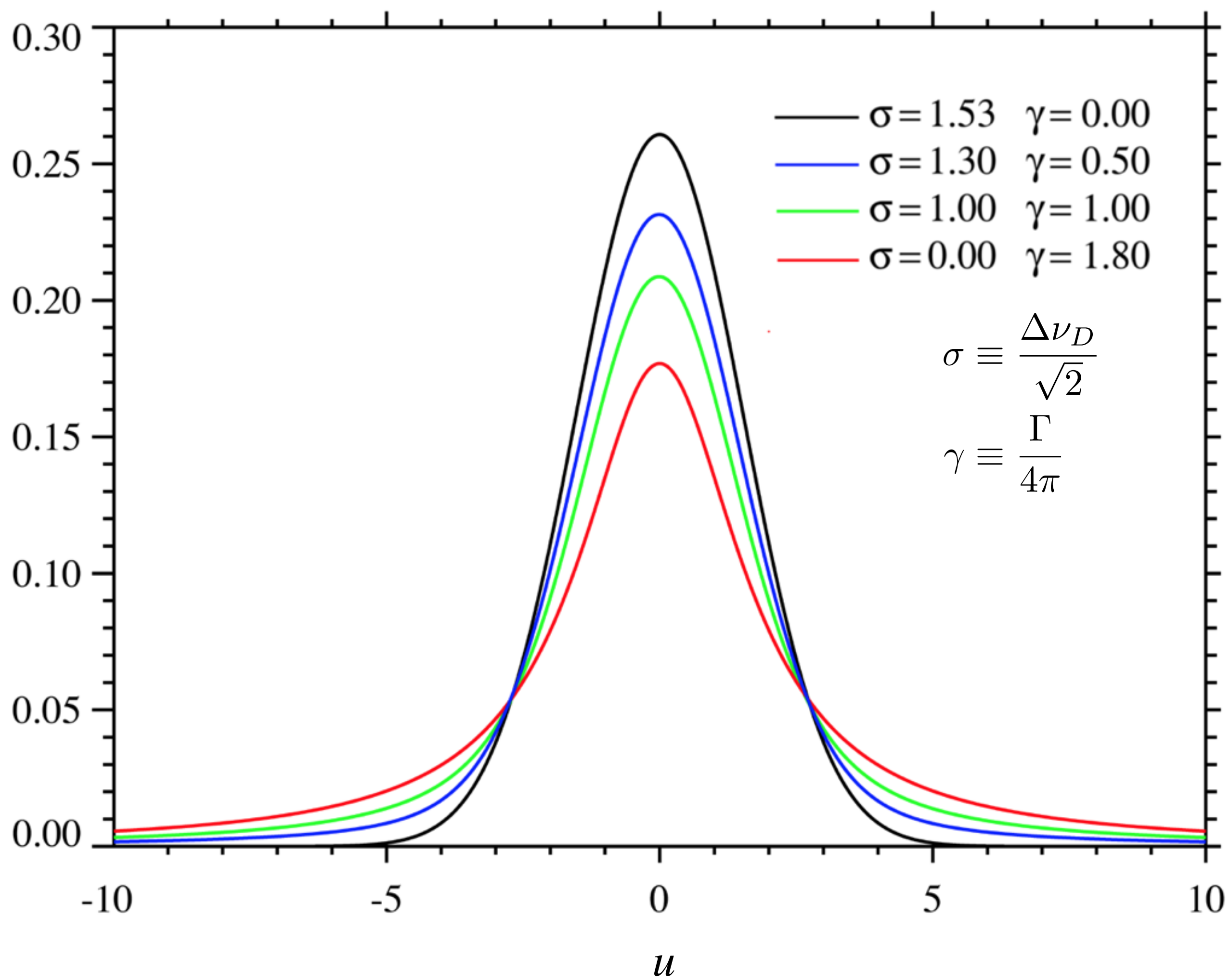
$$\Delta\nu_{\rm D} = \nu_0\frac{v_{\rm th}}{c} \ \rightarrow \ \Delta\nu_{\rm D} = \nu_0\frac{b}{c}$$

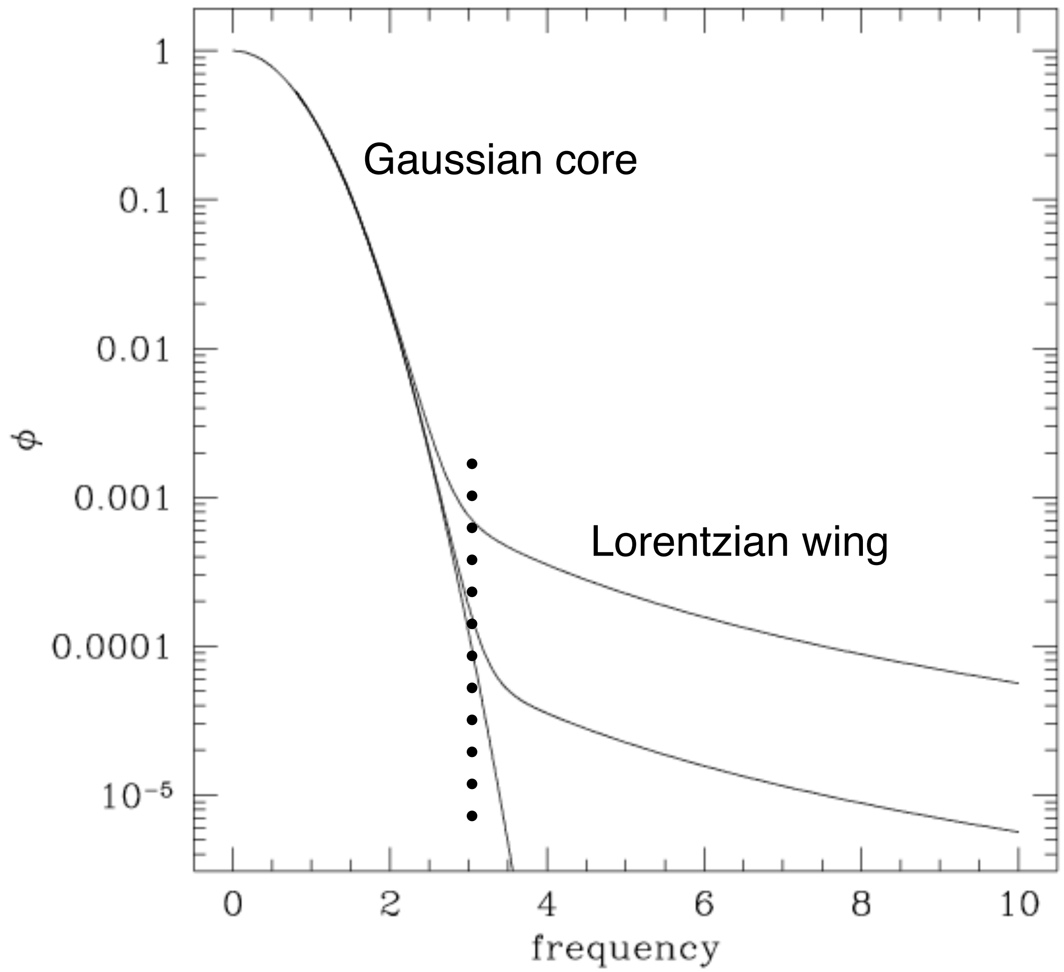
$$\text{where } b = \sqrt{v_{\rm th}^2 + v_{\rm turb}^2}, \ \ v_{\rm th} = \sqrt{\frac{2kT}{m}}$$

# Properties of Voigt Function

- For small $a$, the "core" of the line is dominated by the Gaussian (Doppler) profile, whereas the "wings" are dominated by the Lorentz profile.

$$H(a,u) \equiv \frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}dy}{(u-y)^2+a^2}$$




- In most case, $a \ll 1$. For Ly$\alpha$ at $T$ = 100 K, $a \sim 0.05$.

# Excitation Equilibrium

- Consider a system that has many energy states (for instance, electronic energy levels of an atom, or two rotational or vibrational states of a molecule, or the two hyper fine states of a hydrogen atom)
- A large population of such systems is said to be in **excitation equilibrium** if the relative level populations follows a Boltzmann distribution: $\dfrac{n_u}{n_\ell} = \dfrac{g_u}{g_\ell} \exp\left(-\dfrac{E_{u\ell}}{kT}\right)$, where $g_i = 2J_i + 1$ is the statistical weight of the $i^{\rm th}$ energy level, and $T$ is the kinetic temperature of the system.
  - In the limit $kT \gg E_{u\ell},\ n_u/n_\ell = g_u/g_\ell$ (the two levels are populated according to their statistical weights.)
  - In the limit $kT \ll E_{u\ell}$, $n_u \approx 0$.
  - The excitation equilibrium implies the thermal equilibrium.
  - However, not every system in kinetic equilibrium is in excitation equilibrium. (for instance, masers).
  - For any two energy states, we define an **excitation temperature** using the population ration $n_u/n_\ell$ such that $\dfrac{n_u}{n_\ell} = \dfrac{g_u}{g_\ell} \exp\left(-\dfrac{E_{u\ell}}{kT_{\rm exc}}\right)$. In general, $T_{\rm exc} \neq T_{\rm kinetic}$.
  - The excitation temperature is nothing but a convenient way to parameterize the relative level populations.
  - For a system like a **maser** with inverted energy levels ($n_u/n_\ell > g_u/g_\ell$), *the excitation temperature is negative.*

# Ionization Equilibrium

- First ionization energy of the most abundant elements is $I \sim 10\ \mathrm{eV}$.
  - hydrogen : $I_\mathrm{H} \sim 13.6\ \mathrm{eV}$, carbon: $I_\mathrm{C} \sim 11.26\ \mathrm{eV}$, magnesium: $I_\mathrm{H} \sim 7.65\ \mathrm{eV}$
  - The only regions where we expect collisional ionization of these neutral atoms are where $T > 1.2 \times 10^5\ \mathrm{K}$ and thus $\langle E \rangle > 10\ \mathrm{eV}$. This temperature is attained only in the HIM.

- In practice, much of the ionization in the ISM is photoionization.

$X^r + \gamma \rightarrow X^{r+1} + e^-$ ($\gamma$ represents a photon with $E_\gamma > I_{X^r}$ and "r" the r$^{\mathrm{th}}$ ionization state.)

  - For element $X$ to be in the photoionization equilibrium, we require a balance between photoionization and radiative recombination:

$$n(X^r) n_\gamma \sigma_\mathrm{pho} c = n(X^{r+1}) n_e \sigma_\mathrm{rec} \upsilon$$

$$\frac{n(X^{r+1}) n_e}{n(X^r)} = \frac{n_\gamma \left\langle \sigma_\mathrm{pho} \right\rangle_{h\nu} c}{\left\langle \sigma_\mathrm{rec} \upsilon \right\rangle_\upsilon}$$

$\sigma_\mathrm{pho}$ = cross-section for photoionization, depending on the photon energy $h\nu$

$\sigma_\mathrm{rec}$ = cross-section for recombination, depending on the electron velocity $\upsilon$

averaged over the photon energy spectrum

averaged over the Maxwellian velocity distribution

# Multiphase ISM

# Five Phases of the ISM

## Molecular clouds

- $H_2$ is the dominant form of molecules.
- **Number density ~ $10^6$ cm$^{-3}$ in the molecular cloud cores**, which are self-gravitating and form stars. (Note that $10^6$ cm$^{-3}$ is comparable to the density in the most effective cryo-pumped vacuum chambers in laboratories.)
- How to observe: for instance, 2.6, 1.3 and 0.9 mm (115, 230 and 345 GHz) emission lines from CO.

## Cold neutral medium (CNM) ($T \sim 10^2$ K)

- The dominant form of CNM is H I (atomic hydrogen).
- The CNM is distributed in sheets and filaments occupying ~1% of the ISM volume.
- How to observe: UV and optical absorption lines in the spectra of background stars and quasars.

## Warm neutral medium (WNM) ($T \sim 5 \times 10^3$ K)

- Its dominant form is H I (atomic hydrogen).
- A leading method of observing the WNM is using 21 cm emission.

## Warm ionized medium (WIM) or Diffuse ionized gas (DIG) ($T \sim 10^4$ K)

- The dominant form is H II (ionized hydrogen or proton).
- The WIM is primarily photoionized by O and B stars.
- Observed using Balmer emission lines (H$\alpha$).

## Hot ionized medium (HIM) or coronal gas ($T \gtrsim 10^{5.5}$ K)

- The HIM is primarily heated by supernovae.
- HIM occupies ~ half of the ISM volume, but provides only 0.2% of the ISM mass.
- soft X-ray emission. O VI, N V, and C IV emission or absorption lines in the spectra of background stars.

| Name | T (K) | $n_{\mathrm{H}}(\mathrm{cm}^{-3})$ | Mass fraction | Volume fraction |
|---|---|---|---|---|
| Molecular Clouds | 20 | $> 100$ | 35% | 0.1% |
| Cold Neutral Medium | 100 | 30 | 35% | 1% |
| Warm Neutral Medium | 5000 | 0.6 | 25% | 40% |
| Warm Ionized Medium | $10^4$ | 0.3 | 3% | 10% |
| Hot Ionized Medium | $10^6$ | 0.004 | 0.2% | 50% |

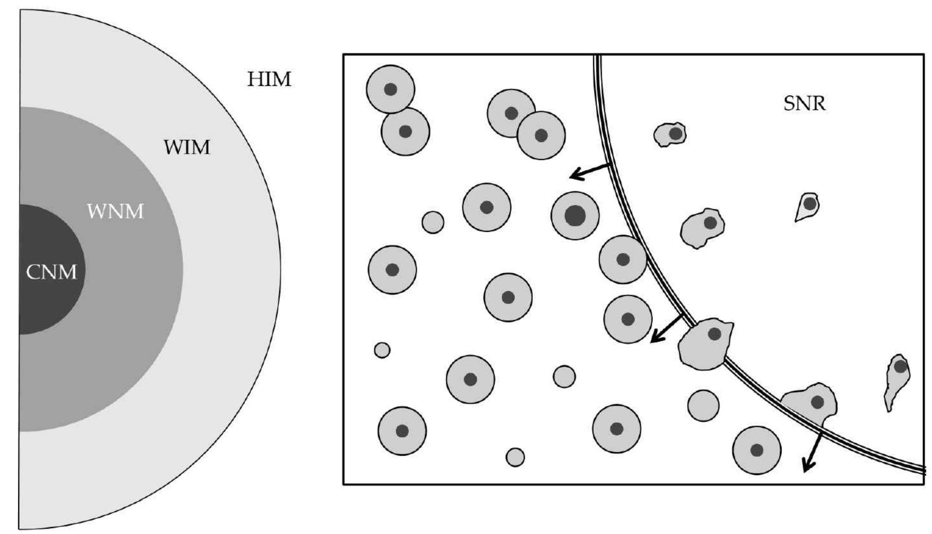
# Pressure Equilibrium

- We already pointed out that all five phases of the ISM have a pressure $P \sim 4 \times 10^{-19}$ atm, equivalent to a thermal energy density $(3/2)nkT \sim 0.4$ eV cm$^{-3}$.
  - Thus, it is tempting to assume that the phases are in pressure equilibrium, with

$$n_1 kT_1 = n_2 kT_2 = 4 \times 10^{-19} \text{ atm}$$

$$n_1 T_1 = n_2 T_2 = 2{,}935 \text{ cm}^{-3}\,\text{K}$$

$$(1 \text{ atm} = 1.013 \times 10^6 \,\text{dyn}\,\text{cm}^{-2})$$




  - Earlier views of the ISM did assume the pressure equilibrium. Denser, cooler “clouds” in a tenuous, hotter “intercloud medium.”
  - However, current studies of the ISM have had reject this simple picture. The ISM has indeed tendencies toward pressure equilibrium, but something always happens to throw things out of equilibrium.
    - ✦ The ubiquity of free electrons indicates that the ISM is coupled to the interstellar magnetic field. The turbulent energy density is not negligibly small. Thus, they have to be taken into account.
    - ✦ Supernova explosions are going off in the ISM, increasing the temperature *T*.
    - ✦ Hot young stars are pouring ionizing radiation into the ISM, splitting up atoms and increasing *n*.

# Heading and Cooling in the ISM

- Balance between heating and cooling in our body.
  - Number density of molecules in your body is $n \sim 3 \times 10^{22}\ \mathrm{cm}^{-3}$ and temperature is $T \sim 310\ \mathrm{K}$.
  - If your temperature drops too low, your body increases the heating rate (by shivering) or decrease the cooling rate (by trying to fluff out fur).
  - If your temperature rises too high, your body increases the cooling rate (by sweating and thus increasing evaporative cooling) or decrease the heating rate (by stopping unnecessary activity).
- The temperature of the ISM is also determined by a balance between heating and cooling.
  - Each phase has a temperature where the balance is a stable one.
- Definitions
  - heating gain $G$, cooling loss $L$ in units of erg $s^{-1}$.
  - volumetric heating rate $g = nG$, volumetric cooling rate $\ell = nL$ in units of erg $cm^{-3}$ $s^{-1}$.
  - cooling function $\Lambda$ in units of erg $cm^3$ $s^{-1}$, which is useful for two-body interactions.
  - $\ell = nL = n^2\Lambda$, where $n$ is the total number density of gas particles.
  - Even when only one type of particle is losing energy, the energy loss is shared among all the gas particles due to the relatively short thermalization time scale in the ISM.

# - Heating -

- Heating processes
  - The primary heating mechanisms of the ISM involve providing free electrons with high energies. Through collisions, the fast free electrons share their kinetic energy with other particles, and through further collisions, the distribution of velocities approaches a Maxwellian distribution.

  - **Source of free electrons**
    - ✦ **Ionization by cosmic rays**
    - ✦ **Photoionization of dust grains by starlight UV.**
    - ✦ **Photoionization of atoms (H, He, C, Mg, Si, Fe, etc) by X-rays or starlight UV.**

  - **Other heating sources:**
    - ✦ **Heating by shock waves and other MHD phenomena.**

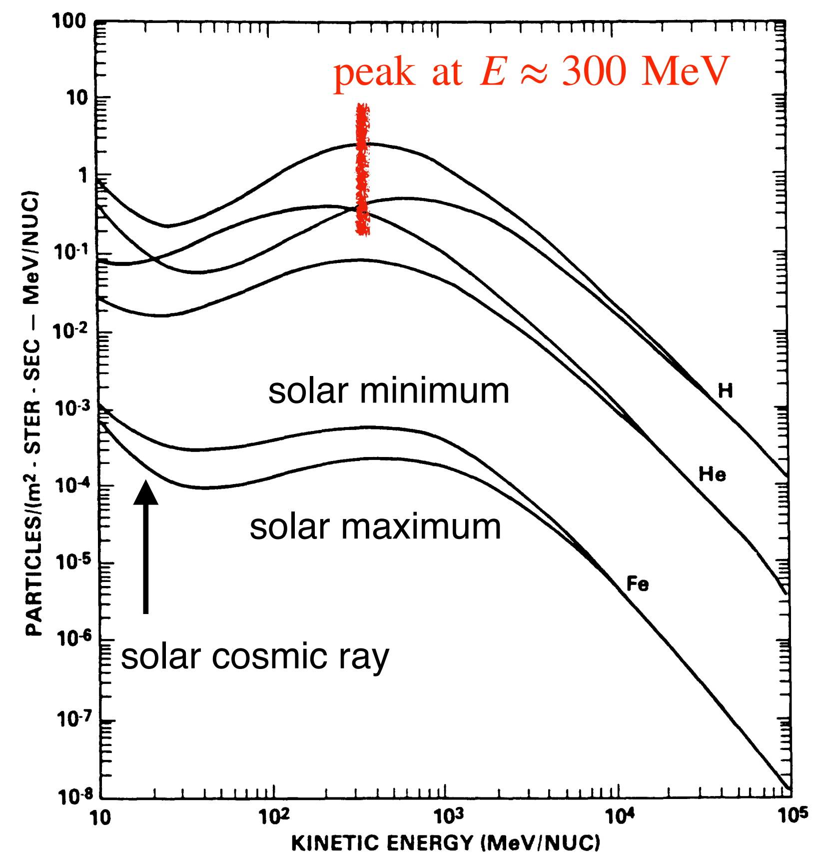
    - Reference: Collisional time scale
      - $t_{\rm coll}({\rm HH}) \sim 2.2\,{\rm yr}$ for atom-atom collisions
      - $t_{\rm coll}(e{\rm H}) \sim 120\,{\rm yr}$ for atom-electron collisions
      - $t_{\rm coll}(ee) \sim 1.2\,{\rm hr}$ for electron-electron collision

# (1) Cosmic Ray Heating

- Cosmic Rays
  - Cosmic rays consist primarily of protons and helium nuclei, with heavier nuclei, electrons, positrons, and antiprotons making a small contribution (~1%). They have relativistic energies as high as $10^{20}$ eV.
  - Cosmic rays are of galactic origin, and not universal except perhaps at very high energies.
  - The energy distribution of cosmic rays peaks at $E \approx 300\text{MeV}$.
  - The solar wind expels cosmic rays of low energy.
- The relatively low-energy cosmic rays ($1 < E < 50$ MeV) can collisional ionize hydrogen atoms:

$$H + p \rightarrow p + p + e^-$$

  - The cosmic ray ionization produces electrons with a spectrum of energies. The ejected electron carries away a mean energy of $\langle E \rangle \approx 35$ eV.
  - Some of this kinetic energy will go into secondary ionization and excitation of H, $H_2$, and He that will then deexcite radiatively, but a fraction of the secondary electron energy will ultimately end up as thermal kinetic energy.




Differential energy spectra of cosmic-ray protons (H), $\alpha$ particles (He), and iron, near solar minimum and maximum (Silberberg et al. 1987)

- The heating efficiency depends on the fractional ionization.
    - ✦ If the ionization is high, then the primary electron has a high probability of losing its energy by long-range Coulomb scattering off free electrons, and ~ 100% of the initial kinetic energy will be converted to heat.
    - ✦ When the gas is neutral, a fraction of the primary electron energy goes into secondary ionization or excitation of bound states.
    - ✦ Heat per primary ionization (Dalgarno & McCray 1972):

$$E_h \approx 6.5\,\mathrm{eV} + 26.4\,\mathrm{eV}\left(\frac{x_e}{x_e + 0.07}\right)^{1/2}, \quad x_e \equiv \frac{n_e}{n_\mathrm{H}} \ \ \text{(ionization fraction)}$$

    - ✦ Heating rate due to cosmic ray ionization:

$$g_\mathrm{CR} \approx \left(n_\mathrm{H} + n_\mathrm{He}\right)\zeta_\mathrm{CR} E_h$$

$$G_\mathrm{CR} \approx 1.03 \times 10^{-27}\left(\frac{\zeta_\mathrm{CR}}{10^{-16}\ \mathrm{s}^{-1}}\right)\left[1 + 4.06\left(\frac{x_e}{x_e + 0.07}\right)^{1/2}\right] \ \ \mathrm{erg\ s^{-1}}$$

Here, $\zeta_\mathrm{CR}$ is the primary cosmic ray ionization rate (the average rate at which a hydrogen atom is ionized by cosmic rays).

- Primary ionization rate by cosmic rays
  - From the observed spectrum of cosmic rays and the definition of the cosmic ray ionization rate:

$$\zeta_{\rm CR} \gtrsim 7 \times 10^{-18}\ {\rm s}^{-1}$$ with a substantially larger rate being allowed by uncertainties

  - The observations of $H_3^+$ appear to indicate a cosmic ray ionization rate, in diffuse molecular gas,

$$\zeta_{\rm CR} \approx (0.5 - 3) \times 10^{-16}\ {\rm s}^{-1}$$

  - Note that $\zeta_{\rm CR} \approx 10^{-16}\ {\rm s}^{-1} \sim 3\,{\rm Gyr}^{-1}$.

- ***Heating by cosmic rays is the dominant heating mechanism in molecular clouds***, where the dust opacity prevents high-energy photons from entering.

# (2) Photoelectric Heating by Dust

- UV and X-ray photons can knock electrons free from dust grains. The ejected electrons carry kinetic energy, which can be effective at heating the surrounding gas.
- ***Photoelectrons emitted by dust grains dominate the heating of the diffuse neutral ISM (CNM and WNM) in the Milky Way.***
- The work function, analogous to the ionization energy of an atom, for graphite is $4.50 \pm 0.05\,\mathrm{eV}$. Therefore, UV photons with $h\nu \gtrsim 5\,\mathrm{eV}$ can kick out photoelectrons from dust grains. The photoelectric heating by dust is dominated by photons with $h\nu \gtrsim 8\,\mathrm{eV}$.

$$G_{\mathrm{pe}} \approx 1.4 \times 10^{-26} \frac{n_{\mathrm{ph}}(8 - 13.6\,\mathrm{eV})}{3 \times 10^{-3}\,\mathrm{cm}^{-3}} \frac{\left\langle \sigma_{\mathrm{abs}} \right\rangle}{10^{-21}\,\mathrm{cm}^2} \frac{\langle Y \rangle}{0.1} \frac{\left\langle E_{\mathrm{pe}} \right\rangle - \left\langle E_c \right\rangle}{1\,\mathrm{eV}} \ \ \mathrm{erg\ s^{-1}}$$

Here,

$n_{\mathrm{ph}}(8 - 13.6\,\mathrm{eV})$ = number density of $8 < h\nu < 13.6\,\mathrm{eV}$ photons
$\left\langle \sigma_{\mathrm{abs}} \right\rangle$ = total dust photo absorption cross section per H nucleon, averaged over the photon spectrum.
$\langle Y \rangle$ = photoelectric yield averaged over the spectrum of 8 to 13.6 eV photons absorbed by the interstellar grain mixture.
$\left\langle E_{\mathrm{pe}} \right\rangle$ = mean kinetic energy of escaping photoelectrons.
$\left\langle E_{\mathrm{c}} \right\rangle$ = mean kinetic energy of electrons captured from the plasma by grains.

- Photoelectric heating from dust may be an order of magnitude larger than the cosmic ray heating rate.

# (3) Photoionization Heating

- Photons in the energy range $11.26\,\mathrm{eV} < h\nu < 13.60\,\mathrm{eV}$ $(911.6\text{Å} < \lambda < 1101\text{Å})$ are likely to end up ionizing a carbon atom. When carbon is photo ionized, a free electron is released.

$$C^0 + h\nu \rightarrow C^+ + e^-$$

- The released electron (photoelectron) carries away the energy between 0—2.34 eV.
- If there aren't many photons with $h\nu > 13.6\,\mathrm{eV}$, hydrogen is predominantly in neutral form and most of positively charged ions are C II ($C^+$).
- The heating gain from the photoionization of carbon is approximately:

$$\begin{aligned} G_{\mathrm{CII}} &= 2.2 \times 10^{-22} f(\mathrm{CI}) \mathscr{A}_C \chi_0 \ \mathrm{erg\ s^{-1}} \\ &\approx 10^{-29}\ \mathrm{erg\ s^{-1}} \end{aligned}$$

Eq (3.8) of The Physics and Chemistry of the Interstellar Medium (A. G. G. M. Tielens)

Here,

$f(\mathrm{CI})$ = neutral fraction of carbon ( $\sim 3.3 \times 10^{-4}$)
$\mathscr{A}_C$ = atomic carbon abundance in the gas phase ( $\sim 2.70 \times 10^{-4} \times 0.5$)
$\chi_0$ = intensity of the radiation field in units of the average interstellar radiation field.

- In the dusty ISM, the heating by carbon photoionization can't compete with the heating by electrons ejected from dust grains.
- H II regions and the diffuse IGM are the regions where photoionization becomes an important heating source.

# (4) Shock Heating

- Shocks are propagating disturbances, characterized by abrupt, nearly discontinuous change in the temperature, pressure, and density.
  - ✦ In the ISM, shocks can be created by a supernova explosion or by the collision between molecular clouds.
  - ✦ On larger scales, shocks can be created by the collision of two galaxy clusters.
  - ✦ Shocks convert the kinetic energy of bulk flow into the thermal energy associated with random particle motion.
  - ✦ By a supernova shock, the temperature can rise to more than $10^6$ K.

- Shock heating is the dominant heating mechanism in the HIM of the ISM and in the warm-hot intergalactic medium (WHIM).

# - Cooling -

- Decreasing the average kinetic energy of particles in the ISM is usually done by ***radiative cooling***.
  - In the CNM, cooling is performed by infrared photons emitted by carbon and oxygen.
    - ✦ Oxygen is nearly all in the form of neutral O I. (the ionization energy = 13.26 eV)
    - ✦ Carbon will be nearly all in the form of singly ionized C II. (ionization energy = 11.26 eV) The background starlight in our galaxy has enough photons in the relevant energy range $11.26\,\mathrm{eV} < h\nu < 13.60\,\mathrm{eV}$ to keep the C atoms ionized.

- [C II] 158µm (collisionally excited line emission)
  - The electronic ground state of C II is split into two fine levels, separated by an energy $E_{u\ell} = 7.86 \times 10^{-3}\,\mathrm{eV}$, which corresponds to $\lambda = 158\,\mu\mathrm{m}$ and $T = E_{u\ell}/k = 91.2\,\mathrm{K}$.
  - The upper level is populated by collisions with hydrogen atoms and free electrons.
  - If C II is excited by collisions with free electrons, the cooling function is given by, for a C abundance $n_\mathrm{C}/n_\mathrm{H} = 3 \times 10^{-4}$,

$$\frac{\Lambda^{e}_{[\mathrm{CII}]}}{10^{-25}\,\mathrm{erg\ cm^3\ s^{-1}}} \approx 0.03 \left(\frac{x}{10^{-3}}\right) \left(\frac{T}{100\,\mathrm{K}}\right)^{-1/2} \exp\left(-\frac{91.2\,\mathrm{K}}{T}\right)$$

Here, $x = n_e/n$ is the ionization fraction.

- If the C II is excited by collisions with hydrogen atoms, the cooling function is

$$\frac{\Lambda^{\mathrm{H}}_{[\mathrm{CII}]}}{10^{-25}\,\mathrm{erg\ cm^3\ s^{-1}}} \approx 0.06\left(\frac{T}{100\,\mathrm{K}}\right)^{0.13}\exp\left(-\frac{91.2\,\mathrm{K}}{T}\right)$$

- In the CNM, both contribute significantly to the excitation of C II.

- [O I] 63.2µm (collisionally excited emission line)
  - The electronic ground state of O I has a fine splitting of $E_{u\ell}/k = 228\,\mathrm{K}$.
  - The upper level is populated primarily by collisions with hydrogen atoms.
  - The resulting cooling function due to the emission of 63.2µm is, for an abundance of $n_{\mathrm{O}}/n_{\mathrm{H}} = 5.4\times10^{-4}$,

$$\frac{\Lambda^{\mathrm{H}}_{[\mathrm{OI}]}}{10^{-25}\,\mathrm{erg\ cm^3\ s^{-1}}} \approx 0.04\left(\frac{T}{100\,\mathrm{K}}\right)^{0.42}\exp\left(-\frac{228\,\mathrm{K}}{T}\right)$$

- Note:
  - [C II] and [O I] are the dominant form of cooling in molecular clouds and the CNM.
  - Molecular clouds can also cool by emission from the vibrational and rotational transitions of molecules.

- Ly$\alpha$ 1216Å
  - The first excited level of atomic hydrogen is $E_{21} = 10.20\,\mathrm{eV}$ above the ground state.
  - Although the first excited level will not be highly populated by collisions until the temperature reaches $T \sim E_{21}/k = 118{,}000\,\mathrm{K}$, hydrogen is extremely abundant. Thus the calling by Ly$\alpha$ can compete with cooling by IR fine-structure lines at temperature as low as T ~ 8000 K.
  - The cooling function for H excited by collisions with free electrons is

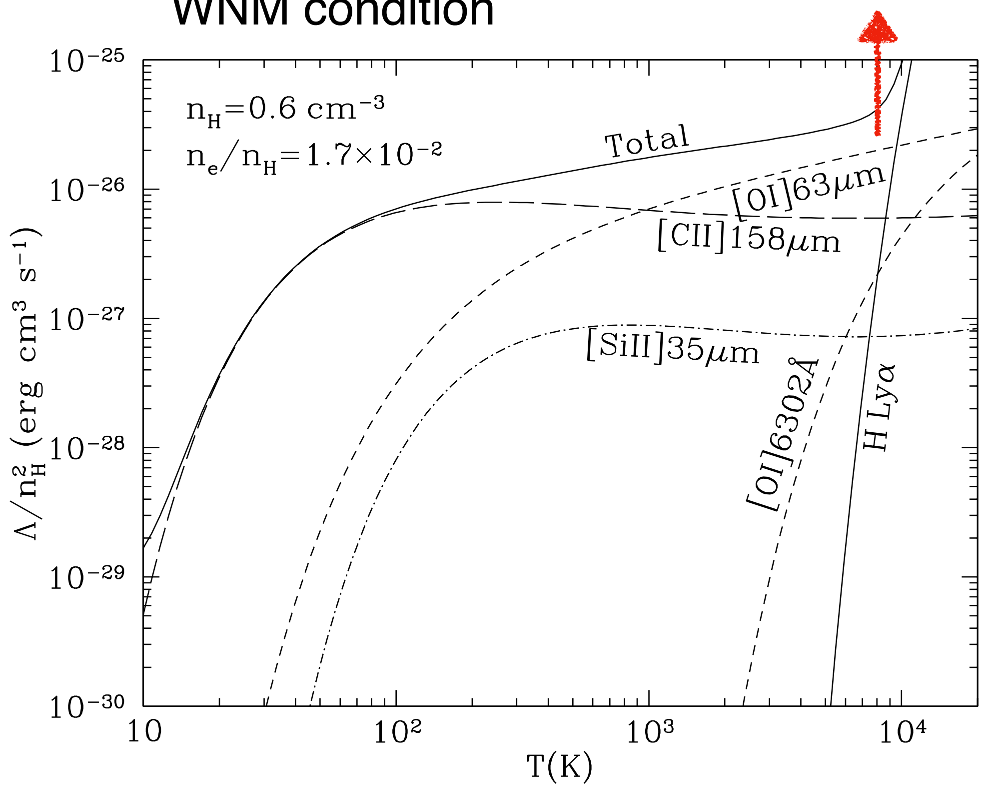
$$\frac{\Lambda^{\mathrm{e}}_{[\mathrm{Ly}\alpha]}}{10^{-25}\,\mathrm{erg\ cm^3\ s^{-1}}} \approx 7000\left(\frac{x}{10^{-3}}\right)\left(\frac{T}{100\,\mathrm{K}}\right)^{-0.5}\exp\left(-\frac{118{,}000\,\mathrm{K}}{T}\right)$$

- When T > 15,000 K,
  - atomic hydrogen can be collisionally ionized, followed by radiative recombination to a high energy level, and followed by a cascade down to the ground state.
  - The recombination lines are an important cooling mechanism in the WNM and WIM.
  - These phases are also cooled by line emission from more highly ionized atoms such as O III, C IV, and O VI.

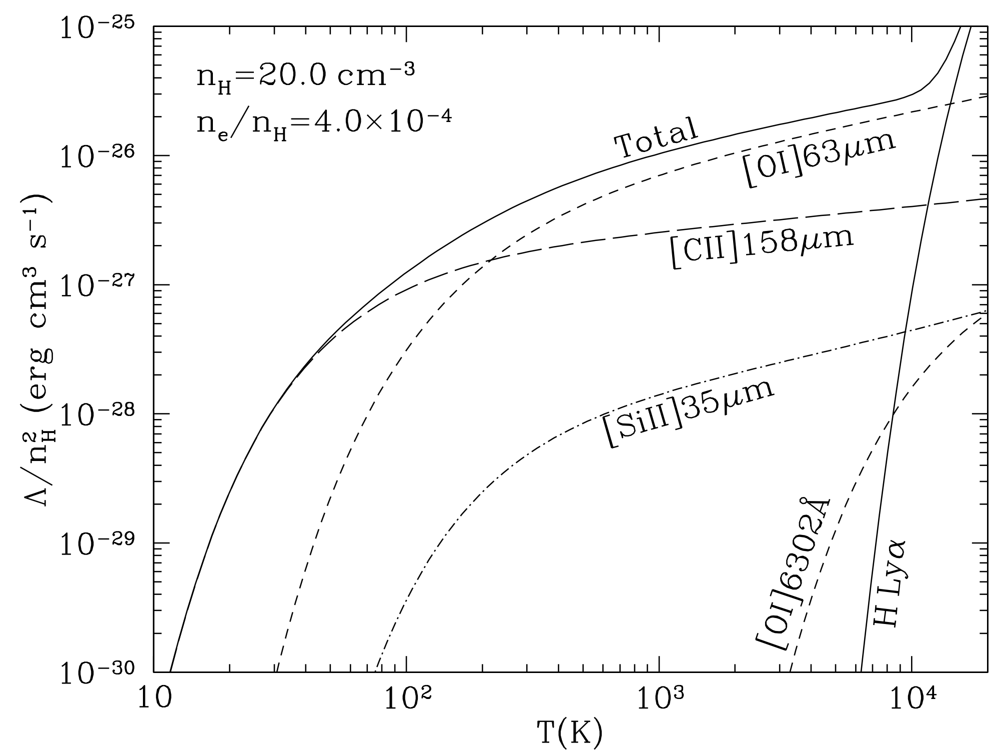
- Thermal Bremsstrahlung
  - In the HIM at T > $10^6$ K, the “braking radiation” emitted by electrons when they are accelerated by other charged particles can be a significant cooling mechanism.
  - The cooling function is $\Lambda \propto T^{1/2}$.
- Cooling Function

Onset of Ly$\alpha$ at T ~ 8,000 K

WNM condition




CNM condition




  - For 10 < T < $10^4$ K, [C II] 158µm line is a major coolant. The [O I] 63µm line is important for T > 100 K. Ly$\alpha$ cooling dominates only at T > $10^4$ K.

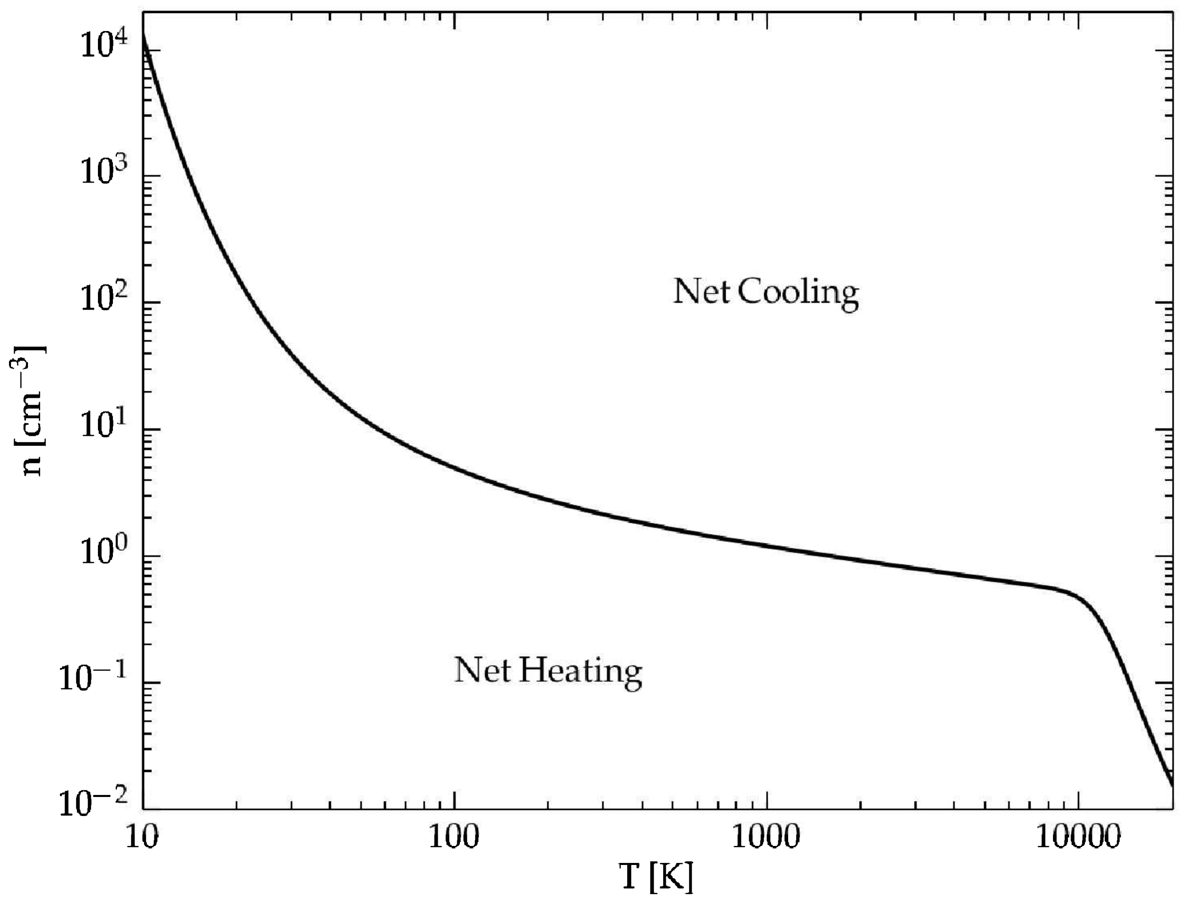
# Stable & Unstable Equilibrium

- A thermal equilibrium must have heating and cooling balanced: $g = \ell$.
  - We assume ***photoelectric heating by dust*** and ***cooling by [C II], [O I], and Ly$\alpha$***. Then, the equilibrium density is obtained by

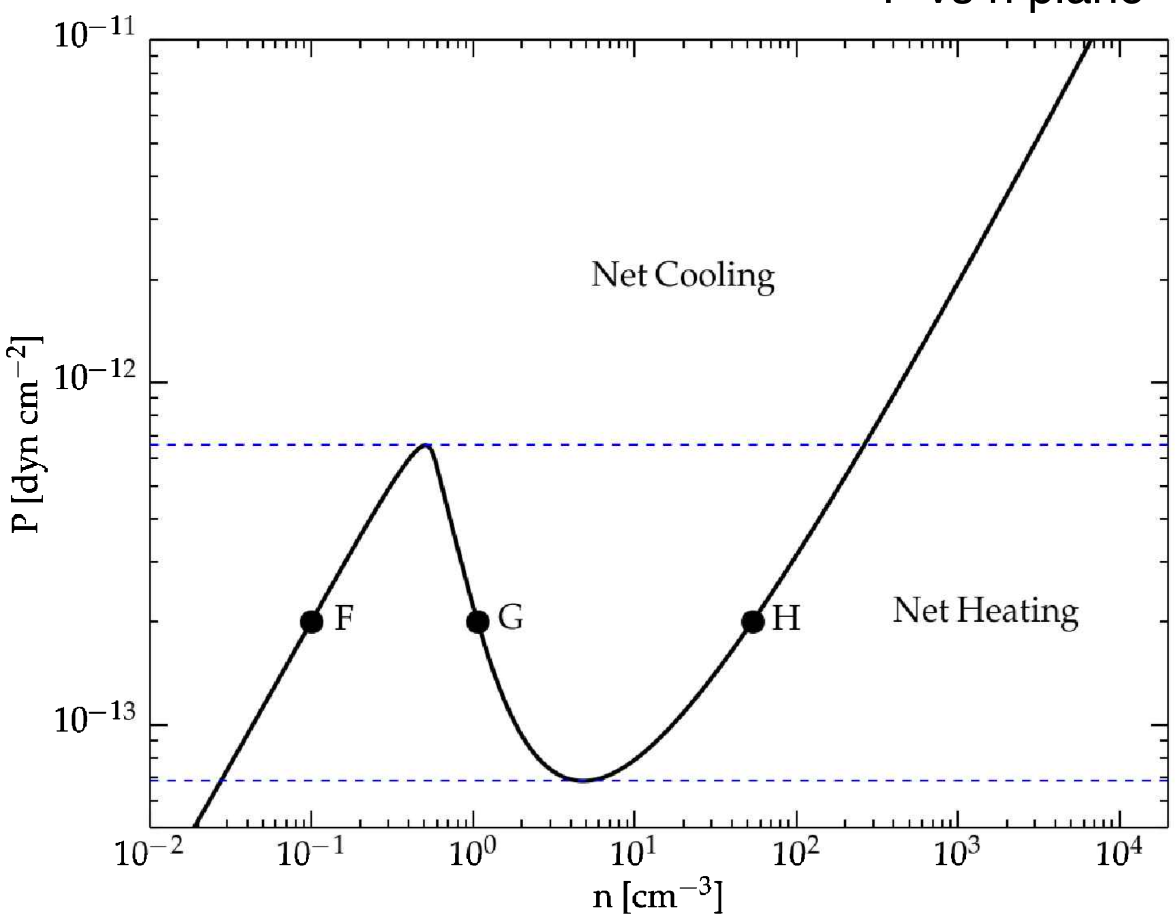
$$n_{\rm eq} G = n_{\rm eq}^2 \Lambda \quad \rightarrow \quad n_{\rm eq}(T) = \frac{G}{\Lambda(T)}$$

Note that G is a (nearly) constant.

n vs T plane



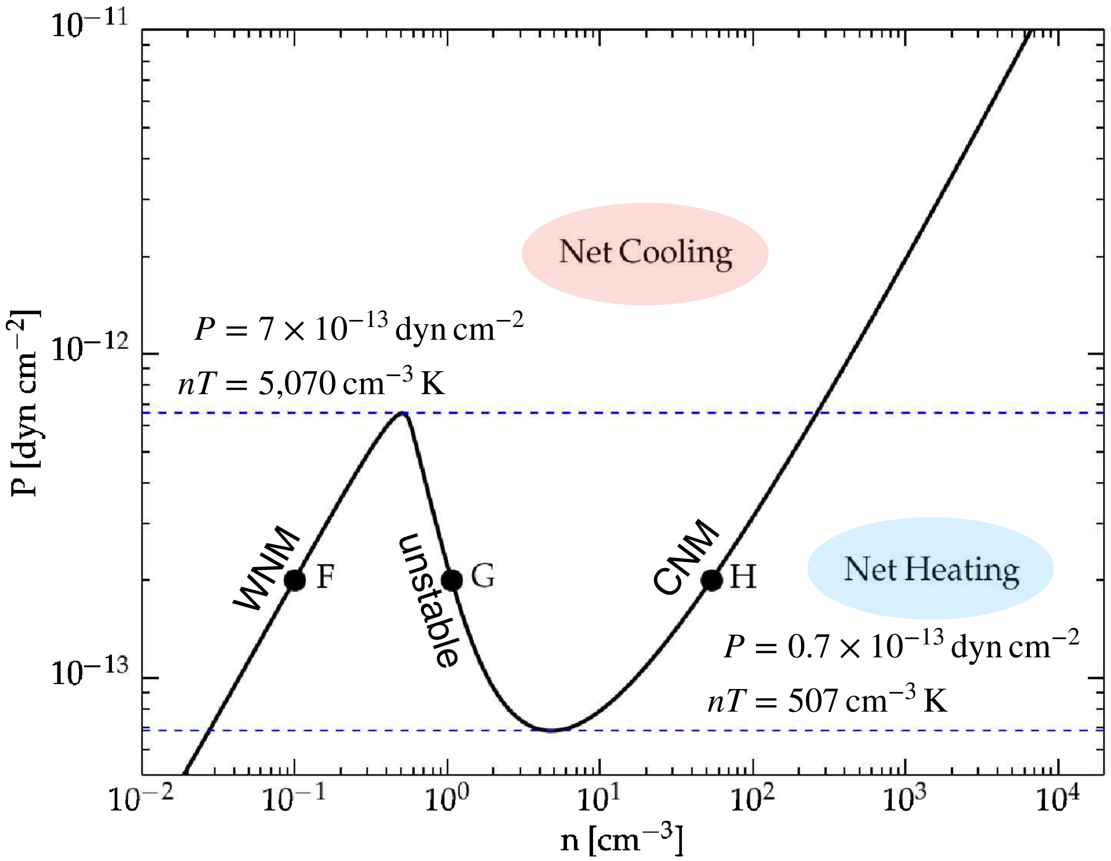

P vs n plane




- If every point along the above equilibrium line represented a stable equilibrium, then there could be a continuous distribution of temperatures, and thus of number densities.
- However, it's not the case. Not every equilibrium point is a stable equilibrium.

# - Pressure Equilibrium

- Let's assume that the interstellar gas is in pressure equilibrium.
  - For pressures in the range $0.7 \times 10^{-13}\,\mathrm{dyn\,cm^{-2}} < P < 7 \times 10^{-13}\,\mathrm{dyn\,cm^{-2}}$, bounded by the dashed lines, there are three possible values of $n_{\mathrm{eq}}$ at a fixed pressure.
  - Consider what happens at a point, for instance F, if you slightly change the temperature while keeping the pressure fixed.
    - If T increases, n must decrease, and you must move left from point F. This moves you into the net cooling portion, and T consequently decreases.
    - If T decrease, n must increase, and this moves you rightward into the net heating portion, and T consequently increases.
    - Thus, a negative feedback restores the original temperature.
  - A similar negative feedback maintains temperature stability at point H.
  - However, now consider what happens at G.
    - If T increases, n must decrease, and you must move left from point G. This moves you into the net heating portion, and T increases further, until you reach F.
    - If T decrease, n must increase, and this moves you rightward into the net cooling portion, and T decrease further, until you reach H.
    - Thus, a positive feedback makes the point unstable.
  - **Consequently, we have two stable equilibrium points (F and H). F = WNM, H = CNM**



# - History: Two-Phase Model & Three-Phase Model

- As a result of their analysis, Field, Goldsmith, and Having (1969) created a two-phase model of the ISM, consisting of Cold Neutral Clouds, with $n \sim 10\ \mathrm{cm}^{-3}$ and $T \sim 100$ K, embedded within a Warm Intercloud Medium, with $n \sim 0.1\ \mathrm{cm}^{-3}$ and $T \sim 10{,}000$ K.

- They were unaware of the role played by dust in heating the ISM, assumed that ***collisional ionization by cosmic rays provided the bulk of the heating***.

- FGH (1969) advocated a two-phase model. However, they also speculated “an existence of a third stable phase at $T > 10^6$ K, with bremsstrahlung the chief cooling process.”

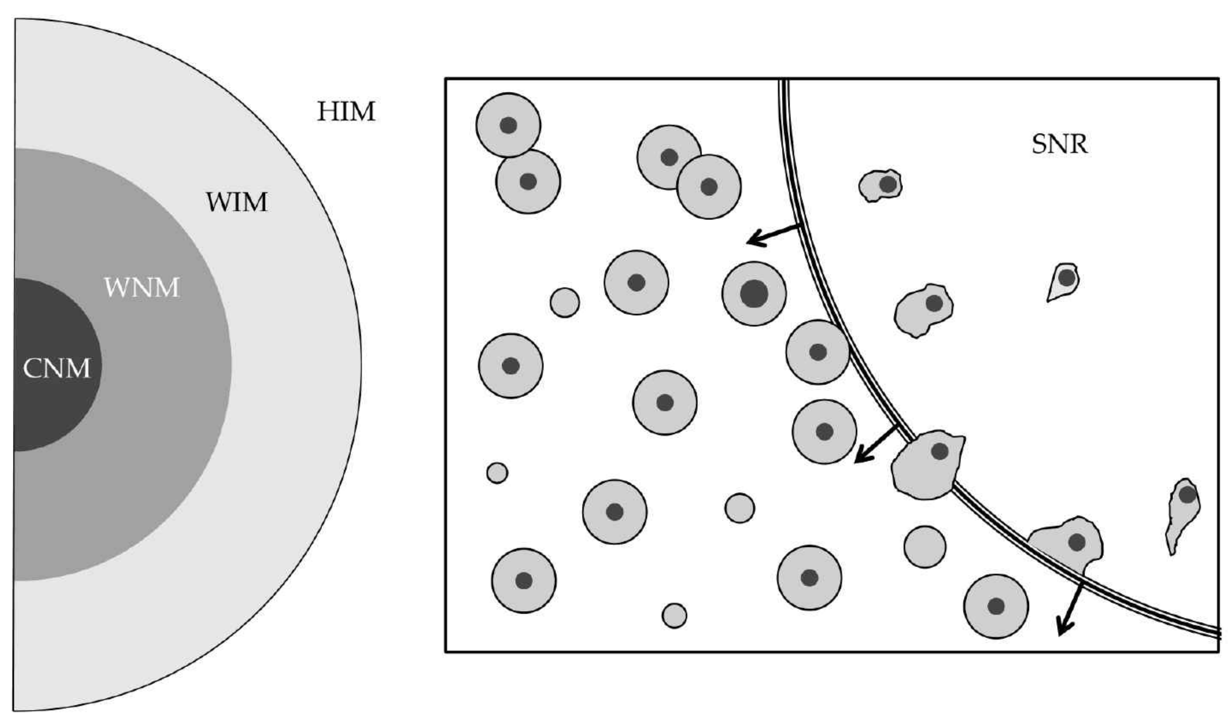
- In the 1970s, detection of a diffuse soft X-ray background and of emission lines such as O VI 1032, 1038Å hinted at the existence of interstellar gas with $T \sim 10^6$ K. In fact, the Sun resides in a “Local Bubble” of hot gas, with $T \sim 10^6$ K and $n \sim 0.004\ \mathrm{cm}^{-3}$.

- Cox & Smith (1974) suggested that supernova remnants could produce a bubbly hot phase, and that the bubbles blown by supernovae would have a porosity factor (volume fraction of the ISM occupied by hot bubbles):

$$q > 0.1 \left( \frac{r_{\mathrm{SN}}}{10^{-13}\,\mathrm{pc}^{-3}\,\mathrm{yr}^{-1}} \right)$$

# - History: McKee & Ostriker's Three-Phase Model

- McKee & Ostriker (1977)
  - They made a more elaborate argument for three phases within the ISM.
  - ***Cold Neutral Medium***, with $T \sim 80\,\mathrm{K}$, $n \sim 40\,\mathrm{cm}^{-3}$, and a low fractional ionization $x = n_e/n \sim 0.001$.
  - ***Warm Medium***, containing both ionized and neutral components, $T \sim 8000\,\mathrm{K}$ and $n \sim 0.3\,\mathrm{cm}^{-3}$, the ionization fraction ranging from $x \sim 0.15$ in the neutral component (WNM) to $x \sim 0.15$ in the ionized component (WIM).
  - ***Hot Ionized Medium***, consisting of the overlapping supernova bubbles, with $T \sim 10^6\,\mathrm{K}$ and $n \sim 0.002\,\mathrm{cm}^{-3}$, and $x \sim 1$ (nearly complete ionization).

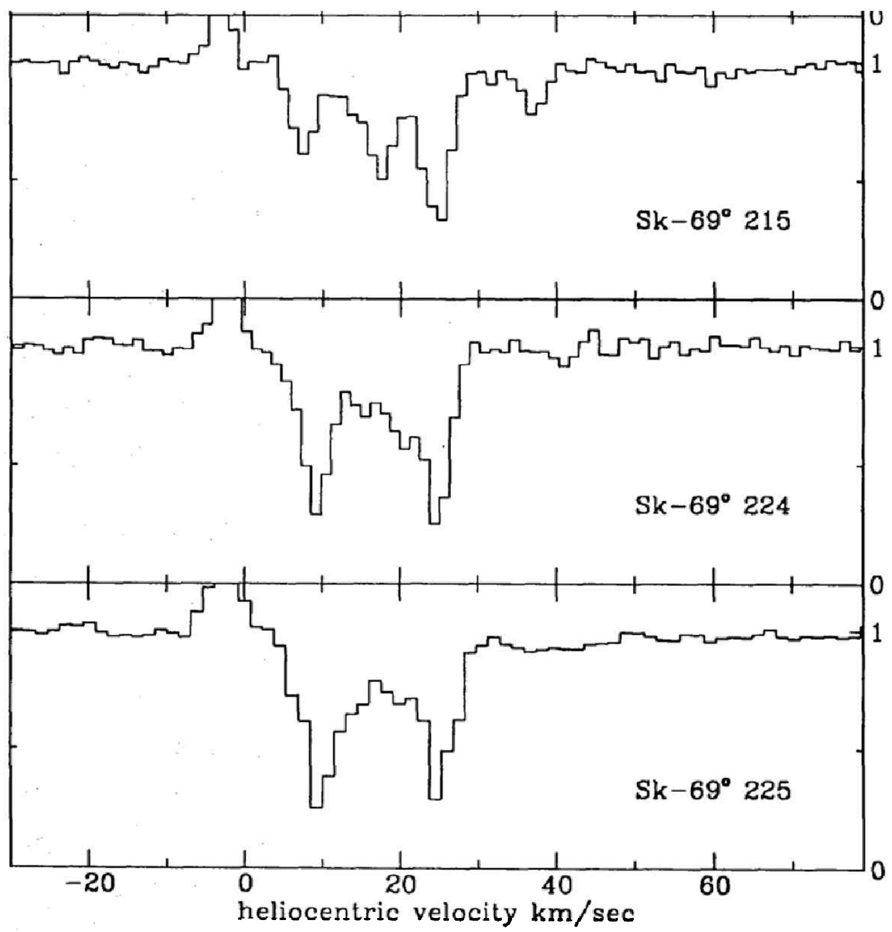



- However, in many ways, the ISM is a dynamic, turbulent, dusty, magnetized place.

# Atomic Gas / Hydrogen Gas

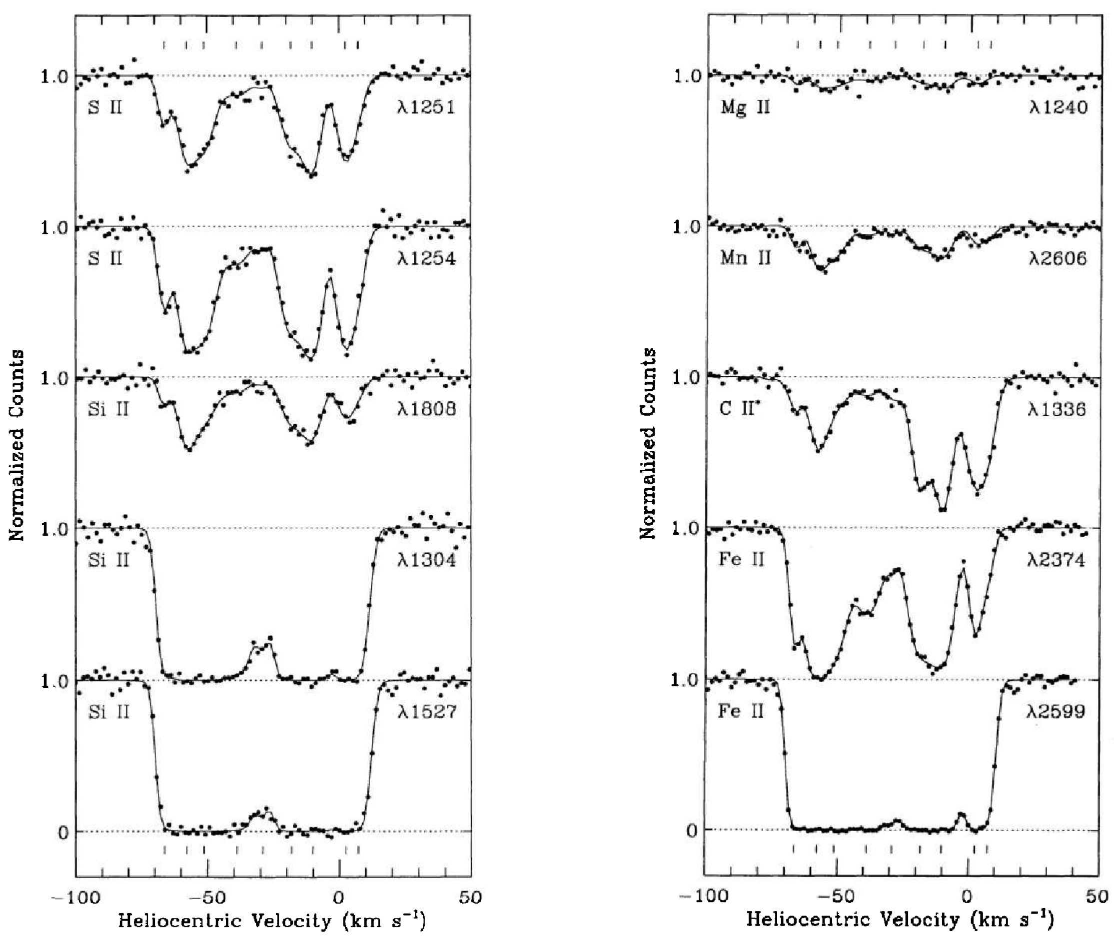
# Observations of Absorption Lines Toward the CNM

- The CNM gives rise to a number of absorption features in the spectra of hot background stars.
  - The most prominent absorption lines at visible wavelengths are Ca II K and H lines at $\lambda = 3933, 3968\ \text{Å}$, and Na I $D_1$ and $D_2$ doublet lines at $\lambda = 5890, 5896\ \text{Å}$.



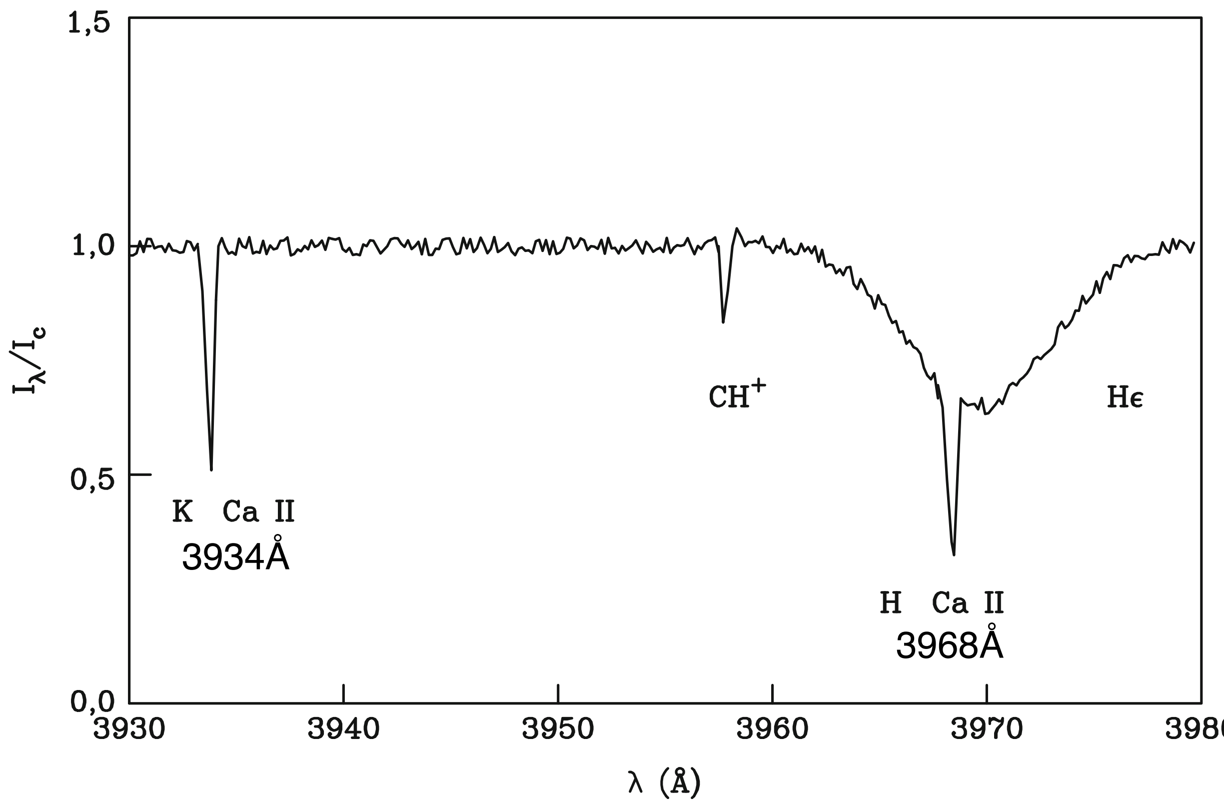

Na I $D_2$ interstellar absorption line seen along 3 lines of sight to stars in LMC (Molaro et al. 1993)

[Note] The cold gas is ~100 pc away from Earth.




UV interstellar absorption lines toward an O-type star HD93521. (Spitzer & Fitzpatrick 1993)

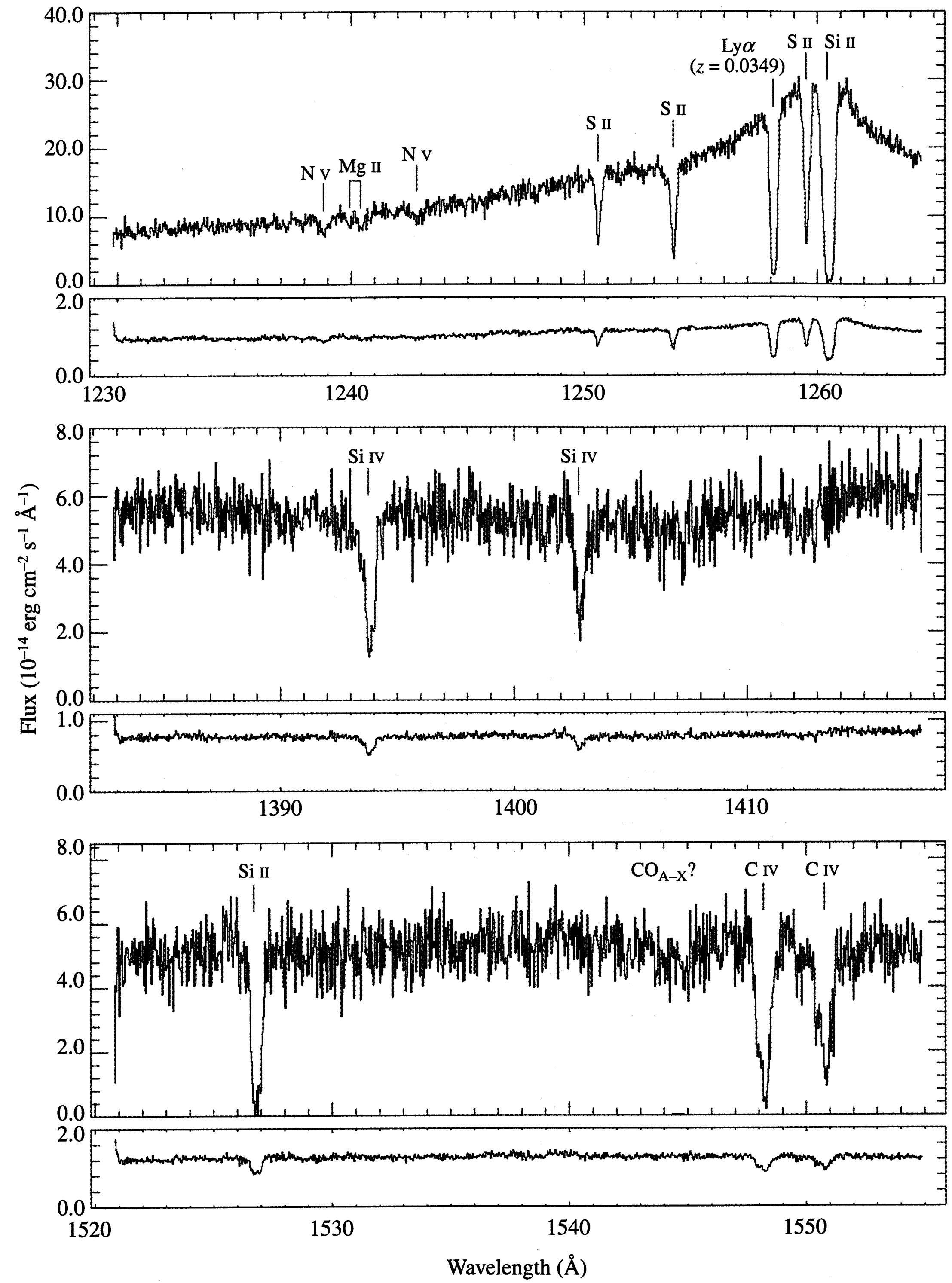
[Note] (1) multiple velocity components and (2) line saturation on Si II and Fe II.
The multiple velocities are due primarily to the differential rotation of our galaxy. (clouds at different distances)




Interstellar absorption lines in the spectrum of $\zeta$ Oph (O9.5V).

Note that the Ca II H line occurs inside the H$\varepsilon$ hydrogen line, which is much broader and of stellar origin.

Figure 4.6 in Astrophysics of the Interstellar Medium [Maciel]



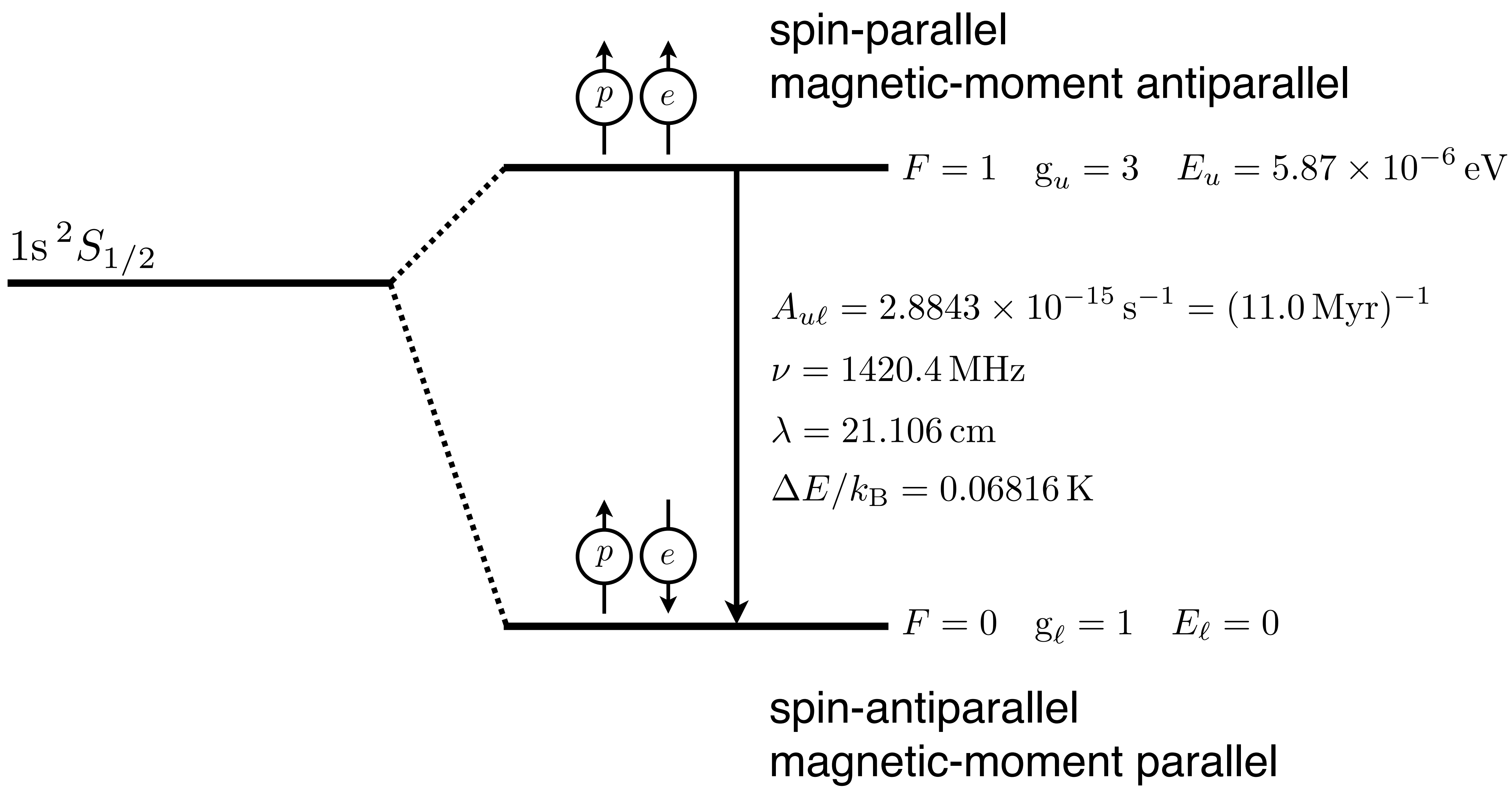

Interstellar absorption lines toward the Seyfert 1 galaxy ESO 141-055.

Figure 5.5 in Physics and Chemistry of the Interstellar Medium [Kwok]

# 21 cm hyperfine line

- The CNM and WNM, taken together, provide over half the mass of the ISM.
  - H is the most abundant element in the universe. In the CNM and WNM, most of the hydrogen is in the form of neutral atoms.
  - The Ly$\alpha$ line of H provides a useful probe of the properties of the CNM and WNM. However, at its wavelength the Earth's atmosphere is highly opaque, and thus observing Ly$\alpha$ absorption requires orbiting UV satellites. In addition, Ly$\alpha$ can be seen in absorption only along those lines of sight toward sources with a high UV flux.
  - To do a global survey of atomic hydrogen in the galaxy, we need some way of easily detecting radiation from hydrogen, regardless of its kinetic temperature or number density.
  - Such a way was first found in 1944, by Henk van de Hulst.
    - He attempted to find emission lines at the wavelengths ~ 1 cm to 20 m, at which the Earth's atmosphere is transparent. He then realized that the hyperfine structure line resulting from a flip of the electron spin within a hydrogen atom should have a wavelength of 21 cm.
    - This was confirmed by Harold Ewen and Edward Purcell in 1951, when they first detected 21 cm emission from the Milky Way.

# Hyperfine splitting of the 1s ground state of atomic H



# Difference between Ly$\alpha$ and 21 cm transitions

- The excitation energy for Ly$\alpha$ (E = 10.2 eV, E/k = 118,000 K) is much higher than the kinetic temperature of the neutral ISM.

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{118,000\,\mathrm{K}}{T}\right) = 1.7 \times 10^{-51} \text{ at } T = 1000\,\mathrm{K}$$

  - Collisional excitation is unimportant, and most hydrogen atoms are in the lower level of the Ly$\alpha$ transition.
  - The Ly$\alpha$ has a higher energy by a factor of $1.7\mathrm{x}10^6$ than the 21 cm.

- The excitation energy for 21 cm is ~ 5.9 μeV, and its equivalent temperature E/k = 0.068 K is much lower than the temperature of the cosmic microwave background.
  - Even the CMB is able to populate the upper level.
  - If collisions are frequent, then the spin temperature will be solely determined by collisions, and thus will be a good tracer of the gas kinetic temperature.
  - Thus, there is ample opportunity to populate the upper energy level of the 21 cm hyperfine transition. The level populations for the 21 cm levels, since $T_{\mathrm{exc}} \gg 0.068\,\mathrm{K}$ in all circumstances of the ISM.

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} e^{-h\nu/kT_{\mathrm{exc}}} = 3\,e^{-0.068\,\mathrm{K}/T_{\mathrm{exc}}} \simeq 3 \longrightarrow \boxed{n_u \simeq \frac{3}{4} n_{\mathrm{H}}, \; n_\ell \simeq \frac{1}{4} n_{\mathrm{H}}}$$

  - However, in many cases (in particular in WNM), the hyperfine levels may not be in excitation equilibrium. Radio astronomers use the term ***spin temperature*** for 21 cm rather than the “excitation temperature.”

# Emissivity and Optical Depth

- ***Emissivity***:
  - The upper level contains ~ 75% of the H I under all conditions of interest, and thus *the 21-cm emissivity is effectively independent of the spin temperature*.

$$j_\nu = n_u \frac{A_{u\ell}}{4\pi} h\nu_{u\ell}\phi_\nu \simeq \frac{3}{16\pi} A_{u\ell} h\nu_{u\ell} n_{\mathrm{H}} \phi_\nu \qquad \left(n_u \simeq \frac{3}{4} n_{\mathrm{H}}\right)$$

- ***Optical depth***

$$\kappa_\nu = n_\ell \sigma_{\ell u} - n_u \sigma_{u\ell} = n_\ell \sigma_{\ell u} \left(1 - e^{-h\nu_{u\ell}/kT_{\mathrm{spin}}}\right)$$

Because $h\nu_{u\ell}/kT_{\mathrm{spin}} \ll 1$ for all conditions of interest, the correction for stimulated emission is very important!

$$\kappa_\nu \simeq n_\ell \sigma_{\ell u} \frac{h\nu_{u\ell}}{kT_{\mathrm{spin}}} \ll n_\ell \sigma_{\ell u} \longleftarrow e^{-h\nu_{u\ell}/kT_{\mathrm{spin}}} \simeq 1 - k\nu_{u\ell}/kT_{\mathrm{spin}}$$

$$\kappa_\nu \simeq \left(\frac{1}{4} n_{\mathrm{H}}\right) \left(\frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{u\ell}^2} A_\ell \phi_\nu\right) \frac{h\nu_{u\ell}}{kT_{\mathrm{spin}}} \qquad \left(n_\ell \simeq \frac{1}{4} n_{\mathrm{H}}\right)$$

$$= \frac{3}{32\pi} A_{u\ell} \frac{hc\,\lambda_{u\ell}}{kT_{\mathrm{spin}}} n_{\mathrm{H}} \phi_\nu$$

*The absorption coefficient is inversely proportional to the spin temperature.*

- Typical optical depths of the 21-cm line:

$$\tau_0 = 0.311 \left( \frac{N_{\mathrm{H\,I}}}{10^{21}\,\mathrm{cm}^{-2}} \right) \left( \frac{100\,\mathrm{K}}{T_{\mathrm{spin}}} \right) \left( \frac{10\,\mathrm{km\,s}^{-1}}{b} \right)$$

- In the CNM, a typical spin temperature is $T_{\mathrm{spin}} \approx 50 - 100\,K$ :

$$\tau_0^{\mathrm{CNM}} \approx 0.3 - 0.6$$
$$e^{-\tau_0} \approx 0.55 - 0.74$$

***The CNM is in general optically thin, but show significant absorption.***

- In the WNM, a typical spin temperature is $T_{\mathrm{spin}} \approx 5000 - 8000\,K$ :

$$\tau_0^{\mathrm{WNM}} \approx 0.004 - 0.006$$
$$e^{-\tau_0} \approx 0.995$$

***The 21-cm absorption is negligible in the WNM.***

# Ionization Equilibrium

- ***Photoionization Equilibrium***:
  - Balance between photo-ionization and the process of recombination.

- ***Collisional Ionization Equilibrium (CIE)*** or coronal equilibrium
  - Balance at a given temperature between collisional ionization from the ground states of the various atoms and ions, and the process of recombination from the higher ionization stages.
  - In this equilibrium, effectively, all ions are in their ground state.

- Ionization balance under conditions of local thermodynamic equilibrium (LTE)
  - The ionization equilibrium in LTE is described by the ***Saha equation***.
  - In LTE, the excited states are all populated according to Boltzmann's law.

# Introduction to Ionized Hydrogen Regions

- Ionized atomic hydrogen regions, broadly termed “H II regions”, are composed of gas ionized by photons with energies above the hydrogen ionization energy of 13.6 eV.
  - ***Ionization Bounded:*** These objects include “***classical H II regions***” ionized by hot O or B stars (or clusters of such stars) and associated with regions of recent massive-star formation, and “planetary nebulae”, the ejected outer envelopes of AGB stars photoionized by the hot remnant stellar core.
  - ***Density Bounded: Warm Ionized Medium*** / Diffuse Ionized Gas: Ionized Gas in the diffuse ISM, far away from OB associations.
  - The UV, visible and IR spectra of H II regions are very rich in emission lines, primarily collisional excited lines of metal ions and recombination lines of hydrogen and helium. H II regions are also observed at radio wavelengths, emitting radio free-free emission from thermalized electrons and radio recombination lines from highly excited states of H, He, and some metals (e.g., H109$\alpha$ and C lines).
- Three processes govern the physics of H II regions:
  - ***Photoionization Equilibrium***: the balance between photoionization and recombination. This determines the spatial distribution of ionic states of the elements in the ionized zone.
  - ***Thermal Balance*** between heating and cooling. Heating is dominated by photoelectrons ejected from hydrogen and helium with thermal energies of a few eV. Cooling is mostly dominated by electron-ion impact excitation of metal ion followed by emission of “forbidden” lines from low-lying fine structure levels. It is these cooling lines that give H II regions their characteristic spectra.
  - ***Hydrodynamics***, including shocks, ionization and photodissociation fronts, and outflows and winds from the embedded stars.

# Case A and B (Radiative Recombination of Hydrogen)

- ***On-the-spot approximation:***
  - In optically thick regions, it is assumed that every photon produced by radiative recombination to the ground state of hydrogen is immediately, then and there, destroyed in photoionizing other hydrogen atom.
  - In the on-the-spot approximation, recombination to the ground state has no net effect on the ionization state of the hydrogen gas.
- Baker & Menzel (1938) proposed two limiting cases:
  - ***Case A:*** ***Optically thin*** to ionizing radiation, so that every ionizing photon emitted during the recombination process escapes. For this case, we sum the radiative capture rate coefficient $\alpha_{n\ell}$ over all levels $n\ell$.
  - ***Case B:*** ***Optically thick*** to radiation just above $I_{\rm H} = 13.60\,{\rm eV}$, so that ionizing photons emitted during recombination are immediately reabsorbed, creating another ion and free electron by photoionization. In this case, the recombinations directly to $n = 1$ do not reduce the ionization of the gas: ***only recombinations to*** $n \geq 2$ ***act to reduce the ionization.***

  - **Case B in photoionized gas**: Photoionized nebulae around OB stars (H II regions) usually have large enough densities of neutral H. For this situation, case B is an excellent approximation.
  - **Case A in collisionally ionized gas**: Regions where the hydrogen is collisional ionized are typically very hot ($T > 10^6$ K) and contain a very small density of neutral hydrogen. For these shock-heated regions, case A is an excellent approximation.

- ***Radiative recombination rate coefficients***:
    - In Case A, the relevant radiative recombination rate coefficient is found by summing over all energy levels of the hydrogen atom:

$$\alpha_{\mathrm{A,H}}(T) \equiv \sum_{n=1}^{\infty} \sum_{\ell=0}^{n-1} \alpha_{n\ell}(T)$$
$$\approx 4.18 \times 10^{-13}\, T_4^{-0.721-0.021 \ln T_4}\ \left[\mathrm{cm}^3\,\mathrm{s}^{-1}\right] \ \text{ for } 0.3 \lesssim T_4 \lesssim 3 \quad \left(T_4 \equiv T/10^4\,\mathrm{K}\right)$$

    - In Case B, the relevant radiative recombination rate coefficient is found by summing over all energy levels other than the ground state:

$$\alpha_{\mathrm{B,H}}(T) \equiv \sum_{n=2}^{\infty} \sum_{\ell=0}^{n-1} \alpha_{n\ell}(T) = \alpha_{\mathrm{A,H}}(T) - \alpha_{1\mathrm{s}}(T)$$
$$\approx 2.59 \times 10^{-13}\, T_4^{-0.833-0.034 \ln T_4}\ \left[\mathrm{cm}^3\,\mathrm{s}^{-1}\right] \ \text{ for } 0.3 \lesssim T_4 \lesssim 3$$

    - The percentage of radiative recombinations that go directly to the ground state is 30% at $T = 3000$ K but increases to 46% at $T = 30{,}000$ K. Thus, the distinction between Case A and Case B becomes increasingly important at higher temperatures.

$$\frac{\alpha_{1\mathrm{s,H}}}{\alpha_{\mathrm{A,H}}} = 1 - \frac{\alpha_{\mathrm{B,H}}}{\alpha_{\mathrm{A,H}}} = 1 - 0.0619\, T_4^{-0.112-0.013 \ln T_4}$$

# H II Regions and Strömgren Spheres

- ***Strömgren Sphere***:
  - Following Strömgren (1939), we consider the simple idealized problem of a fully ionized, spherical region of uniform medium plus a central source of ionizing photons.
  - The ionization is assumed to be maintained by absorption of the ionizing photons radiated by a central hot star. The central source produces ionizing photons, with energy $\nu > \nu_0 = I_{\rm H}/h$ at a constant rate $Q_0$ [photons s$^{-1}$].
  - At a distance $r$ from the central star, the balance equation between ionization and recombination balance is

$$n_{\rm H^0} \int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu} \sigma_\nu d\nu = n_p n_e \alpha_{\rm B,H}$$

From the RT equation,

$L_\nu$ = luminosity of the central star at frequency $\nu$.

$$4\pi J_\nu = \underbrace{\frac{L_\nu}{4\pi r^2} e^{-\tau_\nu}}_{\text{geometrical attenuation + radiative absorption}}, \quad \text{where } \tau_\nu = \int_0^r n_{\rm H^0} \sigma_\nu dr$$

Integrating the balance equation over the whole volume:

$$\int_0^\infty \int_{\nu_0}^\infty \frac{L_\nu/h\nu}{4\pi r^2} e^{-\tau_\nu} n_{\rm H^0} \sigma_\nu d\nu (4\pi r^2) dr = \int_0^\infty n_p n_e \alpha_{\rm B,H} (4\pi r^2) dr$$

$$\int_{\nu_0}^\infty L_\nu/h\nu \left[ \int_0^\infty e^{-\tau_\nu} n_{\rm H^0} \sigma_\nu dr \right] d\nu = \int_0^\infty n_p n_e \alpha_{\rm B,H} (4\pi r^2) dr$$

The square bracket term in the left side is

$$\int_0^\infty e^{-\tau_\nu} n_{\mathrm{H}^0} \sigma_\nu dr = \int_0^\infty e^{-\tau_\nu} d\tau_\nu = 1$$

Then, we obtain

total number of ionizing photons

$$Q_0 = \int_0^\infty n_p n_e \alpha_{\mathrm{B,H}} dV, \quad \text{where } Q_0 \equiv \int_{\nu_0}^\infty \frac{L_\nu}{h\nu} d\nu \text{ and } dV = 4\pi r^2 dr$$

- Assuming that ***the ionization is nearly complete (*** $n_p = n_e = n_{\mathrm{H}}$ ***) within*** $R_s$, and nearly zero ( $n_{\mathrm{H}^0} = n_{\mathrm{H}},\ n_e = 0$ ) outside $R_s$, we obtain the size of the ionized region.

$$Q_0 = n_{\mathrm{H}}^2 \alpha_{\mathrm{B,H}} \frac{4\pi}{3} R_s^3$$

$$R_s = \left( \frac{3}{4\pi} \frac{Q_0}{\alpha_{\mathrm{B,H}} n_{\mathrm{H}}^2} \right)^{1/3}$$

$$= 3.17 \left( \frac{Q_0}{10^{49}\ \mathrm{photons\ s^{-1}}} \right)^{1/3} \left( \frac{n_{\mathrm{H}}}{10^2\ \mathrm{cm^{-3}}} \right)^{-2/3} \left( \frac{T}{10^4\ \mathrm{K}} \right)^{0.28} \quad [\mathrm{pc}]$$

The physical meaning of this is that ***the total number of ionizing photons emitted by the star balances the total number of recombinations within the ionized volume*** $(4\pi/3)R_s^3$ , often called the Strömgren sphere. It's radius $R_s$ is called the Strömgren radius.

# Ionization / Excitation Diagnostics: The BPT diagram

- Ionization / Excitation Mechanisms in galaxies
  - The optical line emission from star-forming galaxies is usually dominated by emission lines from H II regions.
  - Some galaxies have strong continuum and line emission from an active galactic nucleus (AGN). The line emission is thought to come from gas that is heated and ionized by X-rays from the AGN.
    - ***Seyfert galaxies:*** The AGN spectrum normally includes strong emission lines from high-ionization species like C IV and Ne V, which are presumed to be ionized by X-rays from the AGN. Seyfert (1943) discovered that some galaxies had extremely luminous, point-like nuclei, with emission line widths in some cases exceeding 4000 km/s.
    - ***LINERs*** (Low Ionization Nuclear Emission Region): In other cases, the nucleus has strong emission lines but primarily from low-ionization species. LINERs were first identified by Timothy Heckman (1980). [There are debates on the sources of ionization and line emission; AGN or star-forming regions, shock or photoionization]
- ***BPT diagram***:
  - Baldwin, Phillips & Terlevich (1981) found that one could distinguish star-forming galaxies from galaxies with spectra dominated by AGNs by plotting the ratio of [OIII]5008/Hβ vs. [NII]6585/Hα.
  - These lines are among the strongest optical emission lines from H II regions.
  - The line ratios employ pairs of lines with similar wavelengths so that the line ratios are nearly unaffected by dust extinction.

- The structure of H and He ionization zone:
  - In H II regions where He is neutral (no photons with E > 24.6 eV), N and O will be essentially 100% singly ionized throughout the H ionization zone.
  - On the other hand, for O stars that are hot enough (24.6 < E < 54.6 eV) to have an appreciable zone of He ionization, the N and O in this zone can be doubly ionized.
  - Because **N and O have similar second ionization potentials** (29.6 and 35.1 eV for N and O, respectively), to a good approximation, HII regions will have:

$$\mathrm{N}^{+}/\mathrm{N} \approx \mathrm{O}^{+}/\mathrm{O} \quad \text{and} \quad \mathrm{N}^{+2}/\mathrm{N} \approx \mathrm{O}^{2+}/\mathrm{O}$$

  - Essentially all of the gas-phase O and N in the H II region will be either singly or doubly ionized. Hydrogen will fully ionized in the H II region:

$$n(\mathrm{N}) = n(\mathrm{N}^{+}) + n(\mathrm{N}^{2+}), \quad n(\mathrm{O}) = n(\mathrm{O}^{+}) + n(\mathrm{O}^{2+}), \quad \text{and} \quad n(\mathrm{H}) = n(\mathrm{H}^{+})$$

  - Let's define the fraction of doubly-ionized ion.

$$\xi_{\mathrm{N}} \equiv \frac{n(\mathrm{N}^{+2})}{n(\mathrm{N}^{+}) + n(\mathrm{N}^{+2})} = \frac{n(\mathrm{N}^{+2})}{n(\mathrm{N})}$$

$$\xi_{\mathrm{O}} \equiv \frac{n(\mathrm{O}^{+2})}{n(\mathrm{O}^{+}) + n(\mathrm{O}^{+2})} = \frac{n(\mathrm{O}^{+2})}{n(\mathrm{O})}$$

Then, the fractions are approximately equal:

$$\xi_{\mathrm{N}} \approx \xi_{\mathrm{O}} \quad \Longrightarrow \quad \xi$$

- We assume the N abundance to be solar, and the O abundance to be 80% solar (20% is presumed to be in silicate grains).

- In terms of the fraction,

$$\frac{n(\mathrm{N}^+)}{n(\mathrm{H}^+)} = (1-\xi)\frac{n(\mathrm{N})}{n(\mathrm{H})} \qquad\qquad \frac{n(\mathrm{O}^{2+})}{n(\mathrm{H}^+)} = \xi\frac{n(\mathrm{O})}{n(\mathrm{H})}$$

- Then, the line ratios can be written:

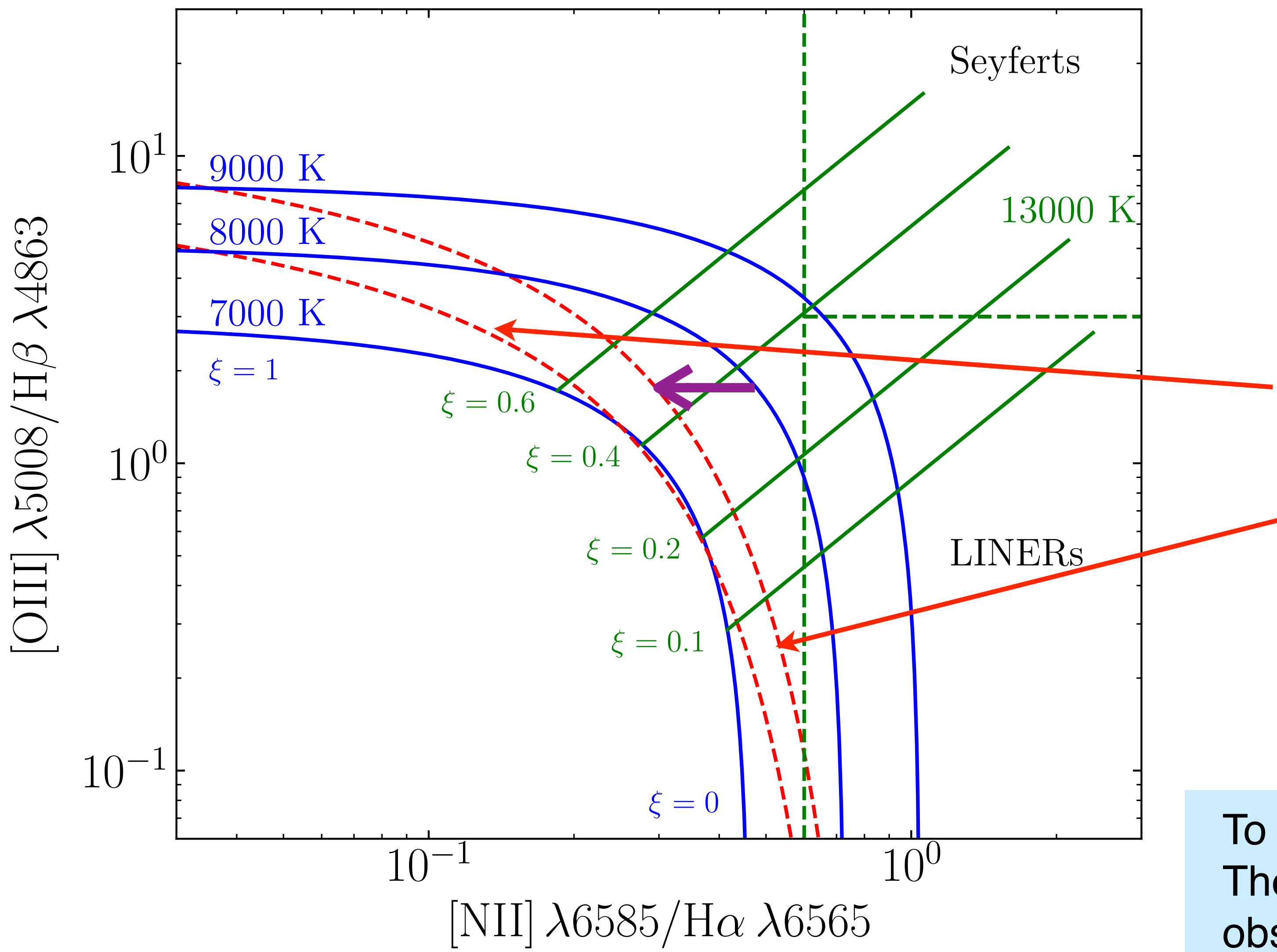
$$\frac{[\mathrm{O\,III}]\,5008}{\mathrm{H}\beta} = 218.7\,\xi\,T_4^{0.494+0.089\ln T_4} e^{-2.917/T_4}\left(\frac{n_\mathrm{O}/n_\mathrm{H}}{0.8\times 5.37\times 10^{-4}}\right)$$

$$\frac{[\mathrm{N\,II}]\,6585}{\mathrm{H}\alpha} = 12.44\,(1-\xi)\,T_4^{0.495+0.040\ln T_4} e^{-2.185/T_4}\left(\frac{n_\mathrm{N}/n_\mathrm{H}}{7.41\times 10^{-5}}\right)$$

- Then, for an assumed temperature T, we can produce a theoretical curve of [OIII]5008/Hβ versus [NII]6585/Hα by varying the fraction ξ of the N and O that is doubly ionized.

The theoretical curve of [OIII]5008/Hβ versus [NII]6585/Hα that is obtained by varying the fraction is shown below:

Blue lines show the tracks of the equations calculated, by varying ξ from 0 to 1, for $T$ = 7000, 8000, and 9000 K.




Empirical curves that discriminate the star-forming galaxies from AGNs.

$$\log_{10}([\mathrm{OIII}]/\mathrm{H}\beta) = 1.10 - \frac{0.60}{0.01 - \log_{10}([\mathrm{NII}]/\mathrm{H}\beta)}$$

$$\log_{10}([\mathrm{OIII}]/\mathrm{H}\beta) = 1.3 - \frac{0.61}{0.05 - \log_{10}([\mathrm{NII}]/\mathrm{H}\beta)}$$

Kauffman et al. (2003, MNRAS, 346, 1055)

To derive the equation, we assumed that $\xi_{\mathrm{N}} = \xi_{\mathrm{O}} = \xi$.
The discrepancy between the simple model with the observations would be due to the assumption.
We need to note that $E(\mathrm{N}^{+} \to \mathrm{N}^{2+}) < E(\mathrm{O}^{+} \to \mathrm{O}^{2+})$, which implies that $\xi_{\mathrm{N}} \gtrsim \xi_{\mathrm{O}}$.

The arrow ← indicates the direction that is expected from $\xi_{\mathrm{N}} > \xi_{\mathrm{O}}$.

- Line ratios for 122,514 galaxies in SDSS DR7 with S/N > 5.

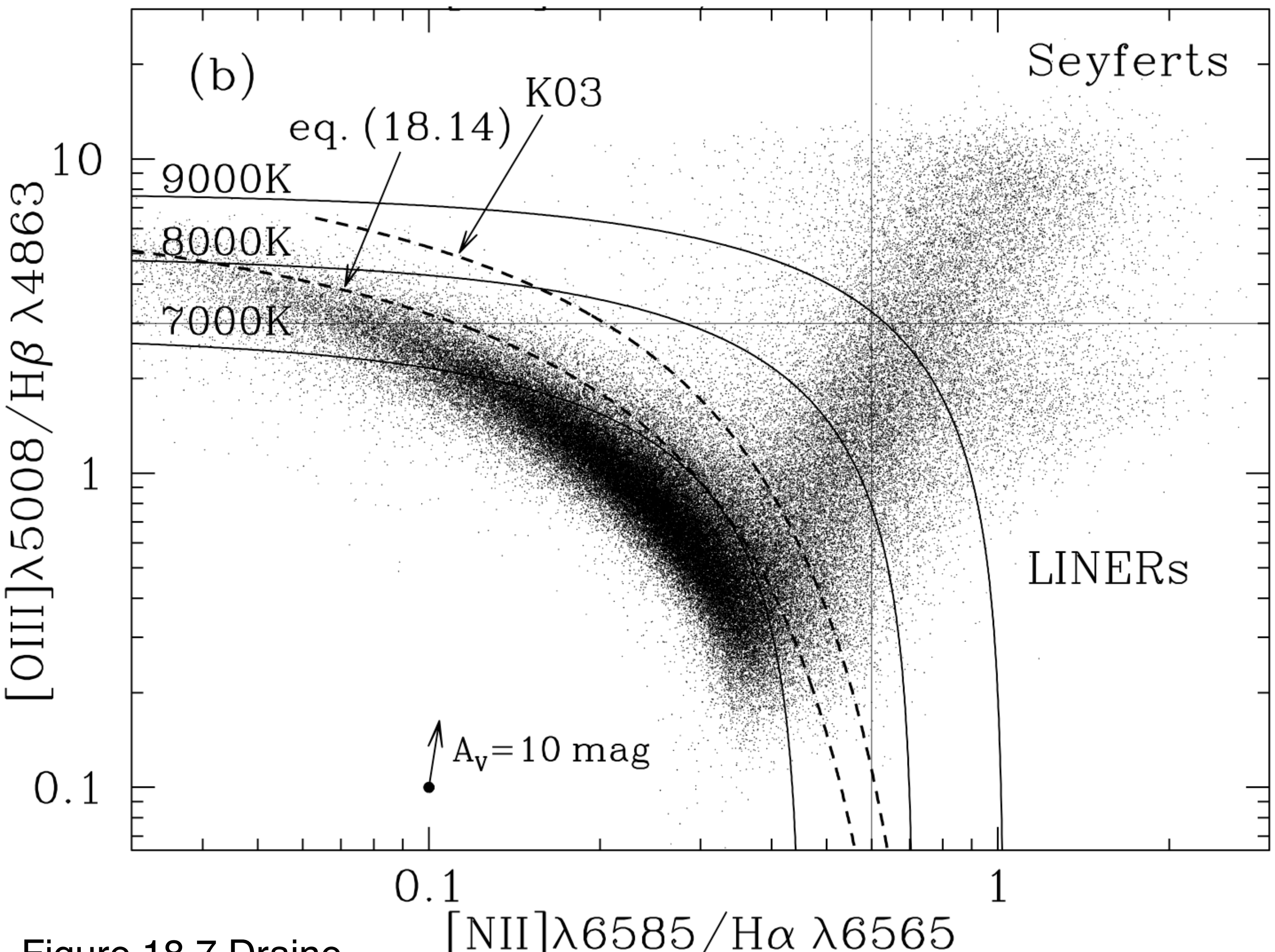


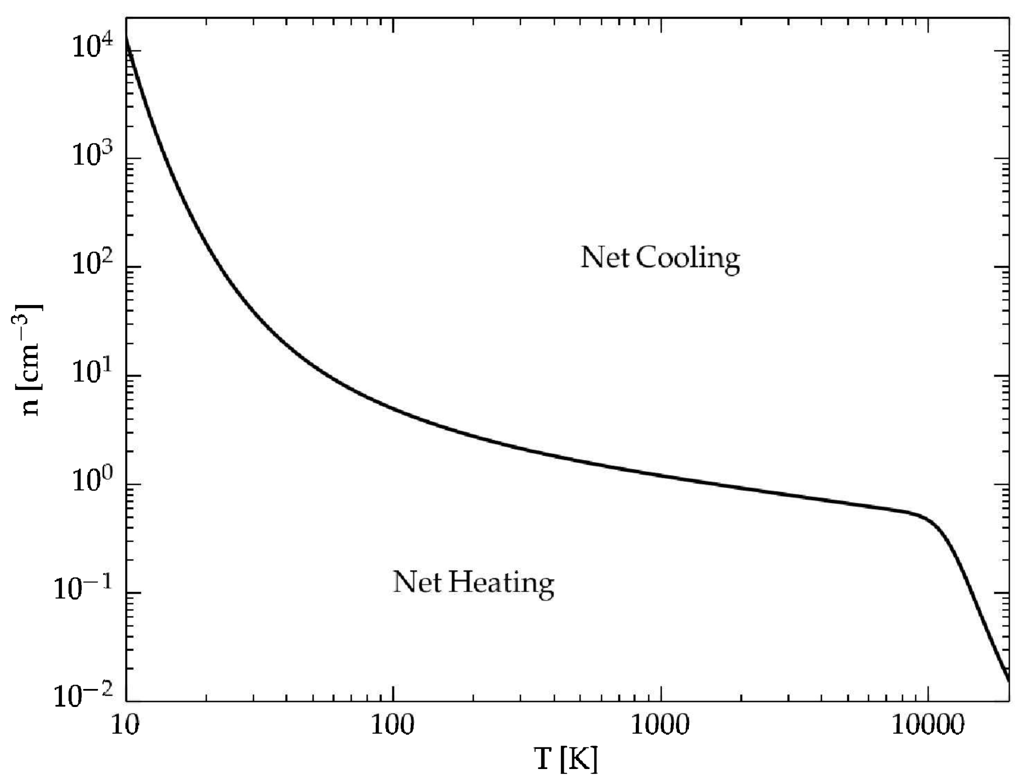

Figure 18.7 Draine

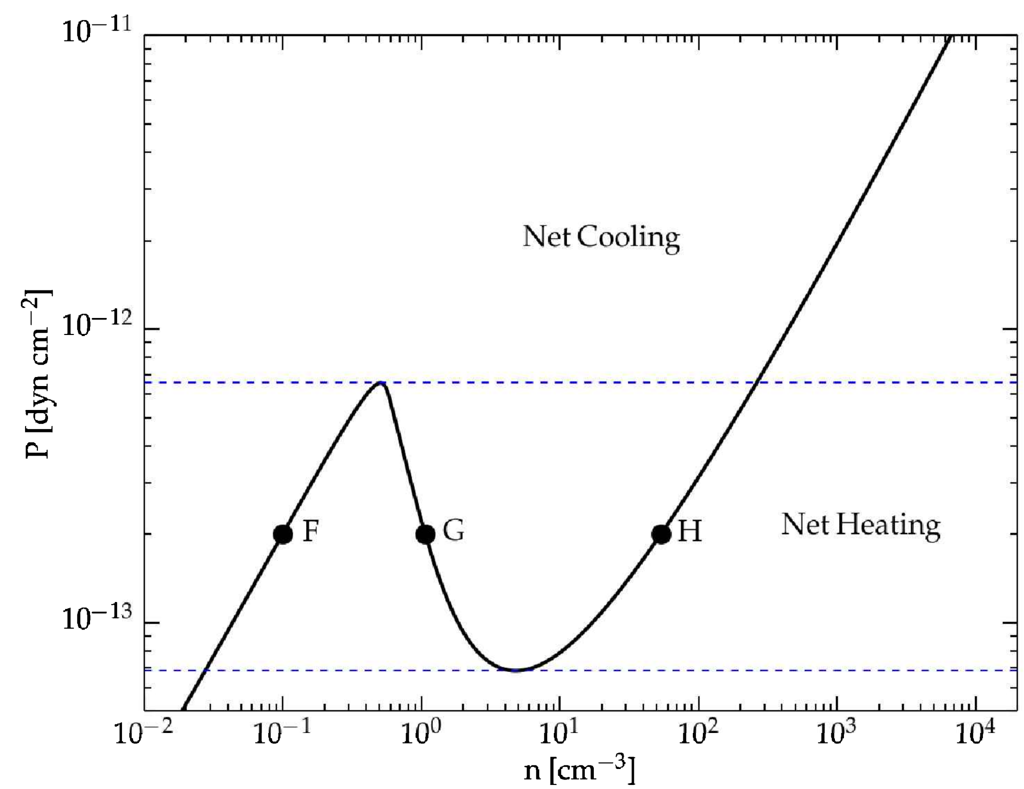

Flying seagull [Stasinska]

Photons from AGNs are harder than those from the massive stars that power H II regions.
***They induce more heating, implying that optical collisionally excited lines will be brighter with respect to recombination lines*** than in the case of ionization by massive stars.
The heating by an AGN boosts the [N II] line and creates a clear separation of the two wings.

# Homework (assignment)

- Problem [1]: Two stable phases
  - Use the formulae for the photoelectric heating rate by dust and the cooling rate by [CII] 158µm, [OI] 63.2µm, and Ly$\alpha$, described in this lecture note (and textbook).
  - Use IDL, python, or whatever you can use.
    - ✦ Reproduce the figures shown below.




    - ✦ Make a plot “P versus T,” in addition to the above plots.
    - ✦ Compute the numerical values of the equilibrium ***density*** and ***temperature*** for two pressures $P = 2 \times 10^{-13}\,\mathrm{dyn\,cm^{-2}}$ and $4 \times 10^{-13}\,\mathrm{dyn\,cm^{-2}}$.

- Problem [2]
  - Suppose that we observe a radio-bright QSO and detect absorption lines from Milky Way gas in its spectra. The 21 cm line is seen in optically-thin absorption with a profile with FWHM(H I) = 10 km s$^{-1}$. We also have high-resolution observations of the Na I doublet lines referred to as D$_1$ (5898Å) and D$_2$ (5892Å) in absorption. The Na I D$_2$ 5892Å line width is FWHM(Na I D$_2$) = 5 km s$^{-1}$. The line profiles are the result of a combination of thermal broadening plus turbulence with a Gaussian velocity distribution with one-dimensional velocity dispersion $\sigma_{v,\,\mathrm{turb}}$.

    You will want to employ the following theorem: If the turbulence has a Gaussian velocity distribution, the overall velocity distribution function of atoms of mass *M* will be Gaussian, with one-dimensional velocity dispersion:

$$v_{\mathrm{rms}}^2 = \sigma_v^2 = \sigma_{v,\,\mathrm{turb}}^2 + \frac{kT}{M}$$

  - If the Na I D$_2$ line is optically thin, estimate the kinetic temperature *T* and $\sigma_{v,\,\mathrm{turb}}$.

    Note hat for a Gaussian function, $\mathrm{FWHM} = 2\sqrt{2\ln 2}\sigma$.