Line transitions

1. Electron changes its binding energy in an atom (bound–bound transition)

1b. Electron changes its binding energy in a molecule (bound–bound transition)

2. A molecule changes its binding energy (vibrations)

3. A molecule changes its rotational energy

➔ ***ALL PROCESSES HAPPENS VIA EMISSION/ABSORPTION OF RADIATION***

(but it is not the whole story…)

Quantum mechanics is at work:

Discrete energies are relevant ⟹ radiative transitions produce line emisson/absorption

no continuum (except ionization/recombination)

Statistical laws in case of Thermal Equilibrium (TE, at least Local …. LTE)

Line transitions (2)

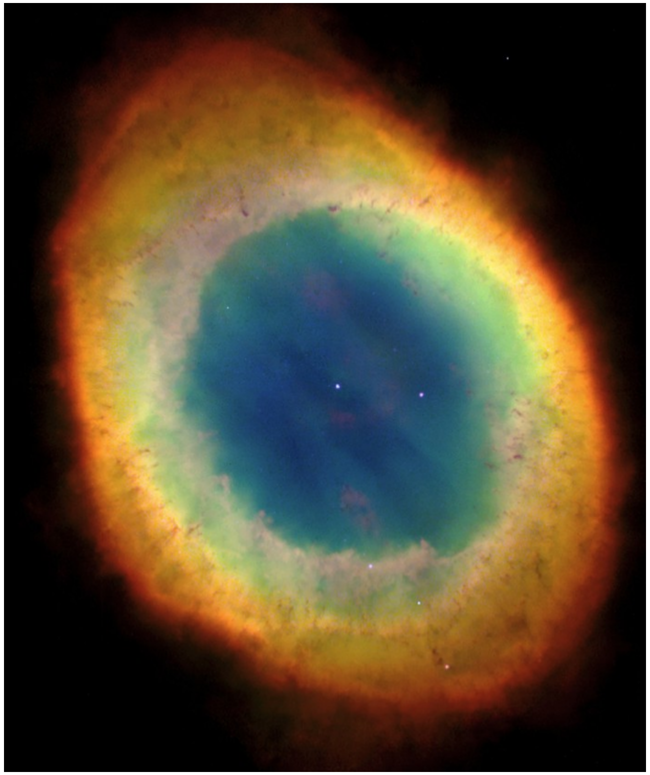
Textbooks and further reading

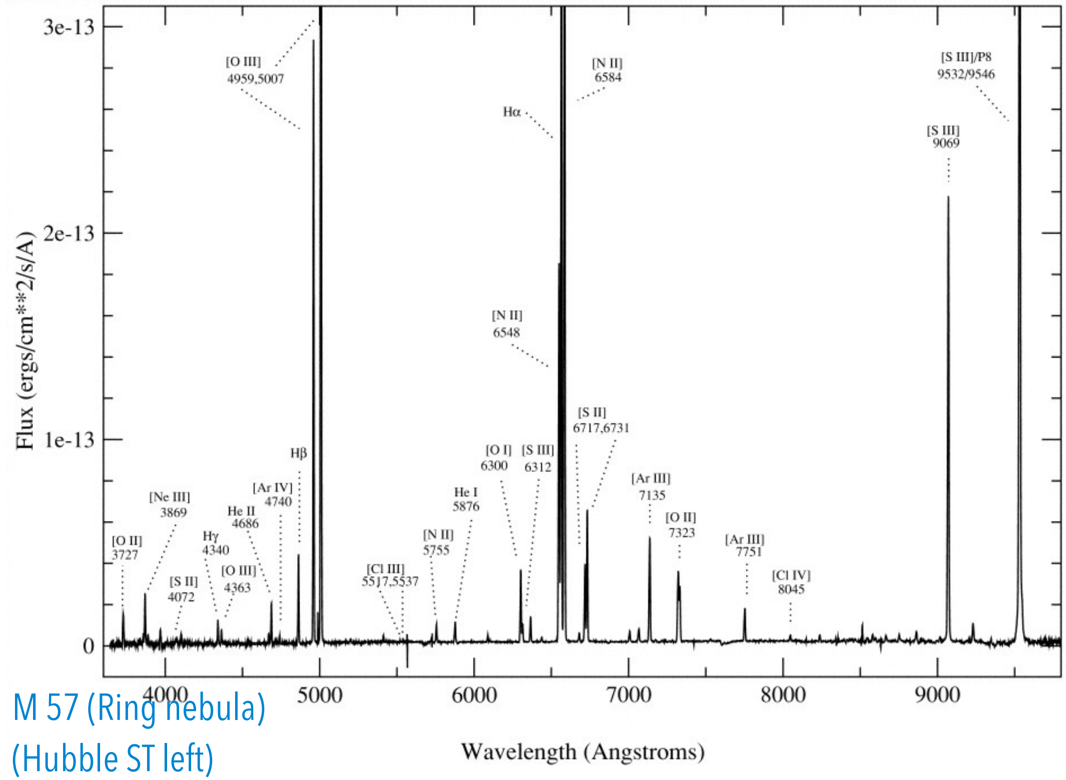
1. Dopita & Sutherland: chap. 2 (more arguments in other chapters)

2. Rybicki – Lightman: chap. 1.6 (Einstein's Coefficients); chap 9; chap10; chap 11

3. Tennison: (H spectrum & similarities, some molecular line theory/observations)

https://www.unitronitalia.com/prodotti/analysis-and-interpretation-of-astronomical-sp.pdf





M 57 (Ring nebula)
(Hubble ST left)

Line transitions (3)

What can we learn?

1. *Composition of a celestial body*

2. *Temperature (and other gas/plasma properties)*

3. *Abundances of various species (intensity of transitions) and excitation/ionization state*

4. *Motions:*
    - *4.1 particles within a cloud (line widths)*
    - *4.2 clouds within a celestial body (line shift)*

5. *Pressure (relation with collisions, line broadening, turbulence)*

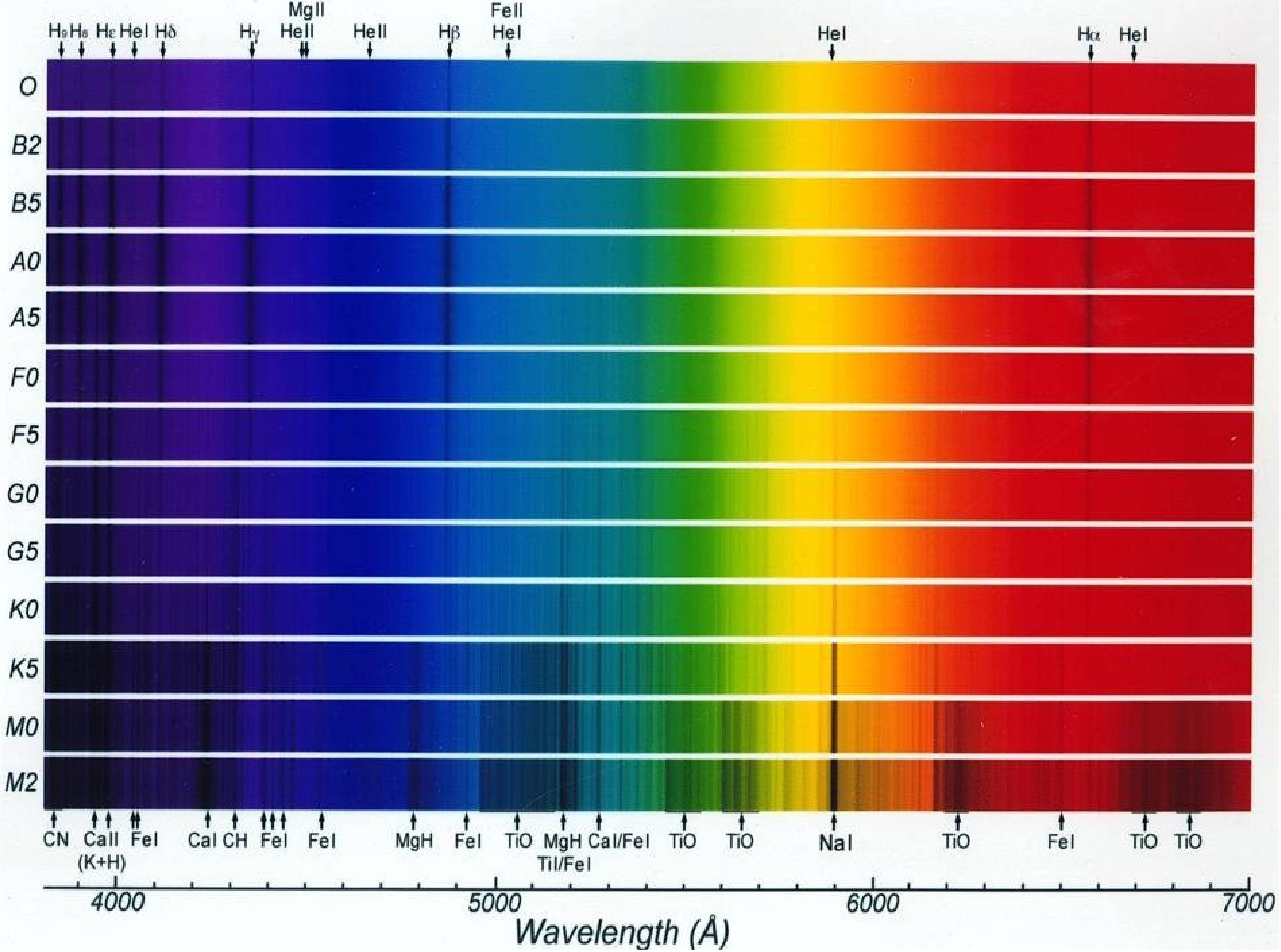
6. *Magnetic field (degenerate state, angular momentum becomes split if H is present)*

Line transitions (4)

Outline

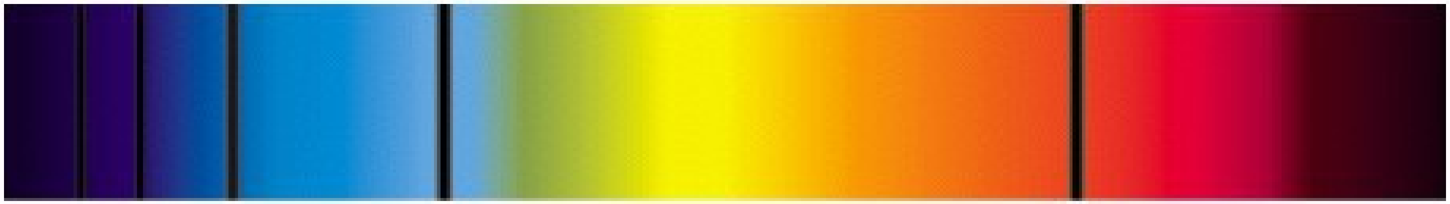
0. *Examples of lines in spectra of celestial bodies*
1. *Very basic definition of tools (atomic structure, orbits/als, energy levels, transitions,...)*
2. *Einstein's Coefficients* (A_{UL}, B_{UL}, B_{LU})
3. *Spectral lines: width, centroid, shift*
4. *Permitted, semi-permitted/forbidden, forbidden transitions*
5. *When density is a key player, and competing transitions!*
6. *Detailed statistical equilibrium and (the clash with) thermal equilibrium*
7. *Neutral hydrogen: a case study*

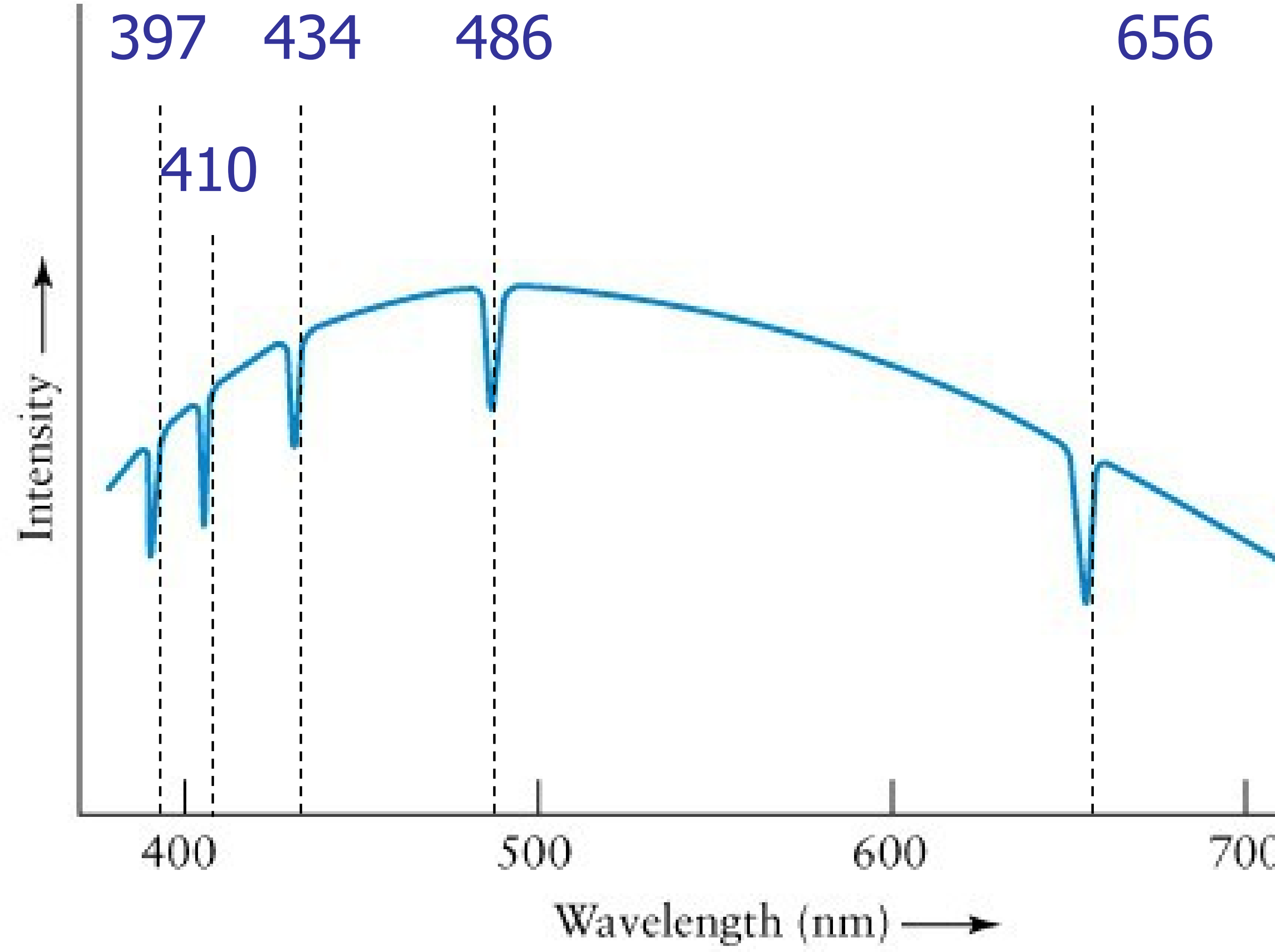
Examples: Spectral lines in optical spectra (mostly atomic transitions)

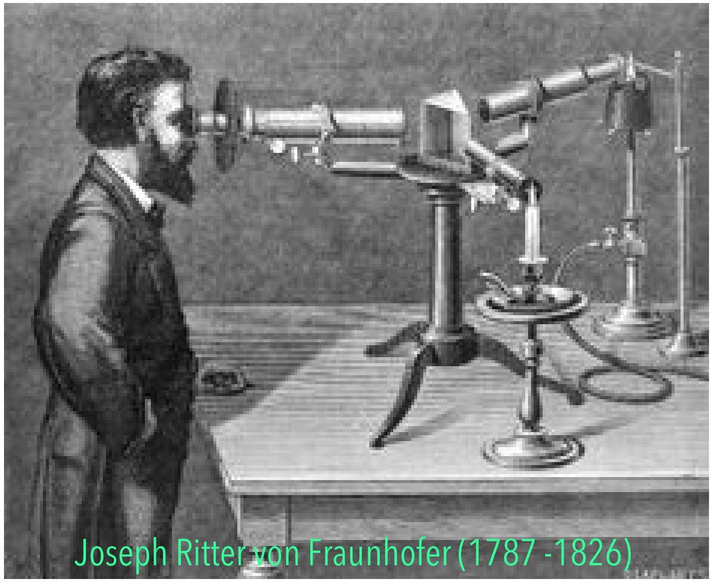


Atomic spectrum

Hydrogen at visual wavelengths

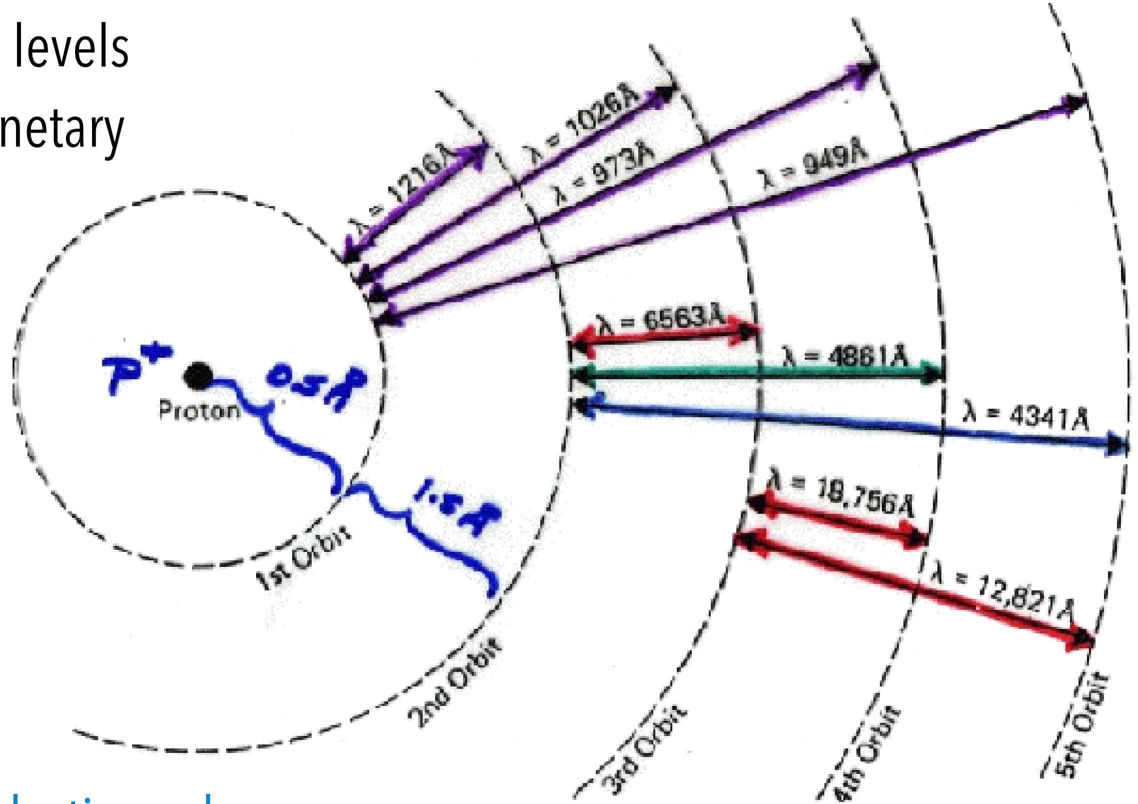





Joseph Ritter von Fraunhofer (1787 -1826)

Basic concept of atomic structure (1)

Each electron **bound** to its nucleus: **binding energy** is **quantized** into various **LEVELS** (as predicted by QM), corresponding to **different distances to the nucleus**, i.e. the various levels correspond to different orbits in a sort of planetary system.



The **outermost electron** **may** change its binding energy, swapping between two LEVELS, either acquiring (absorption) or releasing (emission) energy **hν** via **radiative transitions**

Such radiative transitions must obey strict selection rules.

(warning… there are also **other types of energy transitions**!)

(They will be considered later on)

Basic concept of atomic structure (2)

The Ground State corresponds to the maximum binding energy (which is defined as negative).

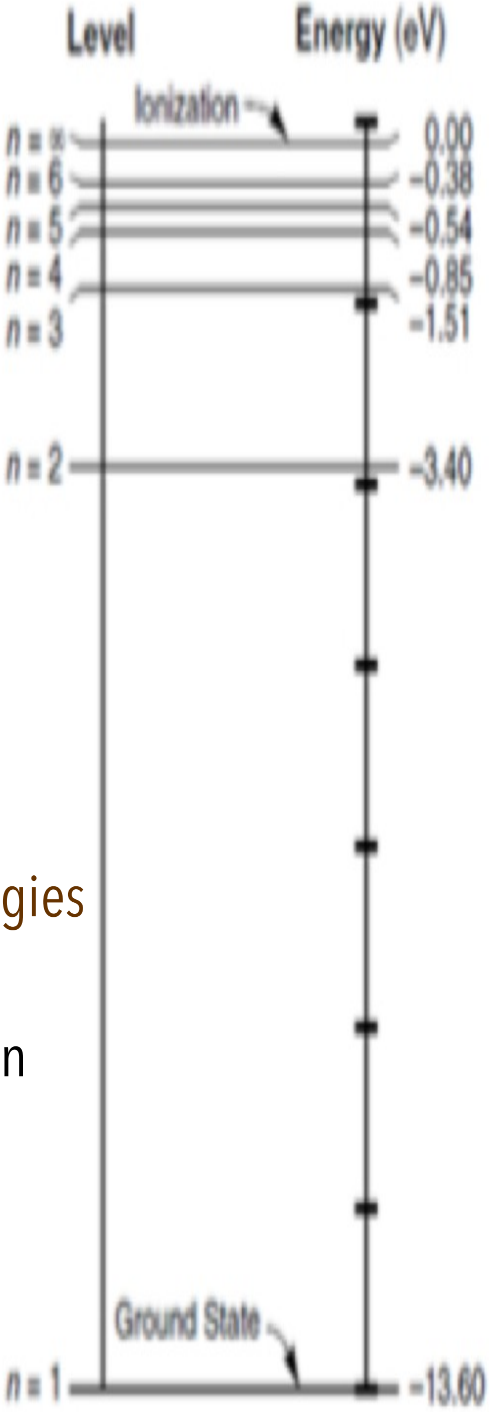
Electrons in states other than the Ground State are defined "**Excited**"

To **IONIZE** an atom in the ground state an energy in excess to this maximum binding energy must be provided.
The maximum binding energy defines the minimum ionization energy.
E.g. for an H atom it is 13.6 eV (UV photons, 912 A)

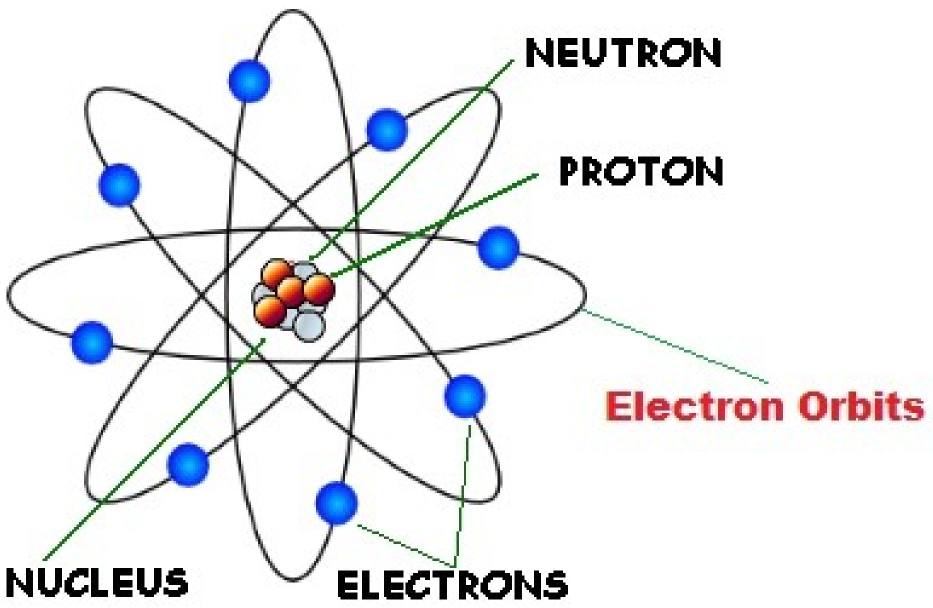
Electrons in states different from the ground state have lower ionization energies

[In general] in polyelectronic atoms, only the outermost (less bound) electron is considered

Obviously, real atoms are more complicated!



Basic concept of atomic structure (3): Bohr .vs. QM



(artist's view of) Bohr's model for O

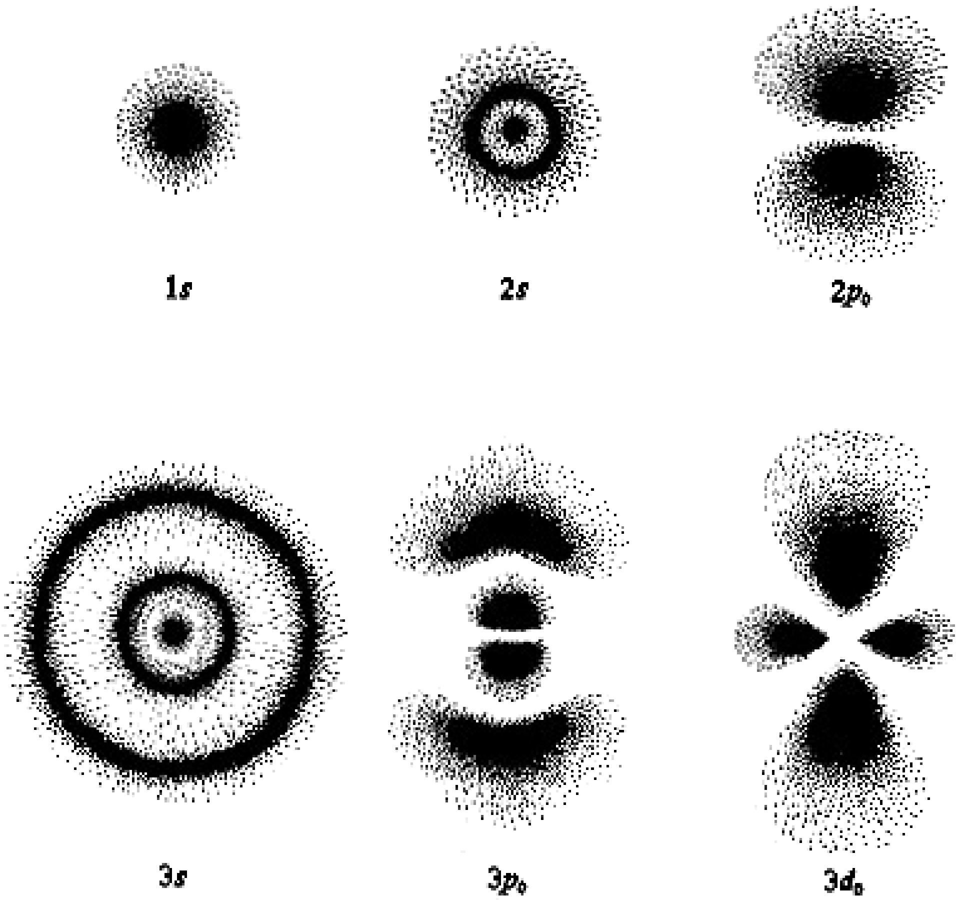
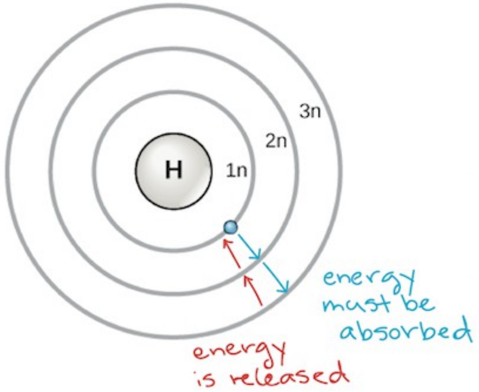


Figure 6-12. Probability density plots of some hydrogen atomic orbitals. The density of the dots represents the probability of finding the electron in that region.

© 1983 University Science Books; "Quantum Chemistry" by Donald A. McQuarrie



basic concepts (4)

Quantum numbers:

n – main number $= 1,2,3,\ldots$ defines the energy and the size of the “orbit”

$$a_n = a_o \frac{n^2}{Z} \qquad a_o = 0.53\,\text{A}$$

l – azimutal number (angular momentum, related to eccentricity, defines the SHAPE)

$0,1,2,\ldots,n-1$

$$\sqrt{1-e^2} = \frac{b}{a} = \frac{l+1}{n} \leq 1$$

m – magnetic number (orbit orientation, relevant in case of magnetic field)

$-l,-l+1,\ldots,0,\ldots l-1,l$

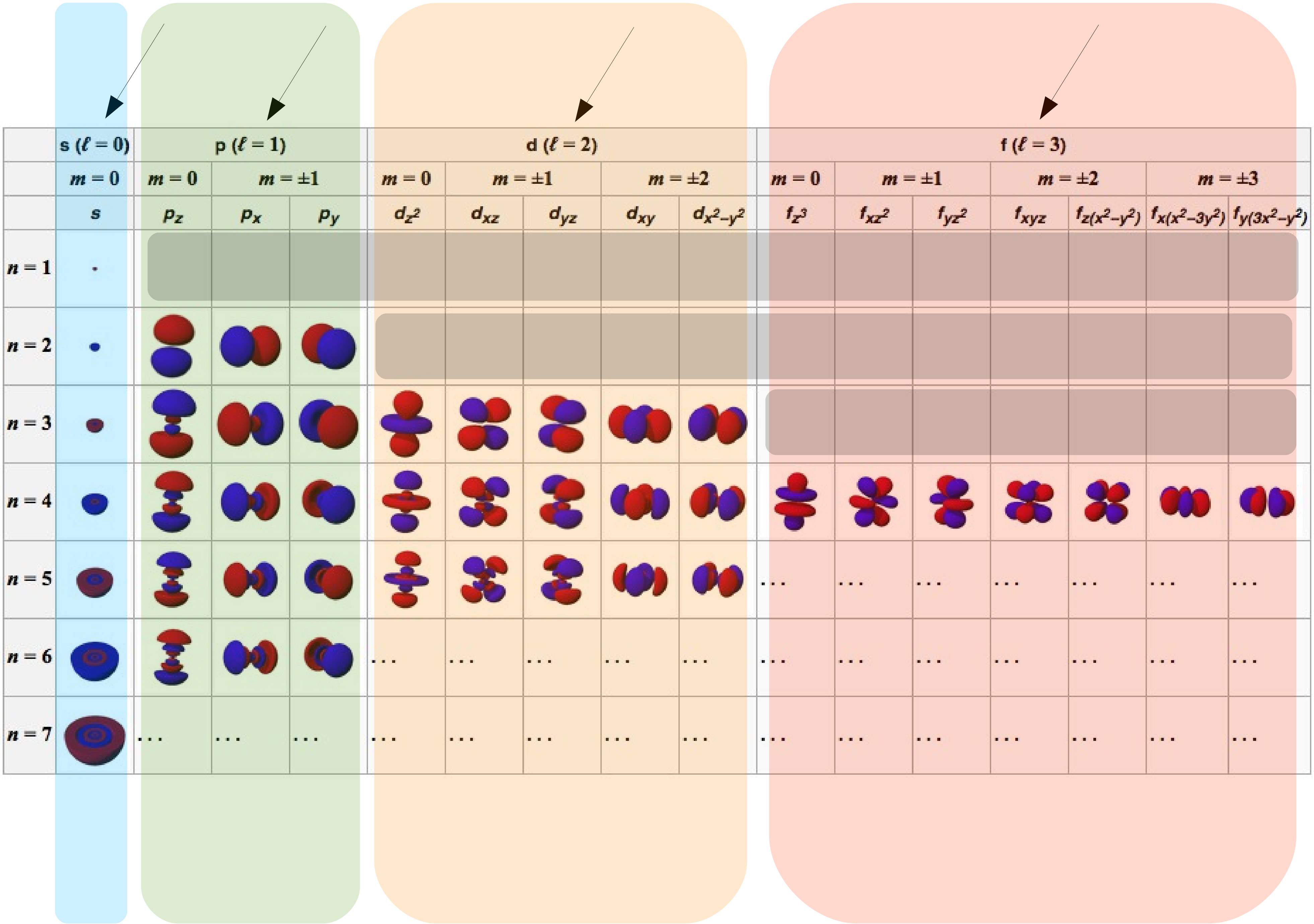
However.... at a given main number (n), there is a tiny difference in energy between levels with different combination of l,m

this is not true (first order) for hydrogen, where there is a high degree of energy degeneracy (fine structure)

further extremely small energy structures (hyperfine structure) can be defined by the spin quantum number $s = (\pm 1/2)$

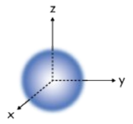
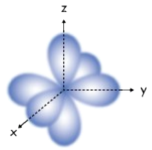
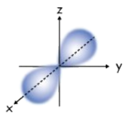
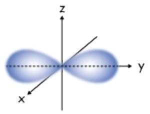
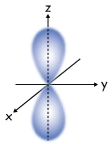
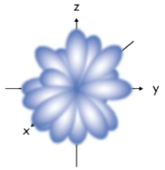
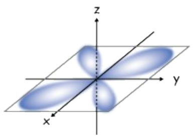
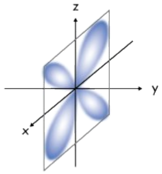
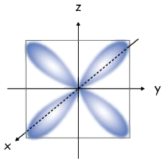
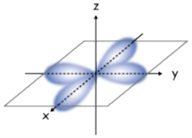
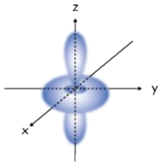
contrary to classical theory of charges in motion, the electrons do not radiate in their curved orbits, except during a “transition”

Basic concept of atomic structure (4): Orbitals, as from n,l,m

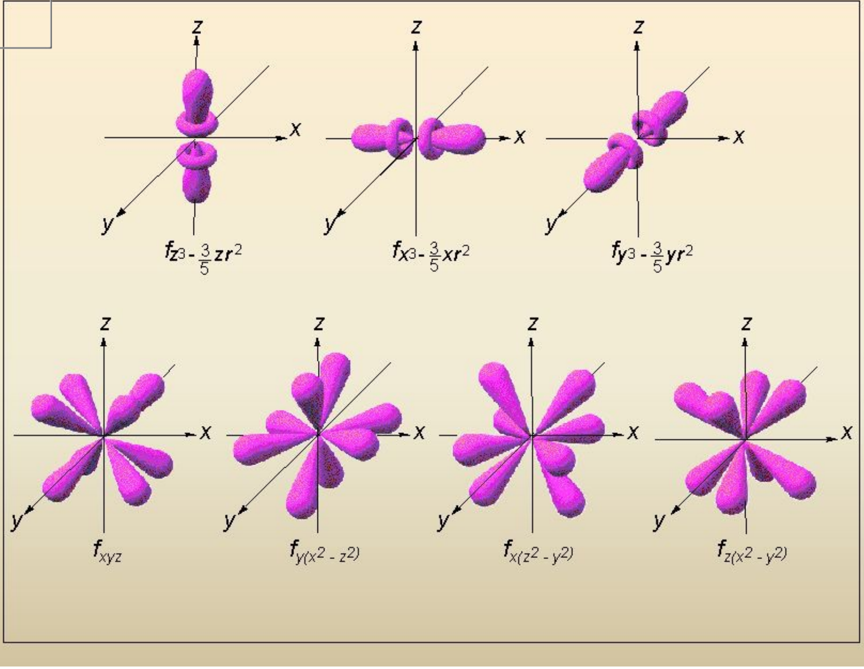


	s ($\ell = 0$)	p ($\ell = 1$)			d ($\ell = 2$)					f ($\ell = 3$)						
	$m = 0$	$m = 0$	$m = \pm1$		$m = 0$	$m = \pm1$		$m = \pm2$		$m = 0$	$m = \pm1$		$m = \pm2$		$m = \pm3$	
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy}	$d_{x^2-y^2}$	f_{z^3}	f_{xz^2}	f_{yz^2}	f_{xyz}	$f_{z(x^2-y^2)}$	$f_{x(x^2-3y^2)}$	$f_{y(3x^2-y^2)}$
$n = 1$																
$n = 2$																
$n = 3$																
$n = 4$																
$n = 5$										…	…	…	…	…	…	…
$n = 6$					…	…	…	…	…	…	…	…	…	…	…	…
$n = 7$		…	…	…	…	…	…	…	…	…	…	…	…	…	…	…

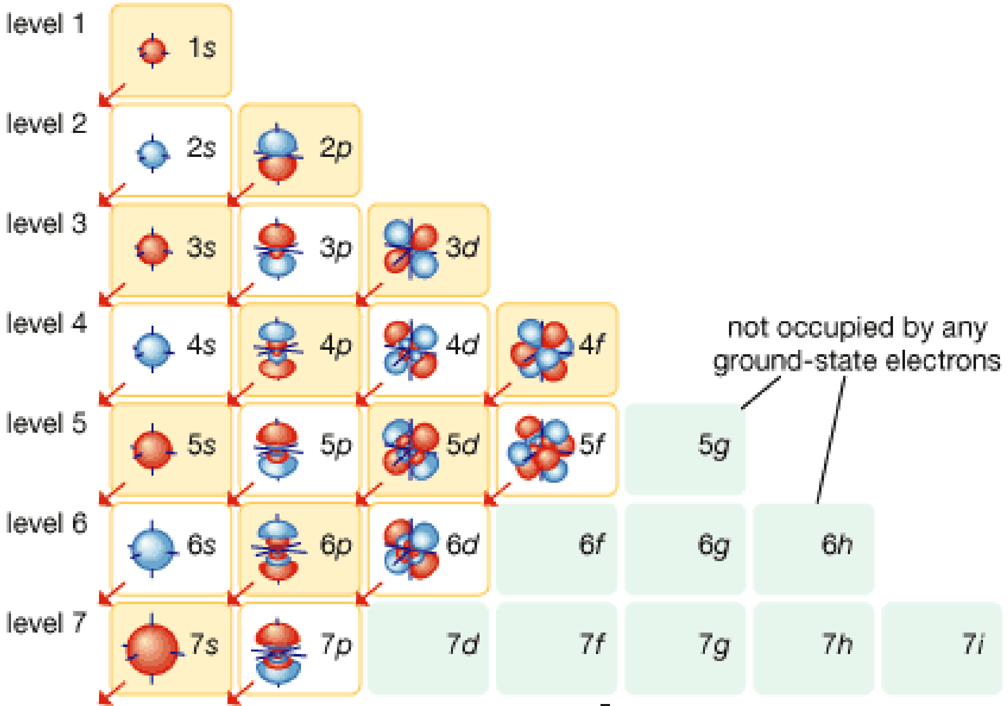
Basic concept of atomic structure (5): Orbitals, as from n,l,m (alternative view)

Orbitals and sub-orbitals of Bound Electrons		
$\ell = 0$ **s**		
$\ell = 1$ **p**		**p_x**  $m_\ell = -1$ **p_y**  $m_\ell = 0$ **p_z**  $m_\ell = +1$
$\ell = 2$ **d**		**d_{xy}**  $m_\ell = -2$ **d_{xz}**  $m_\ell = -1$ **d_{yz}**  $m_\ell = 0$ **$d_{x^2-y^2}$**  $m_\ell = +1$ **d_{z^2}**  $m_\ell = +2$
$\ell = 3$ **f**		7 sub-orbitals not pictured

Shape of f orbitals



Basic concept of atomic structure (6): Filling the orbitals



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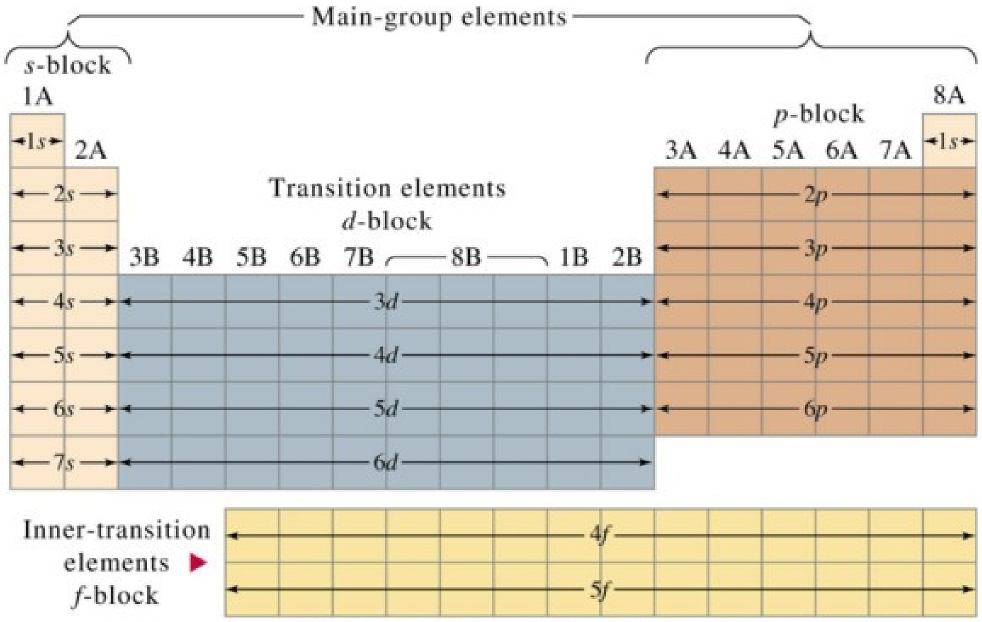
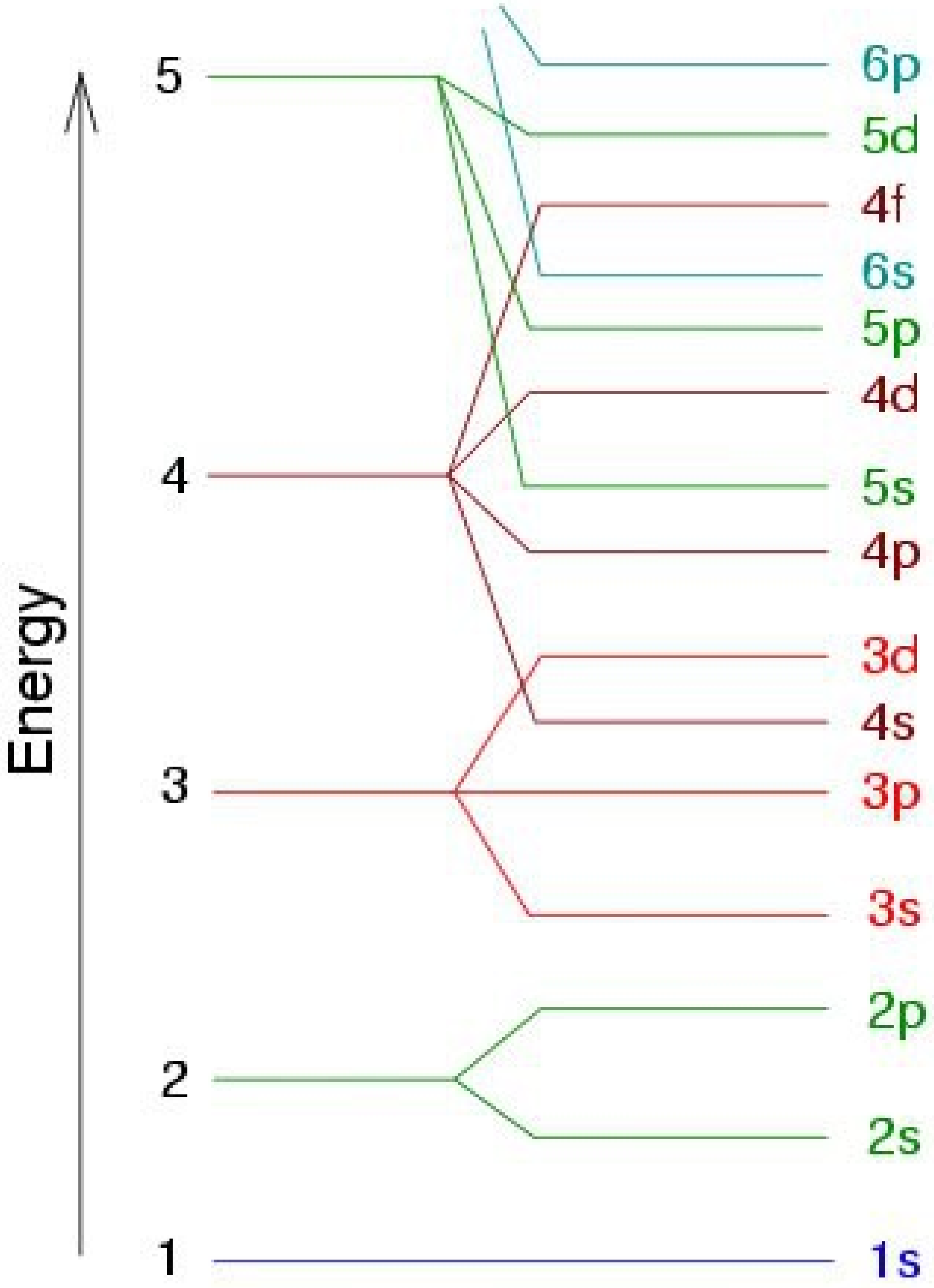




basic concepts (7): Hydrogen

Hydrogen:

simplest example for studying lines between various energy levels

The frequency ν_{UL} of a photon emitted/absorbed during a transition

between two levels U and L is $\boxed{\nu_{UL} = c R_H \left(\frac{1}{L^2} - \frac{1}{U^2} \right) \quad \text{Hz}}$; $U > L > 0$

$$R_H = \frac{2 \pi^2 e^4 m_e}{h^3 c} = 1.1 \cdot 10^5 \ \text{cm}^{-1} \quad \rightarrow \quad \text{Rydberg constant for H}$$

- increasing U, lines get closer to a limiting frequency $\nu = \frac{c R_H}{L^2}$

- if L is large, lines of different series start at very close frequencies and produce a spectrum similar to a continuum (but it is not!)

[hydrogen-like atoms, He+, Li++, Be+++,... obtained assigning the energy $\mathbf{E_n}$ at each "atom"]

$$E_n = -Z^2 \frac{R_H \mu h c}{n^2} + \epsilon(n, l)$$

Hydrogen transitions in terms of energy:

$$\boxed{R_y = \frac{2\pi^2 e^4 m_e}{h^2} = 13.6 \ \text{eV}} \quad \left(\text{called 1 Rydberg (energy unit)} = 2.18\cdot 10^{-18} \ \text{J}\right)$$

$$h\nu_{UL} = R_y \left(\frac{1}{L^2} - \frac{1}{U^2}\right) \ \text{eV} \qquad ; \qquad U > L > 0$$

For a given pair of quantum numbers, decay and excitation can either
generate (emission)
or cancel (absorption)
photons at the appropriate frequency/energy

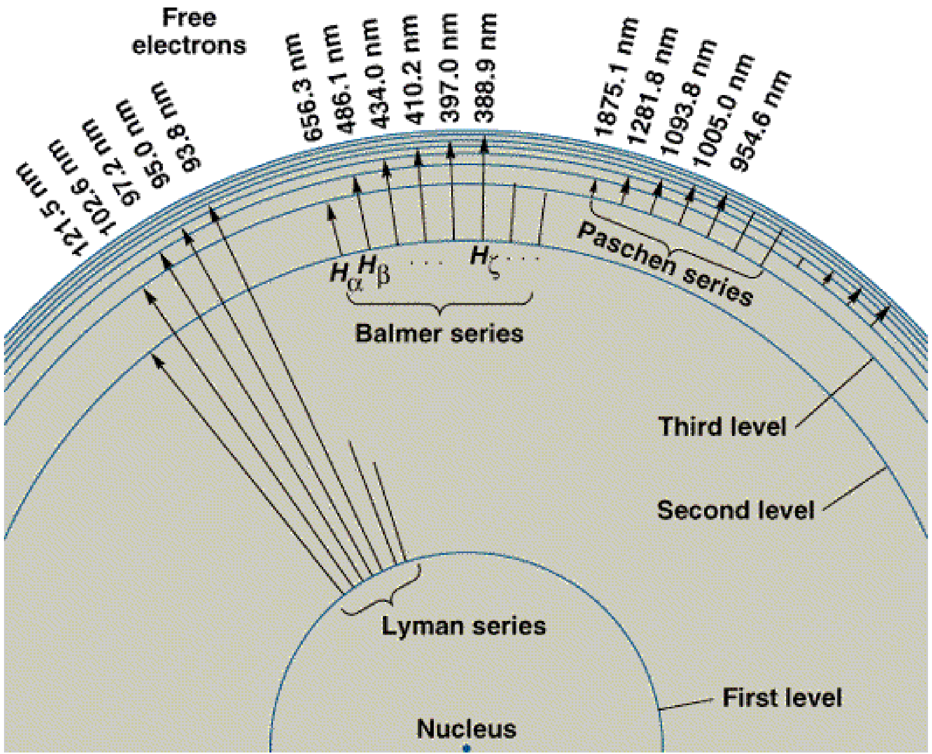
$U \rightarrow \infty$ determines the binding energy of a given L status (quantum number)

Atomic spectra

Hydrogen

Based on the main quantum number various series are defined:

Lyman (n=1, UV)
Balmer (n=2, visible)
Paschen (n=3, IR) ...



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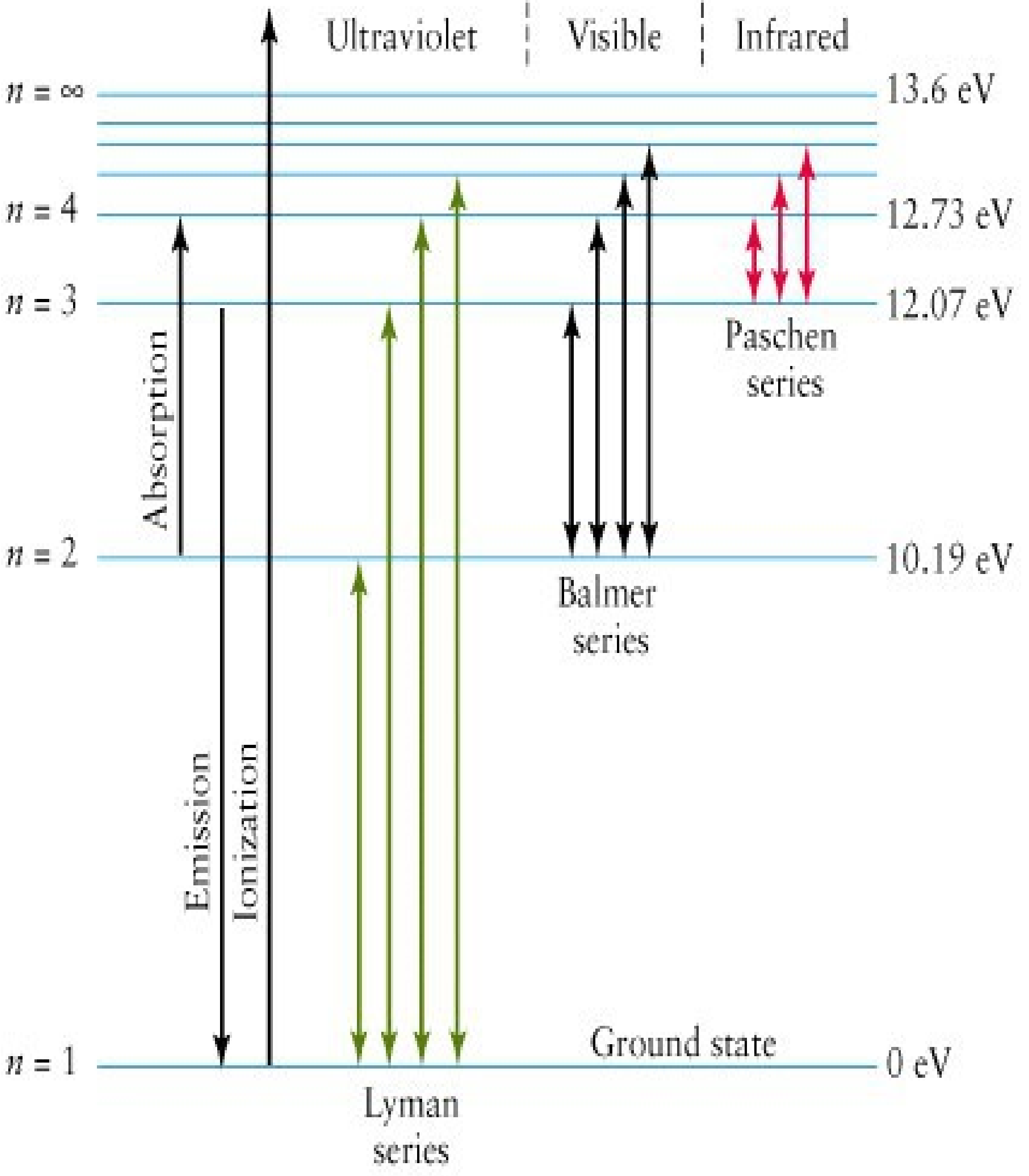
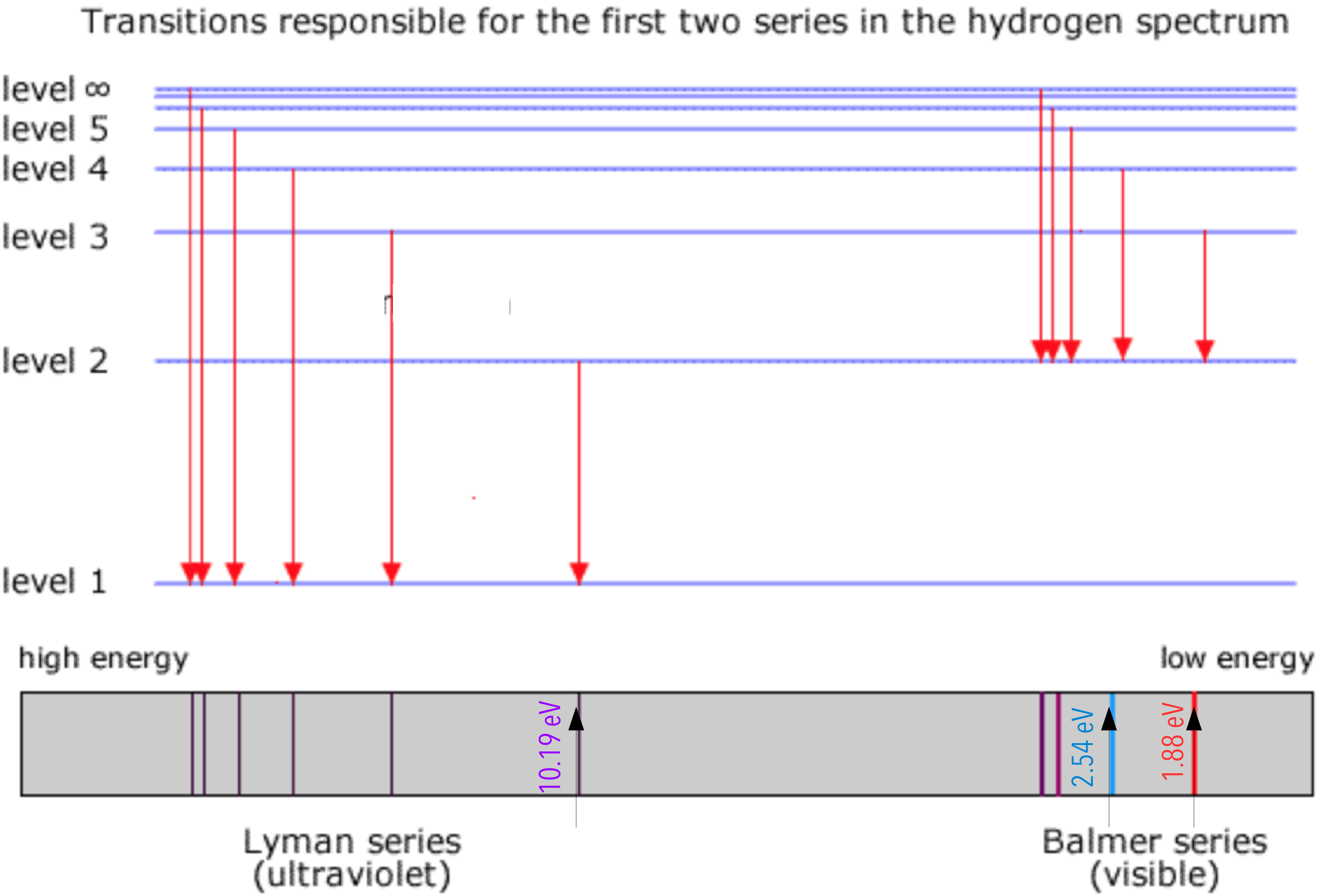
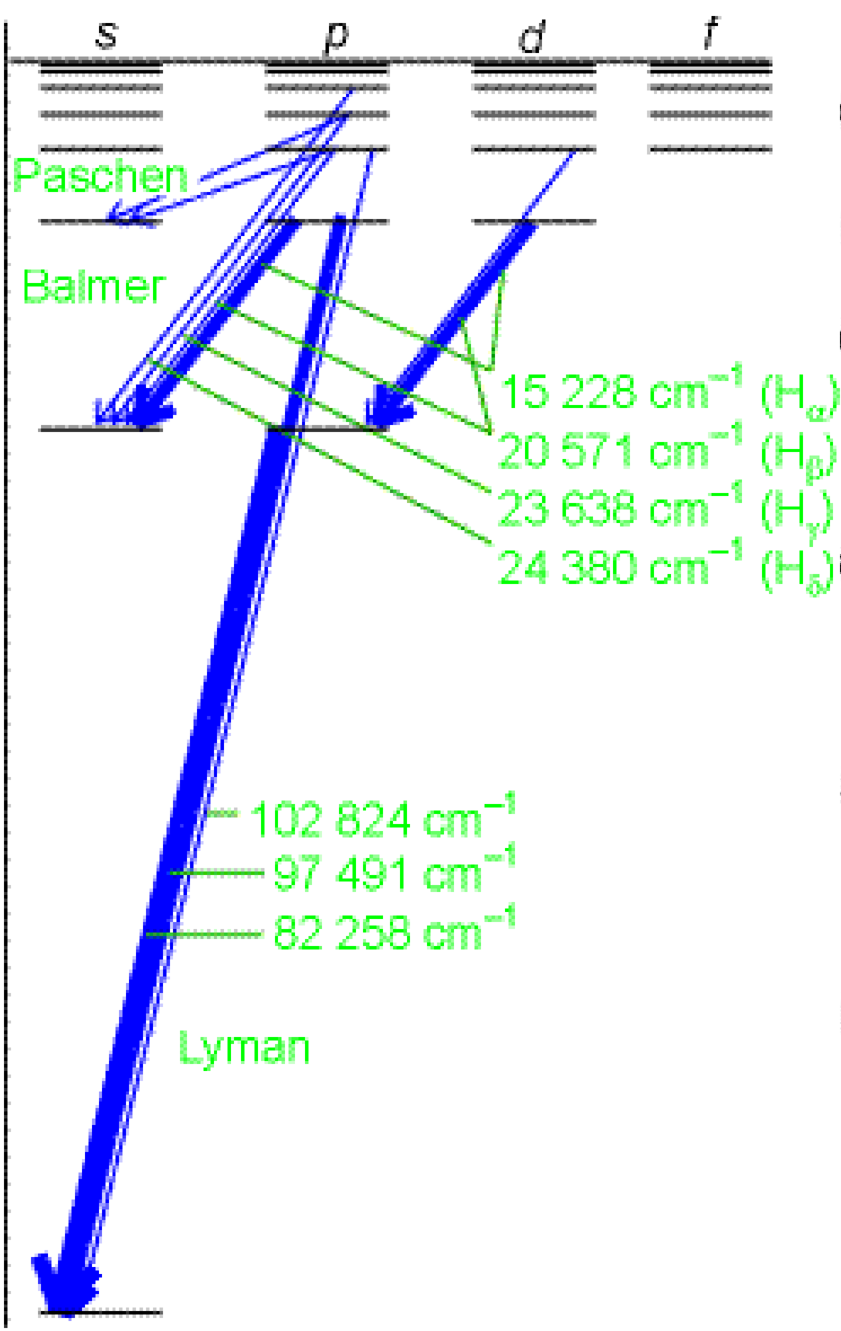


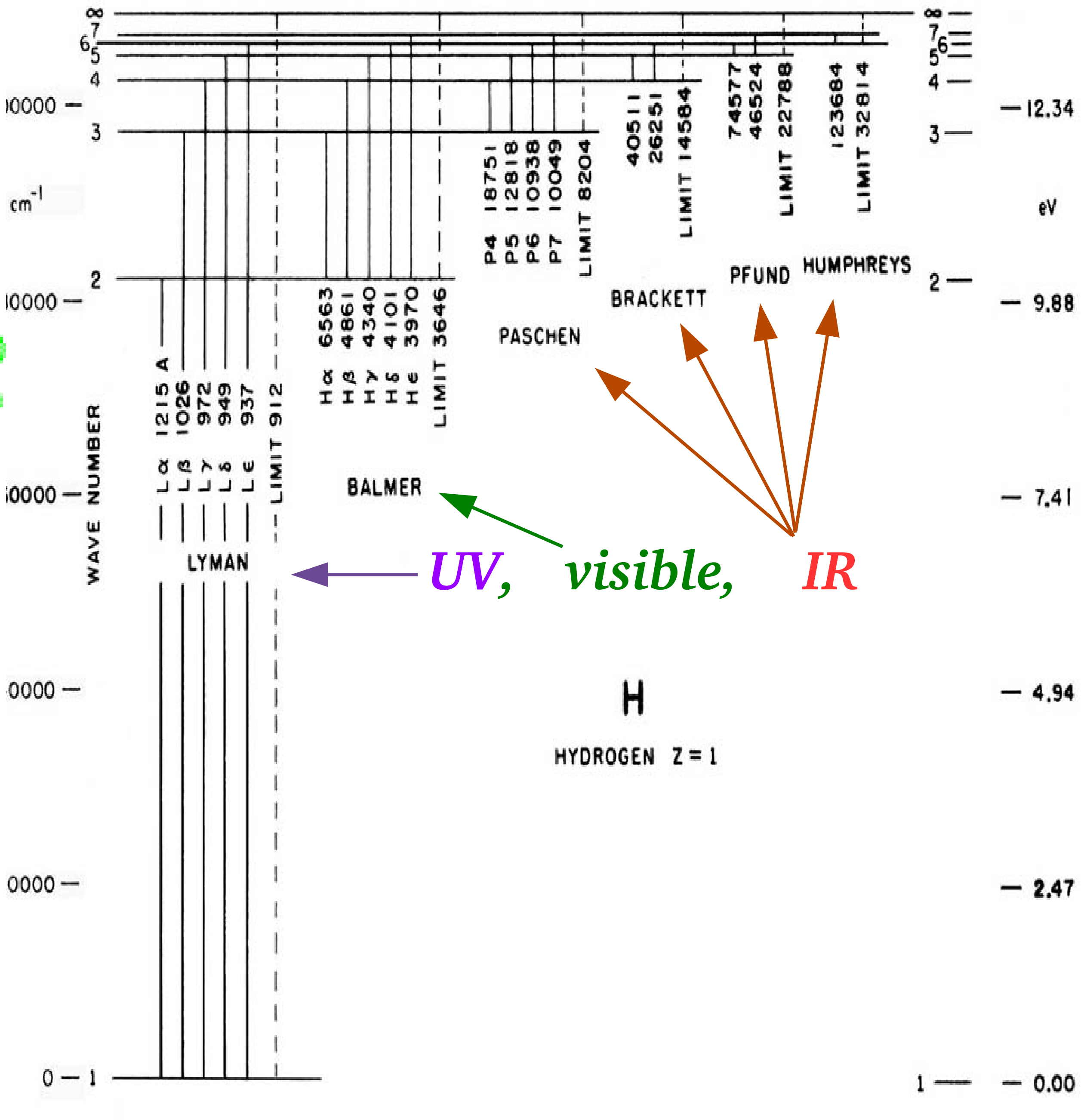
Atomic spectra



Hydrogen: Grotrian diagrams

transitions obey to well known selection rules: Δn, Δl, Δm,



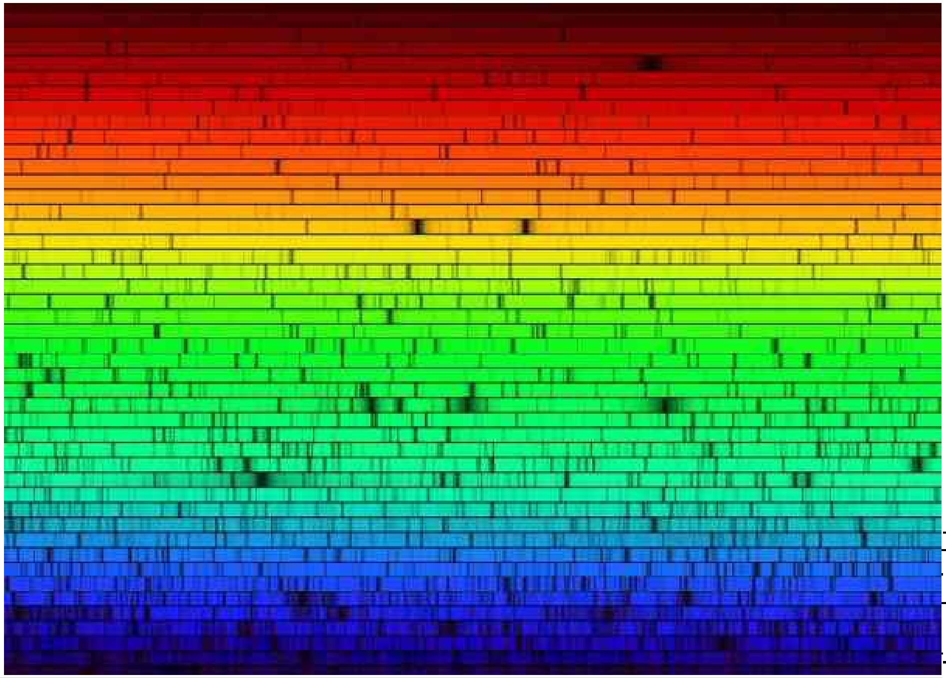


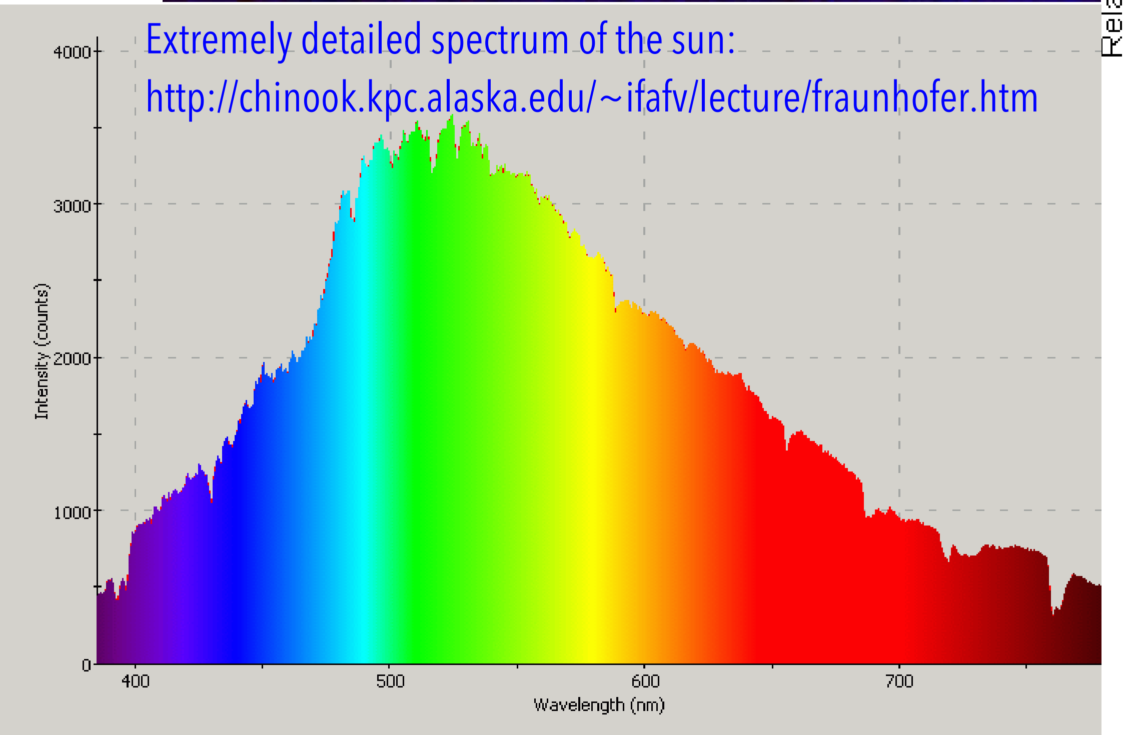
UV, visible, IR

(mostly) Atomic spectra

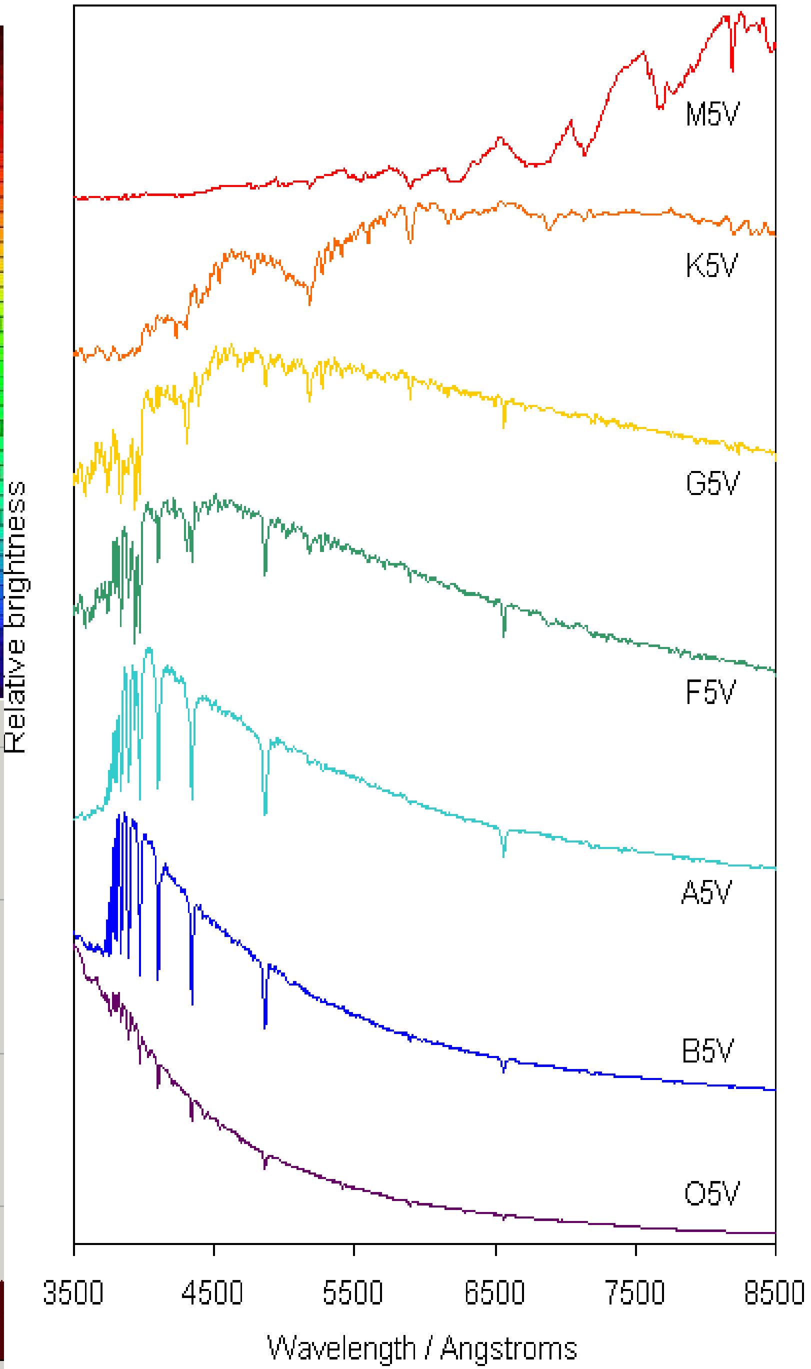
typical spectra of stars

There is a background made of BB continuum

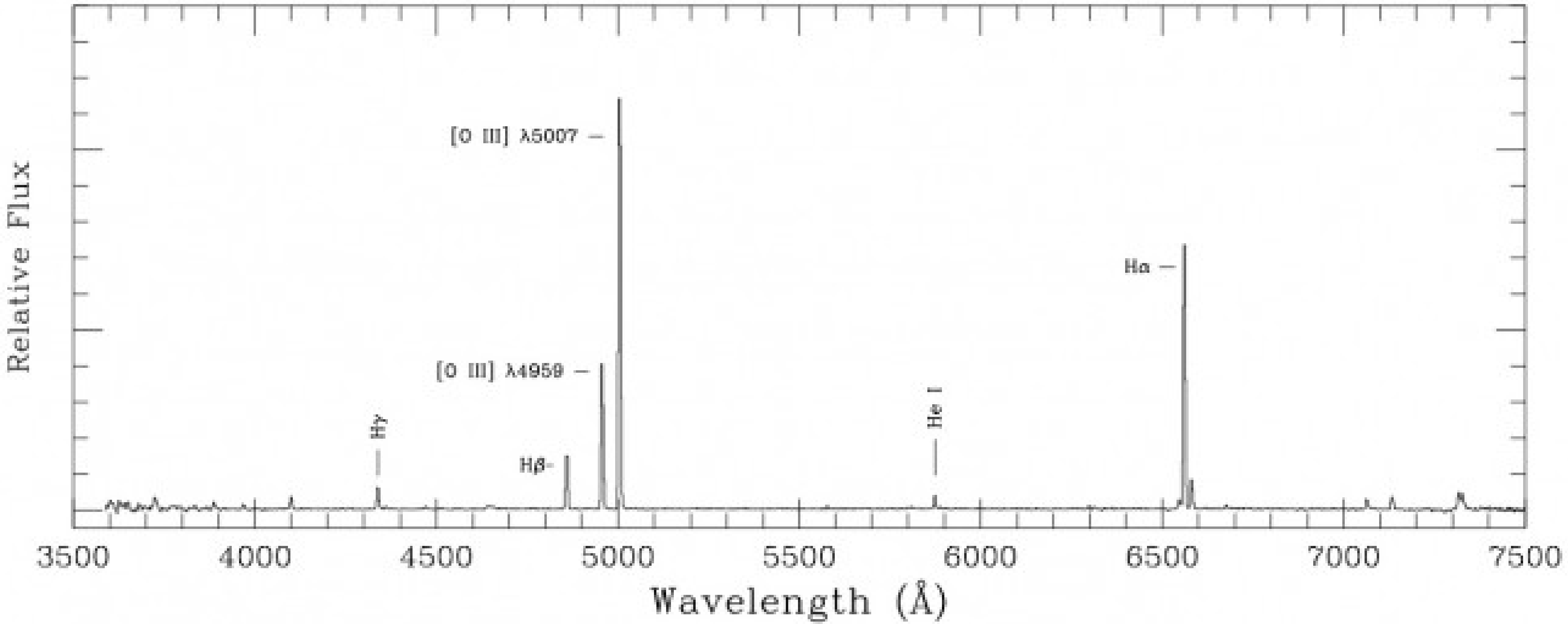




Extremely detailed spectrum of the sun:
http://chinook.kpc.alaska.edu/~ifafv/lecture/fraunhofer.htm



Various elements in an astrophysical plasma



> No continuum photons: nonetheless, we have beautiful optical images!

> Typical of gaseous environments like Planetary Nebulae and HII regions

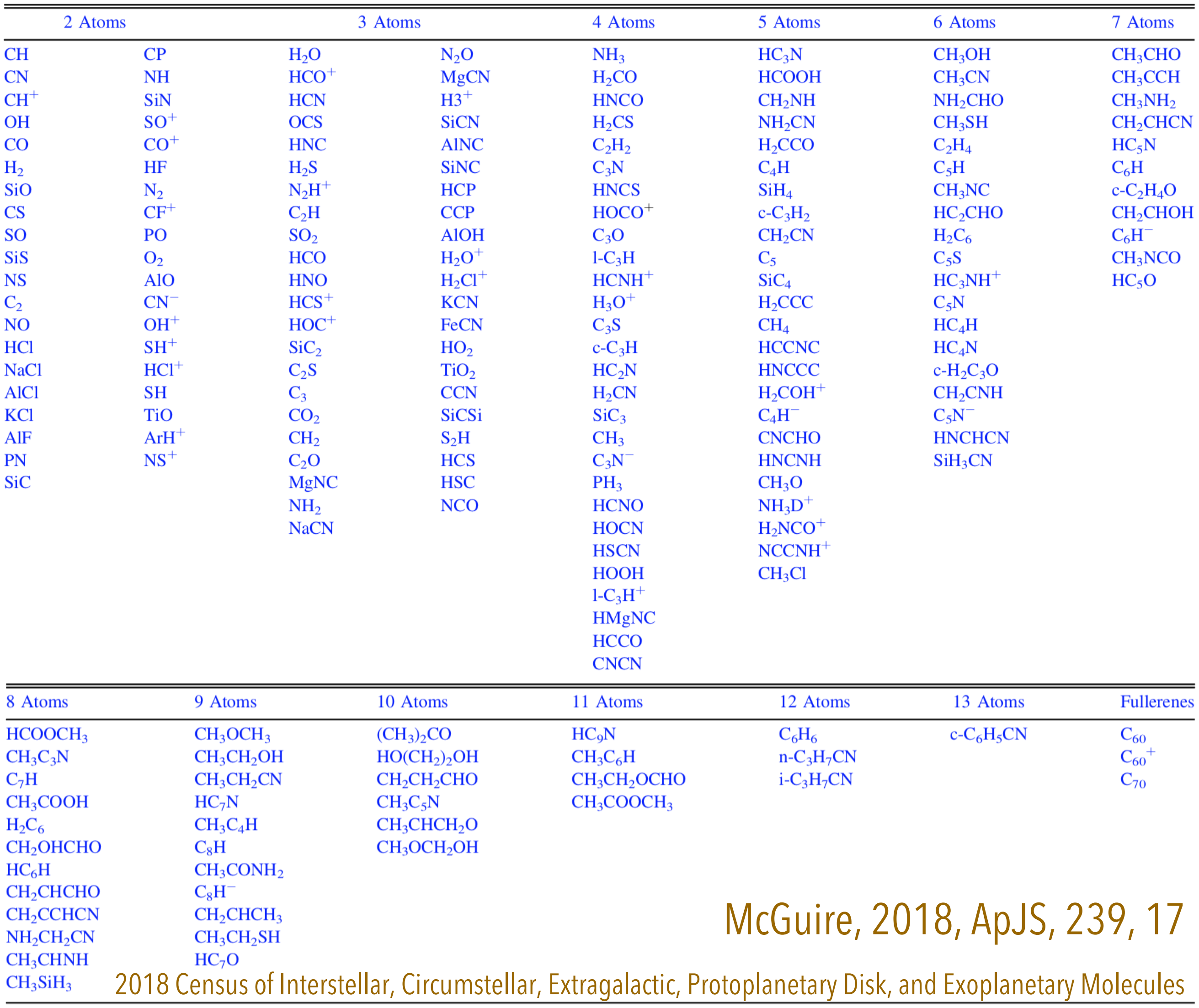
Molecular spectra (0):

Molecules have 3–D structures capable to oscillate around the equilibrium distance (vibrations), and may also change their rotational energy between adjacent levels defined by quantum mechanics.

Animations @ https://en.wikipedia.org/wiki/Molecular_vibration

Molecules are mostly found in low temperature (T from10s to a few 100s °K) and high density ($n > 10^2$ cm^{-3}) regions in the ISM in spiral galaxies.

They can have electronic transitions in any of the atoms in the molecule (see earlier), not considered here (small differences in the binding energy of the electron)



2 Atoms		3 Atoms		4 Atoms	5 Atoms	6 Atoms	7 Atoms
CH	CP	H_2O	N_2O	NH_3	HC_3N	CH_3OH	CH_3CHO
CN	NH	HCO^+	$MgCN$	H_2CO	$HCOOH$	CH_3CN	CH_3CCH
CH^+	SiN	HCN	$H3^+$	$HNCO$	CH_2NH	NH_2CHO	CH_3NH_2
OH	SO^+	OCS	$SiCN$	H_2CS	NH_2CN	CH_3SH	CH_2CHCN
CO	CO^+	HNC	$AlNC$	C_2H_2	H_2CCO	C_2H_4	HC_5N
H_2	HF	H_2S	$SiNC$	C_3N	C_4H	C_5H	C_6H
SiO	N_2	N_2H^+	HCP	$HNCS$	SiH_4	CH_3NC	$c\text{-}C_2H_4O$
CS	CF^+	C_2H	CCP	$HOCO^+$	$c\text{-}C_3H_2$	HC_2CHO	CH_2CHOH
SO	PO	SO_2	$AlOH$	C_3O	CH_2CN	H_2C_6	C_6H^-
SiS	O_2	HCO	H_2O^+	$l\text{-}C_3H$	C_5	C_5S	CH_3NCO
NS	AlO	HNO	H_2Cl^+	$HCNH^+$	SiC_4	HC_3NH^+	HC_5O
C_2	CN^-	HCS^+	KCN	H_3O^+	H_2CCC	C_5N	
NO	OH^+	HOC^+	$FeCN$	C_3S	CH_4	HC_4H	
HCl	SH^+	SiC_2	HO_2	$c\text{-}C_3H$	$HCCNC$	HC_4N	
$NaCl$	HCl^+	C_2S	TiO_2	HC_2N	$HNCCC$	$c\text{-}H_2C_3O$	
$AlCl$	SH	C_3	CCN	H_2CN	H_2COH^+	CH_2CNH	
KCl	TiO	CO_2	$SiCSi$	SiC_3	C_4H^-	C_5N^-	
AlF	ArH^+	CH_2	S_2H	CH_3	$CNCHO$	$HNCHCN$	
PN	NS^+	C_2O	HCS	C_3N^-	$HNCNH$	SiH_3CN	
SiC		$MgNC$	HSC	PH_3	CH_3O		
		NH_2	NCO	$HCNO$	NH_3D^+		
		$NaCN$		$HOCN$	H_2NCO^+		
				$HSCN$	$NCCNH^+$		
				$HOOH$	CH_3Cl		
				$l\text{-}C_3H^+$			
				$HMgNC$			
				$HCCO$			
				$CNCN$			

8 Atoms	9 Atoms	10 Atoms	11 Atoms	12 Atoms	13 Atoms	Fullerenes
$HCOOCH_3$	CH_3OCH_3	$(CH_3)_2CO$	HC_9N	C_6H_6	$c\text{-}C_6H_5CN$	C_{60}
CH_3C_3N	CH_3CH_2OH	$HO(CH_2)_2OH$	CH_3C_6H	$n\text{-}C_3H_7CN$		$C_{60}{}^+$
C_7H	CH_3CH_2CN	CH_2CH_2CHO	CH_3CH_2OCHO	$i\text{-}C_3H_7CN$		C_{70}
CH_3COOH	HC_7N	CH_3C_5N	CH_3COOCH_3			
H_2C_6	CH_3C_4H	CH_3CHCH_2O				
CH_2OHCHO	C_8H	CH_3OCH_2OH				
HC_6H	CH_3CONH_2					
CH_2CHCHO	C_8H^-					
CH_2CCHCN	CH_2CHCH_3					
NH_2CH_2CN	CH_3CH_2SH					
CH_3CHNH	HC_7O					
CH_3SiH_3						

McGuire, 2018, ApJS, 239, 17

2018 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules

Molecular spectra (1):

Vibrational transitions (~0.1 – 0.01 eV → IR)

$n = 0, 1, 2 \ldots$ is the vibrational quantum number

The energy of a given level is

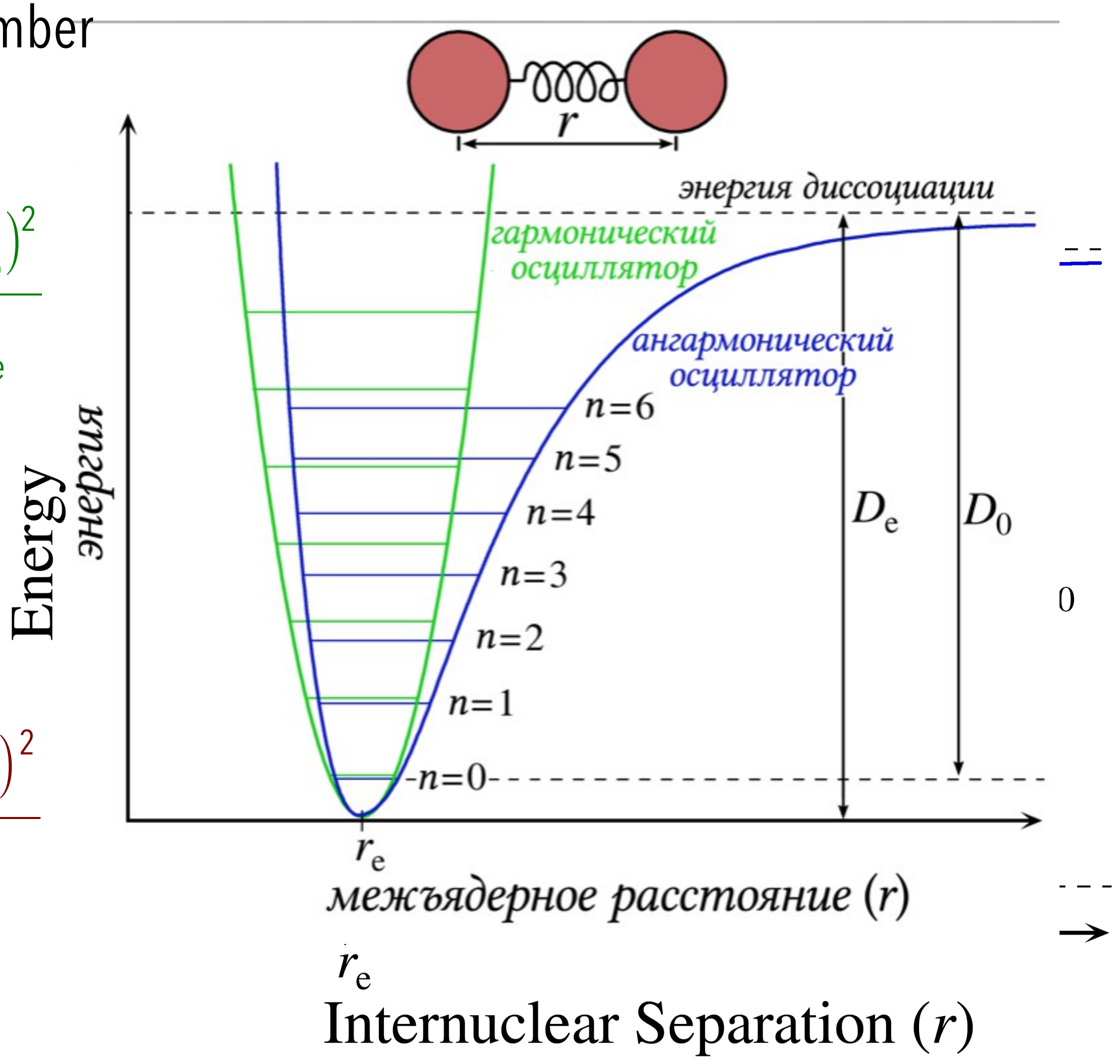
$$E_n = \left(n+\frac{1}{2}\right) h\nu_o - \left(n+\frac{1}{2}\right)^2 \frac{(h\nu_o)^2}{4D_e}$$

Transitions are allowed for $\Delta n = \pm 1$

Difference between two adjacent levels is

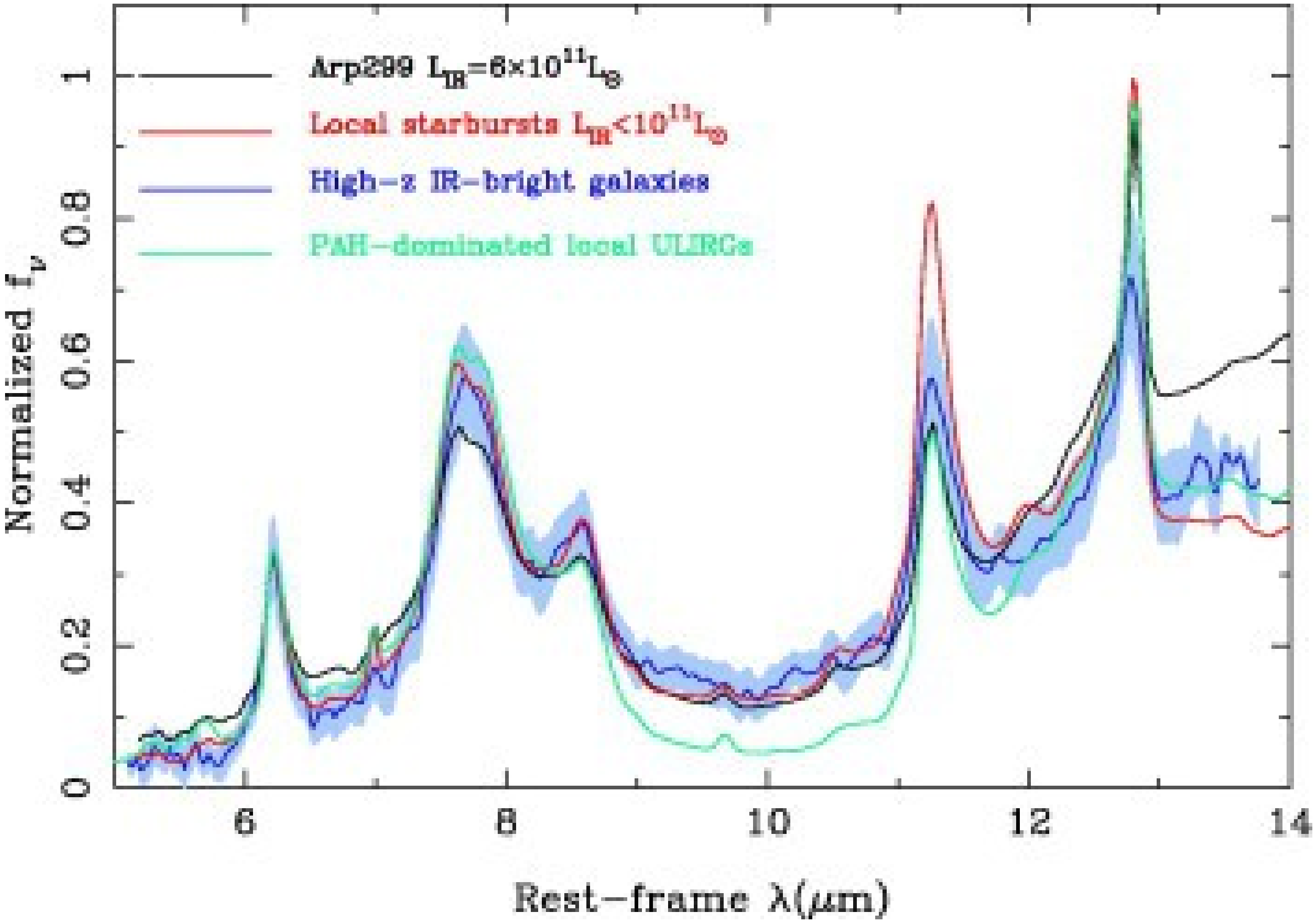
$$E_{n+1} - E_n = h\nu_o - (n+1) \frac{(h\nu_o)^2}{2D_e}$$

FYI,
Computations
never asked

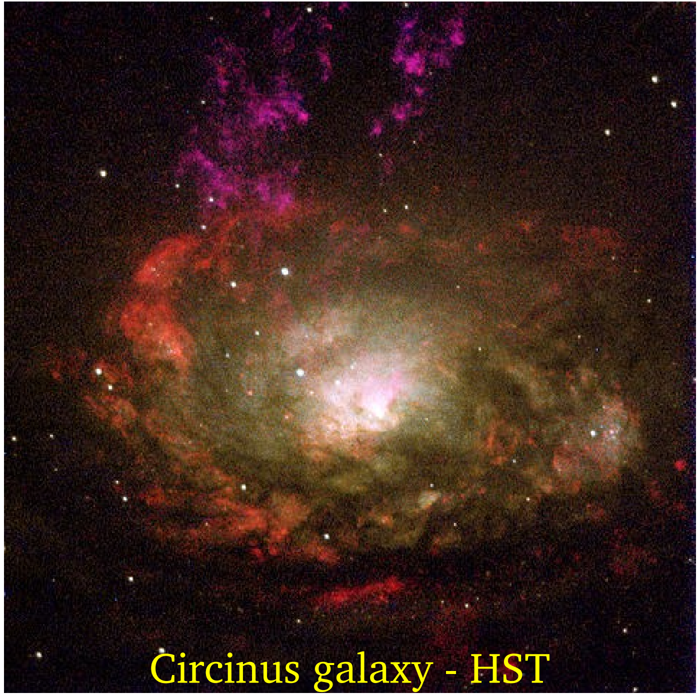


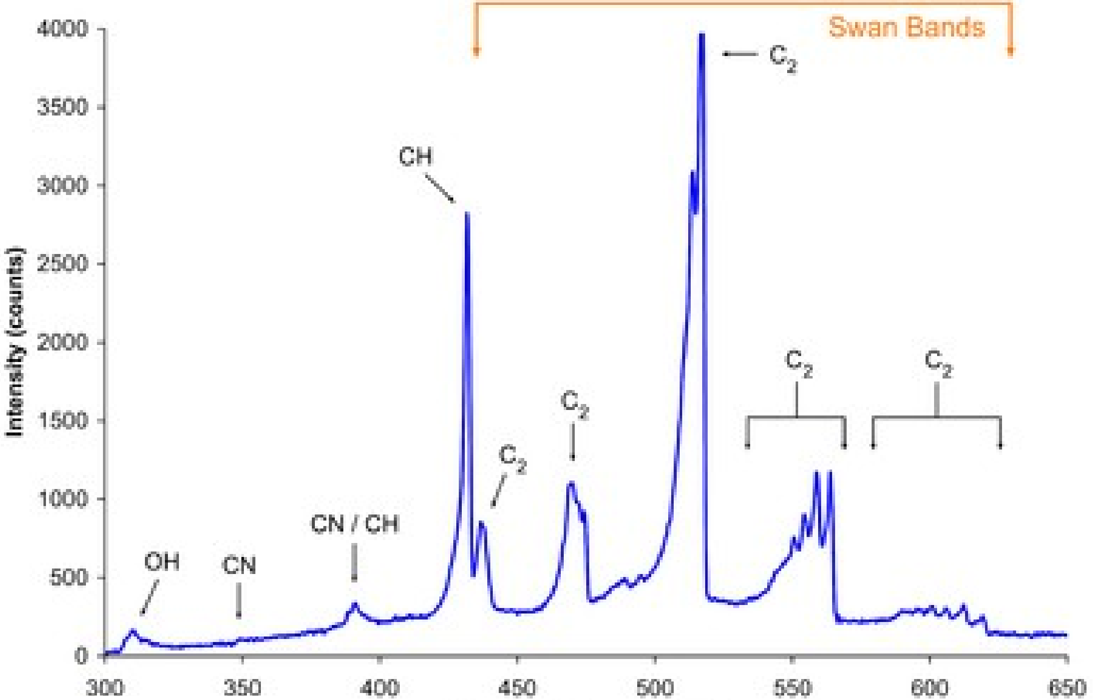
Molecular spectra (1b): NIR from vibrational transitions

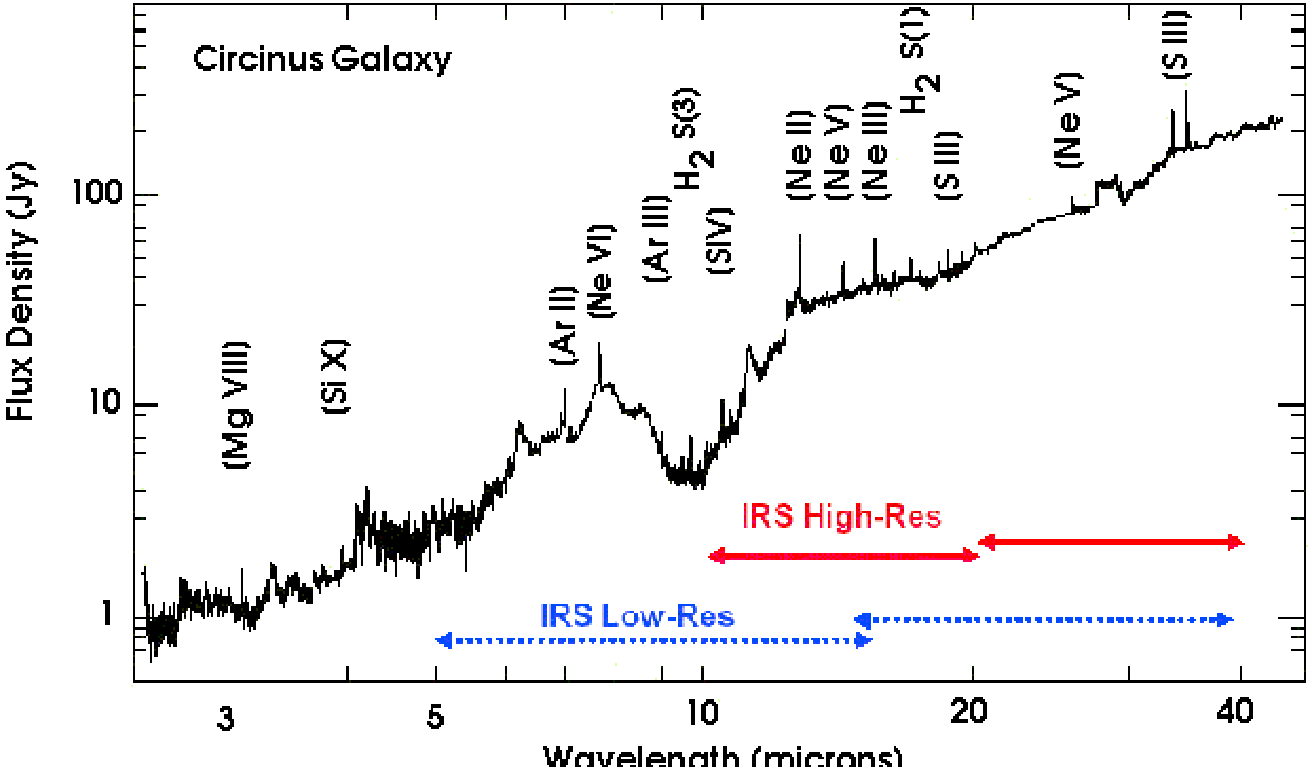
NIR composite spectra for various astrophysical bodies



Molecular spectra (1c): NIR & MIR, from vibrational transitions



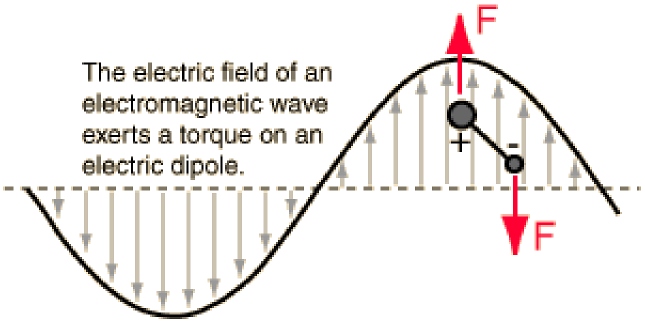


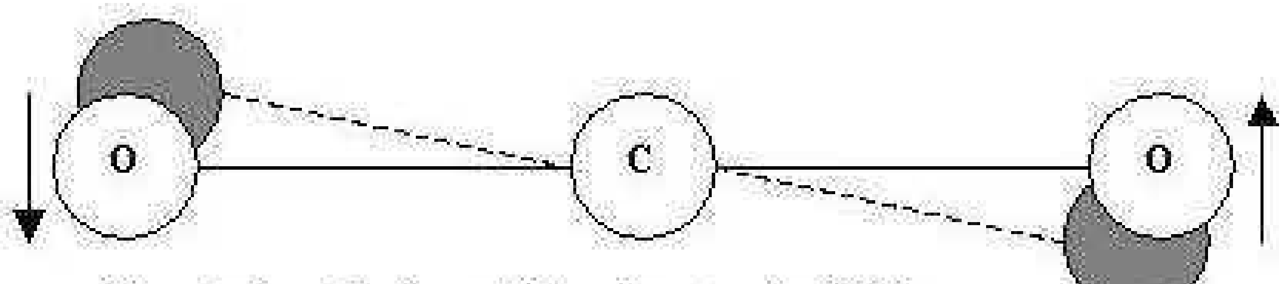


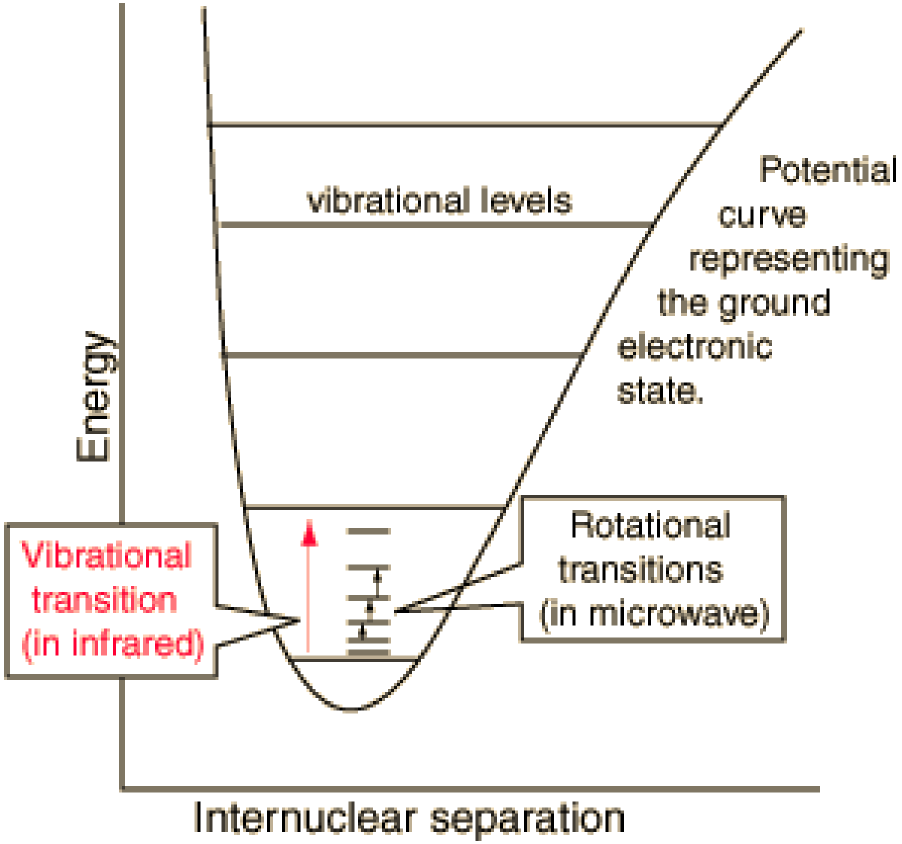
Molecular spectra (2):

rotational (~meV, submm, mm & cm wavelengths)

rotational levels lie within vibrational levels


The electric field of an electromagnetic wave exerts a torque on an electric dipole.

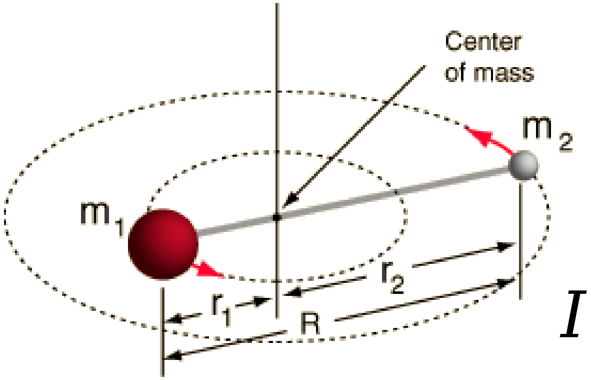

The rotation of a linear triatomic molecule, CO2



The rotational quantum number **J** is related to the moment of inertia **I**, to the distance **r** and to the rotational energy $\mathbf{E_{rot}}$:

$$J(J+1) = \frac{8\pi^2 I (r_1+r_2)^2 E_{rot}}{h^2}$$

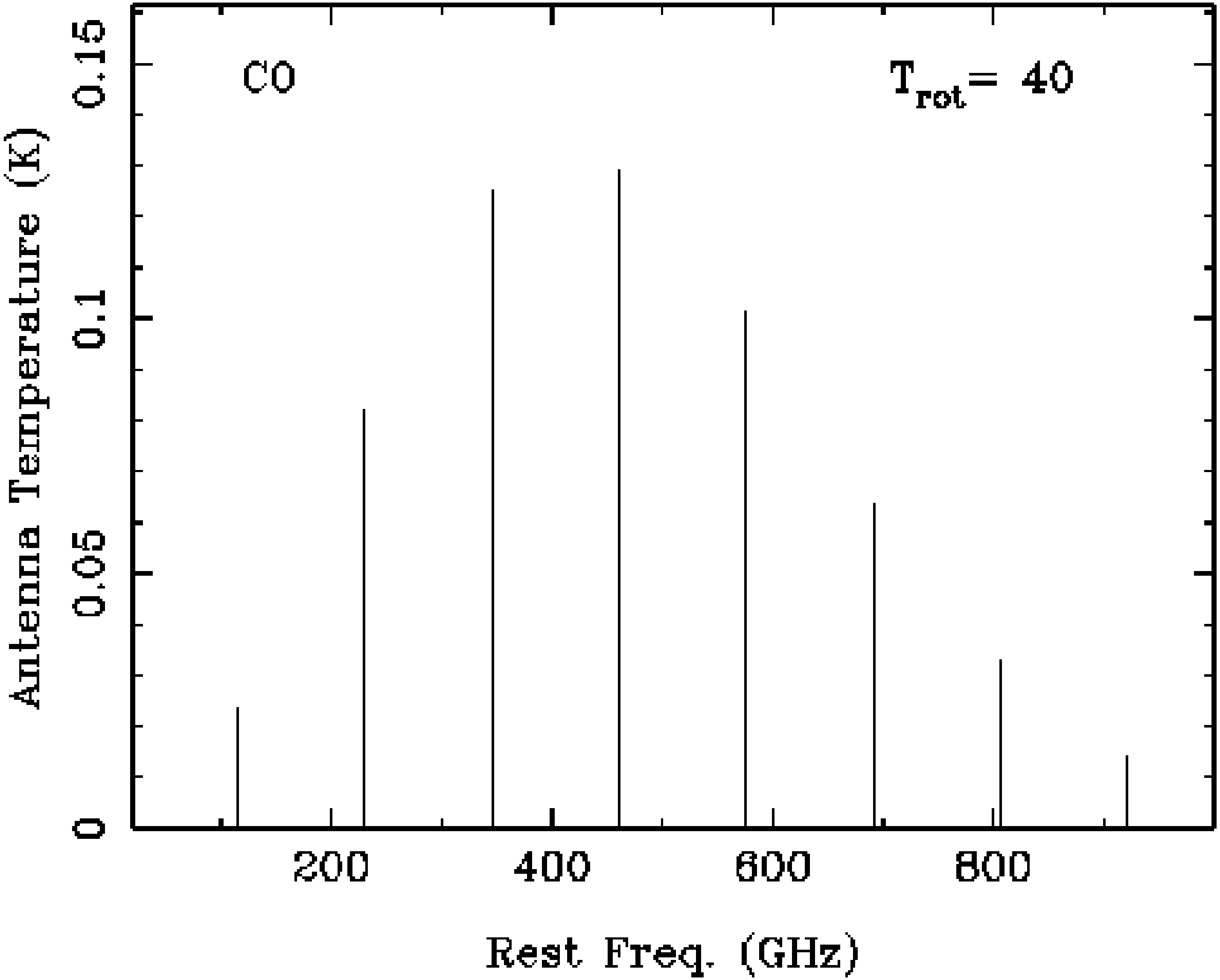
FYI, Computations never asked



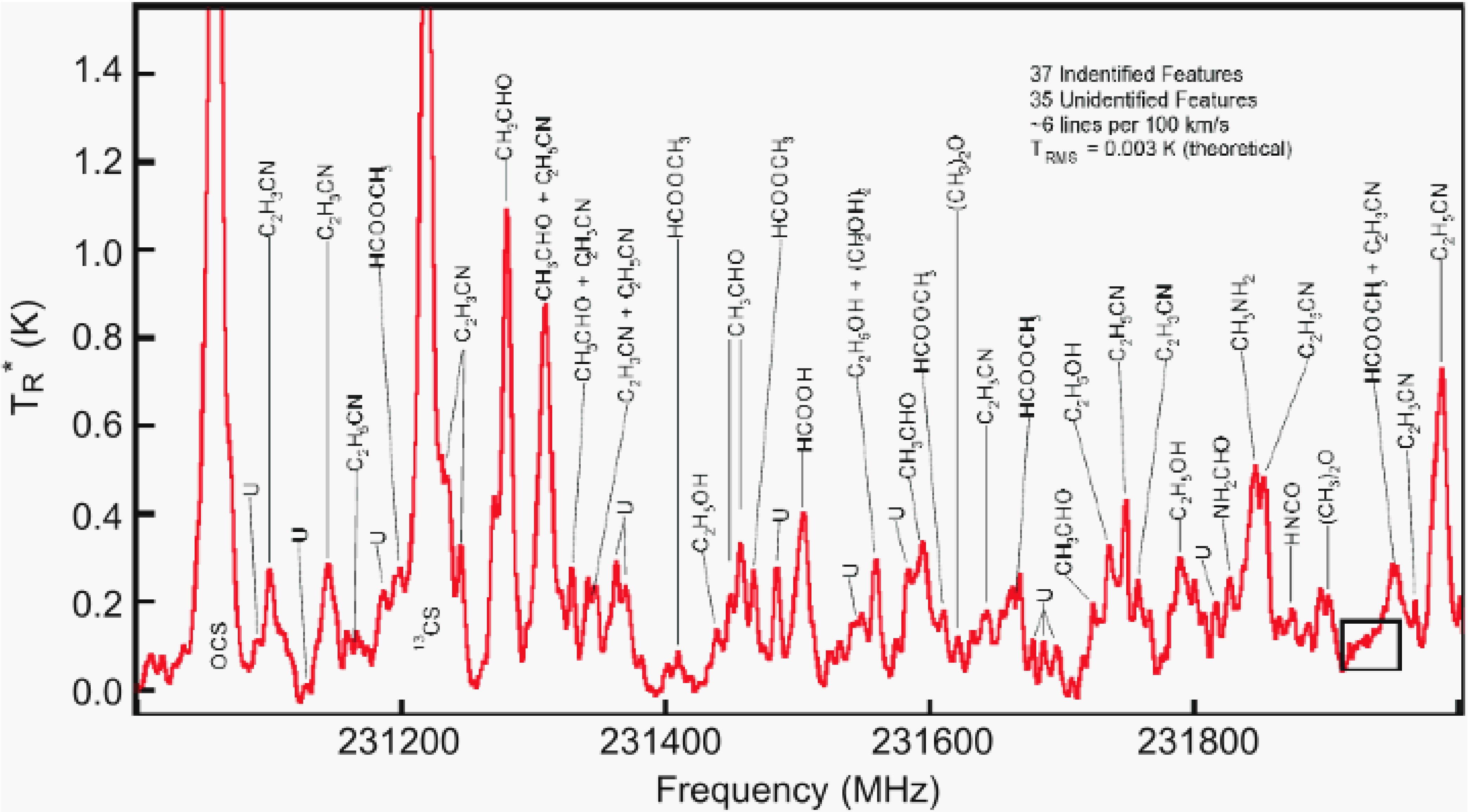
$$I = m_1 r_1^2 + m_2 r_2^2$$

Molecular spectra (2b):

CO emission in a dense, cold cloud (a GMC!)

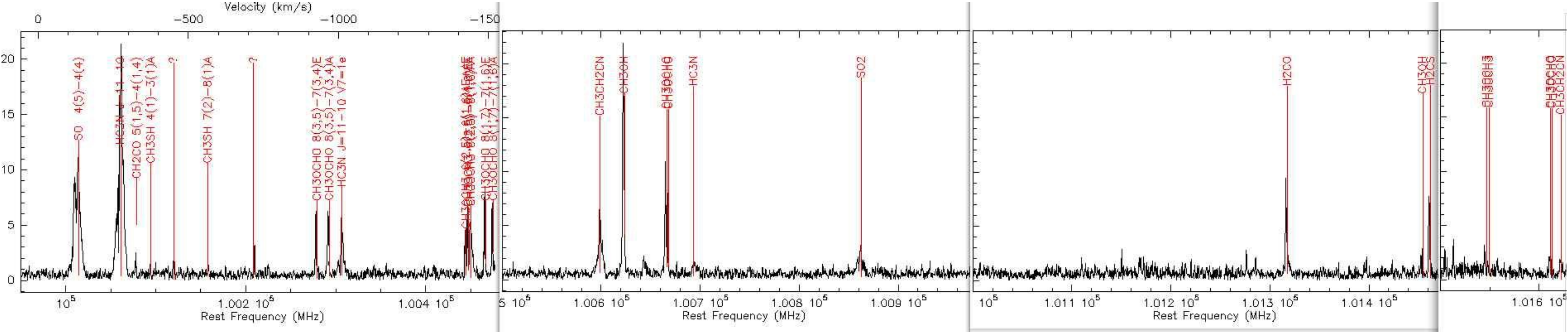


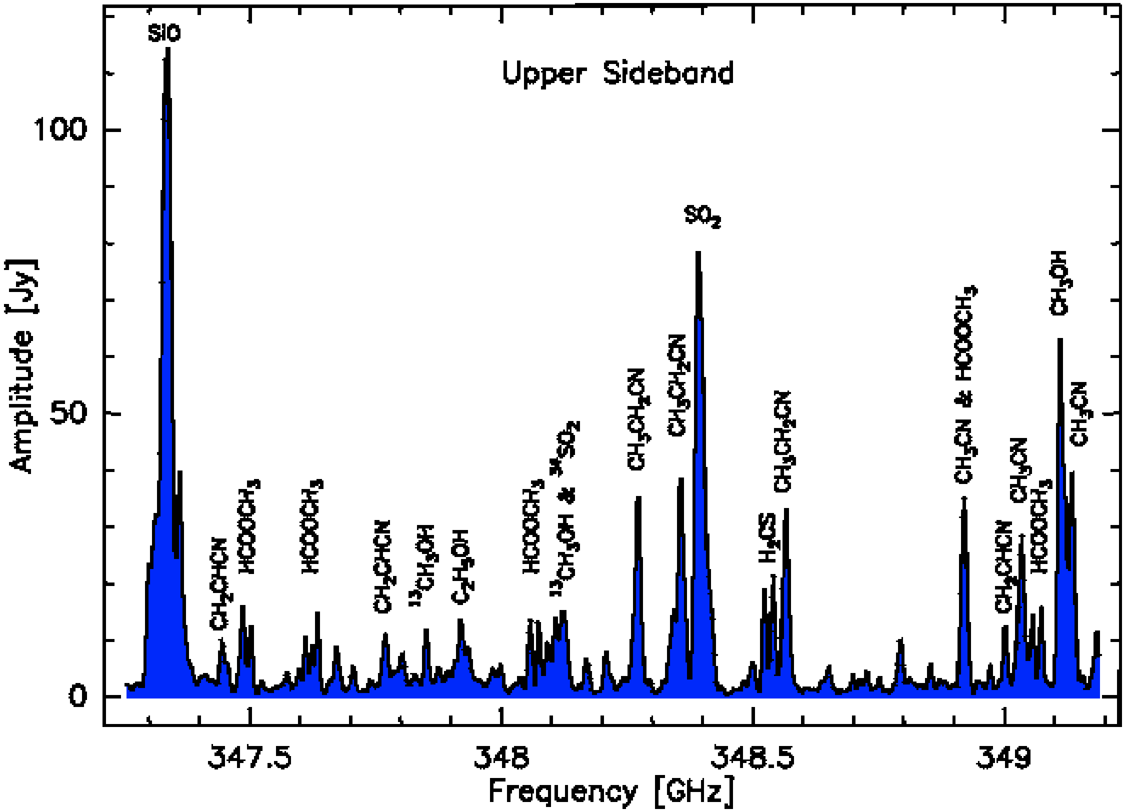
Molecular spectra (2c):



37 Indentified Features
35 Unidentified Features
~6 lines per 100 km/s
T_{RMS} = 0.003 K (theoretical)

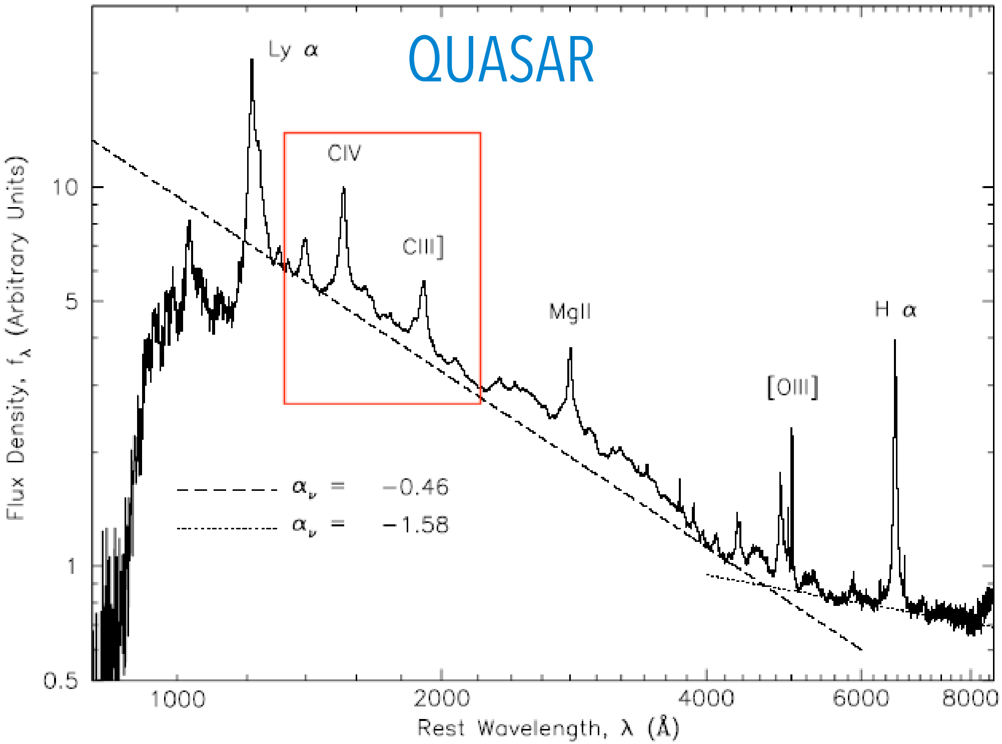
Molecular spectra (2d): transitions with ALMA

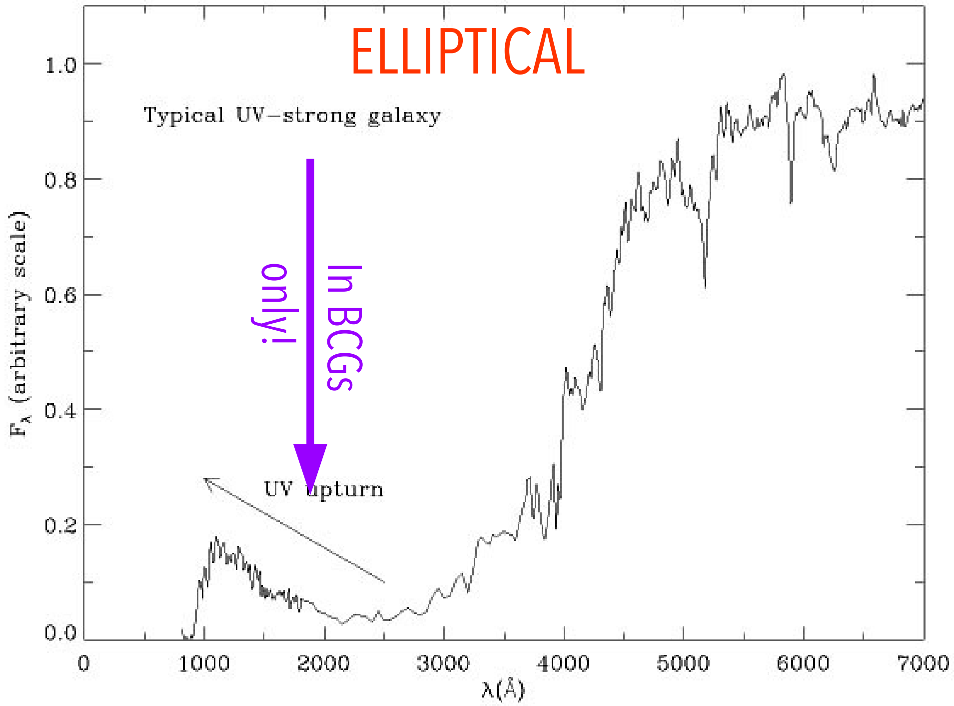


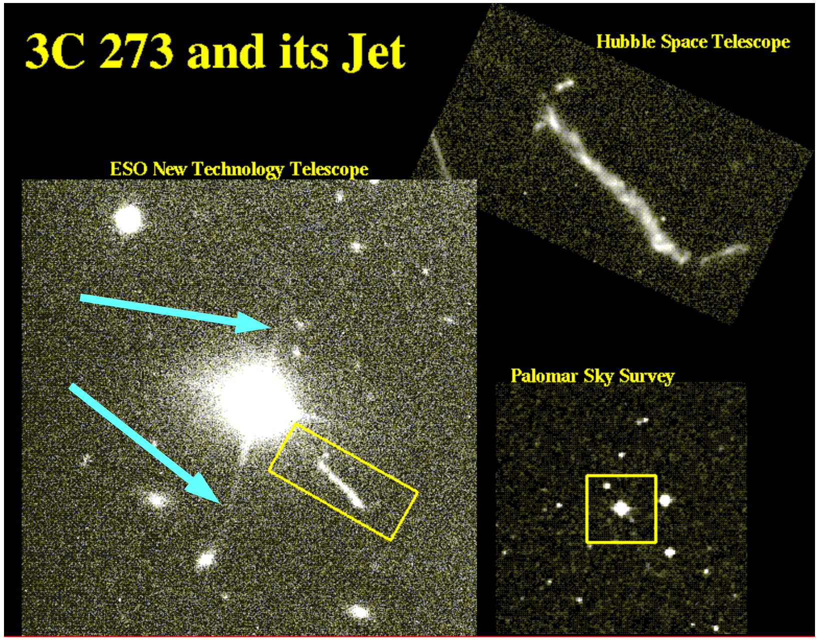


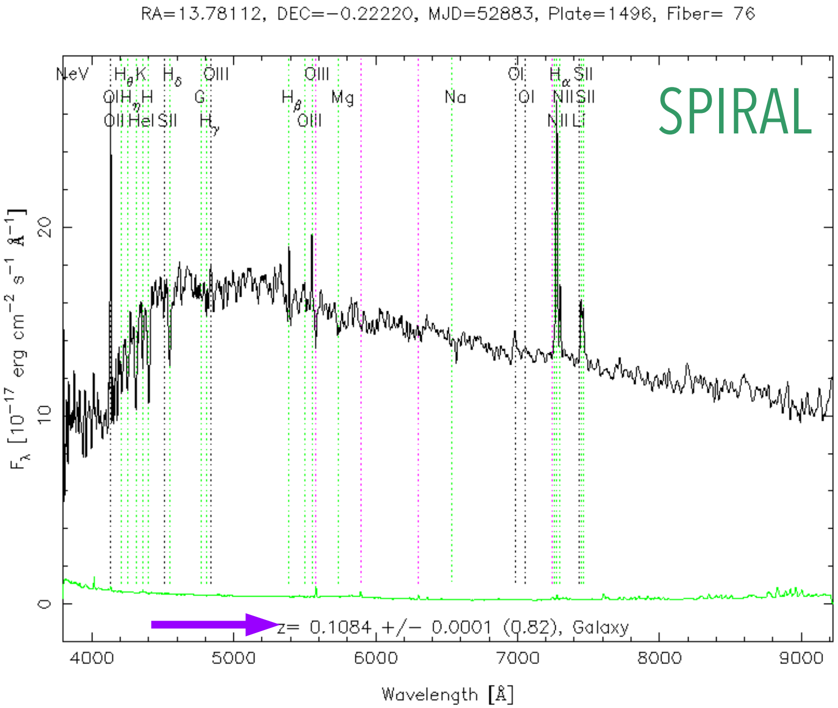
The hot core in Orion KL (high mass SFR)

Optical (& UV) spectra of galaxies









Atomic and molecular spectra: observational constraints

- Lines are generally associated to gaseous (plasma) fluids

- Lines appear either in emission or in absorption (* a background source is required!)

- Lines are not monochromatic

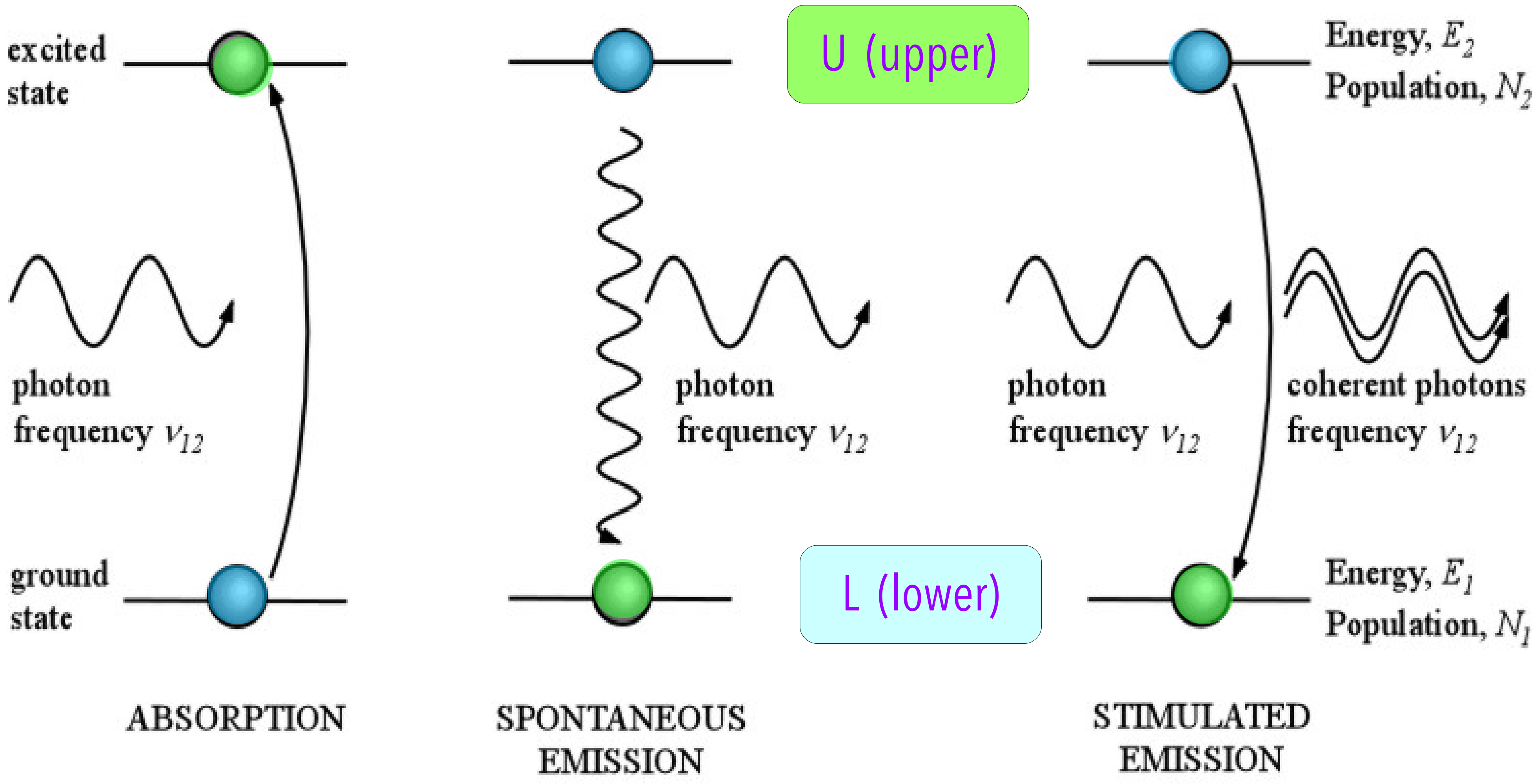
- Lines can be (red – blue) shifted

- Various elements may appear in the same spectrum (i.e. region ?)
  Projection effects ?
  Intrinsic association ? (In that case physical conditions have to be consistent!)

- Are line ratios a diagnostic for temperature?

Einstein's coefficients (1)

They are used to describe radiative interactions involving bound-bound electron transitions, on the basis of quantum mechanics. Simplest example: an atom with two energy levels only (approx)



Transition energy, $E_{12} = E_2 - E_1 = h\nu_{12}$

EINSTEIN A & B COEFFICIENTS

Einstein's coefficients (2)

Given two atomic levels U and $L, (\text{with}\, U > L)$ the following definitions hold:

Spontaneous emission:

A_{UL} = transition probability per unit time to go from level U to L by emission of a photon

Absorption:

$B_{LU}\,\bar{J}$ = transition probability per unit time to go from level L to U via absorption of a photon

Stimulated emission:

$B_{UL}\,\bar{J}$ = transition probability per unit time $U \rightarrow L$ via emission induced by incoming radiation

$\bar{J}$ represents the density of photons at (about) the frequency ν_{UL} so that $h\nu_{UL}$ corresponds to the difference between the energy levels U and L

A_{UL} is given in $\sec^{-1}$ units

$\frac{1}{A_{UL}}$ is the mean lifetime of the excited state

Einstein's coefficients (3)

The set of emitted photons IS NOT monochromatic

→ the energy difference between the two levels is not infinitely sharp.

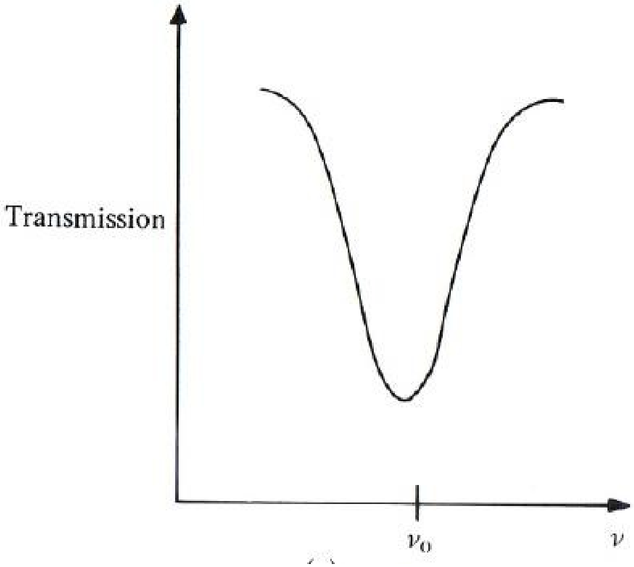
→ described by the line profile function (LPF) $\Phi(\nu)$ (sharply?) peaked at the frequency ν_{UL}

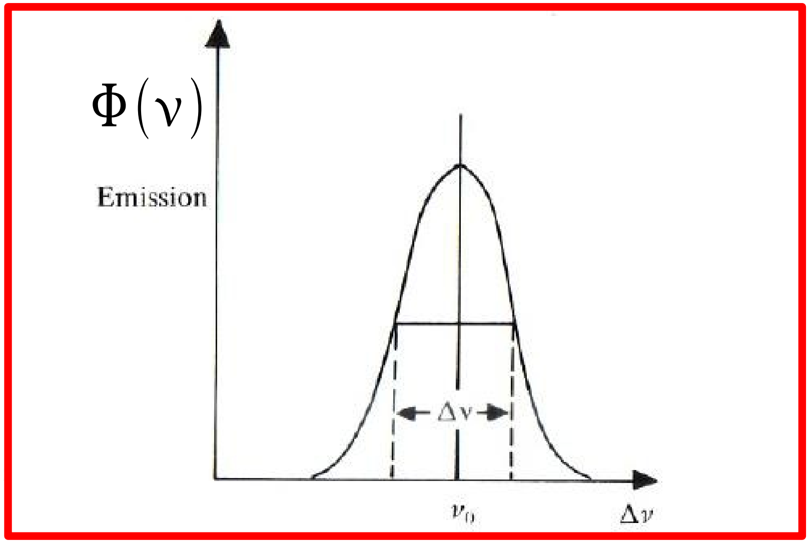
$$\boxed{\int_0^\infty \Phi(\nu)\,d\nu = 1}$$

It represents how effectively photons with frequencies around ν_{UL} can cause transitions

$$\bar{J} \equiv \int_0^\infty J(\nu)\Phi(\nu)d(\nu)$$

If $J(\nu)$ changes slowly with ν, then $\Phi(\nu)$ acts like a δ function





Spectral line broadening (1)

Natural (Lorentz) broadening

An atom at an excited state has a finite lifetime $\Delta t \simeq \frac{1}{A_{UL}}$

The energy difference is finite as well $\Delta E = \Delta h \nu$

The decay therefore follows the Heisemberg's Principle in the form $\Delta E \Delta t \geq \frac{h}{2\pi}$

$$\Delta E \Delta t = \Delta h \nu \frac{1}{A_{UL}} \geq \frac{h}{2\pi}$$

$$\boxed{\Delta \nu \geq \frac{A_{UL}}{2\pi}}$$

and this is the **minimum width** allowed for the transition between levels U, L

WARNING : **large/small** values of A_{UL} imply **broad/narrow** lines

Spectral line broadening (2)

– see Chap 7 in Padmanabhan

Doppler (thermal) broadening

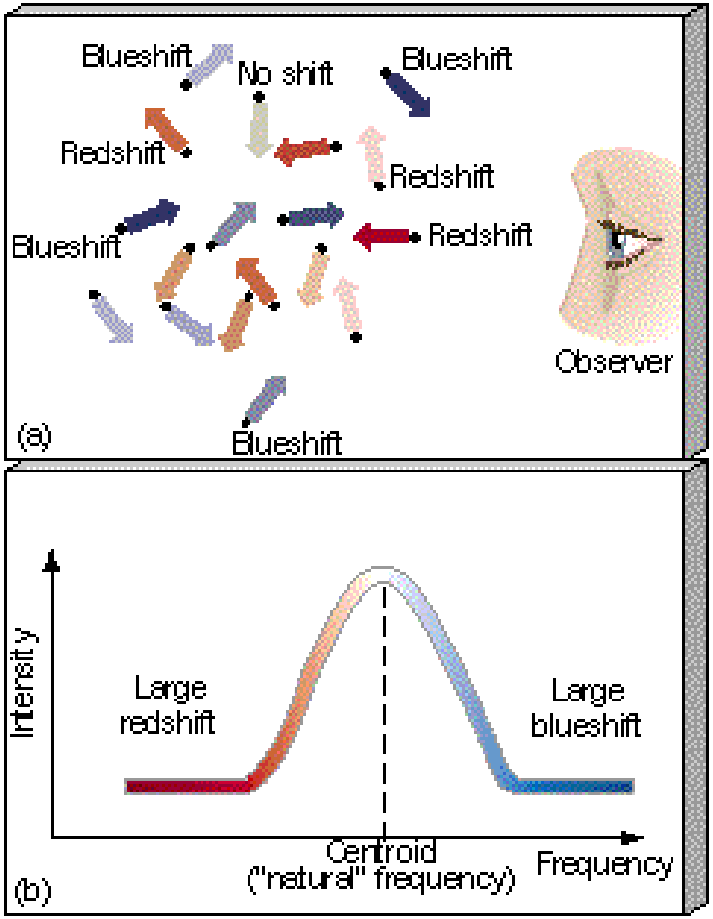
Atoms are in (thermal) motion wrt the observer and the rest (atom) frame frequencies may be either red- or blue- shifted. If v_r is the radial velocity

$$\Delta \nu = \nu_{obs} - \nu_{em} = \nu_{em} \frac{v_r}{c}$$

It is possible to derive the radial velocity (redshift / blueshift)

$$v_r = c \, \frac{\nu_{obs} - \nu_{em}}{\nu_{em}}$$

[OK for small v_r]



→ **the shape of the line is modified, the total energy is not**

N.B. **The centroid** (= "natural frequency") **remains unchanged;**
Only in the case that the **whole cloud is moving, then also the centroid is (Doppler) shifted**

Spectral line broadening (3) – v_r and temperature

In case we are at thermal equilibrium (Maxwell-Boltzmann)

$$N(v_r)\,dv_r \simeq N_o\, v_r^2\, e^{\frac{-m_a v_r^2}{2kT}}\, dv_r$$

where m_a is the mass of the atom

$$N(\nu)\,d\nu \simeq N_o\, e^{\frac{-m_a c^2}{2kT}\,\frac{(\nu_{obs}-\nu_{em})^2}{\nu_{em}^2}}\, d\nu$$

And in this case the Line Profile Function becomes (if we introduce the Doppler width)

$$\boxed{\Delta\nu_D = \frac{\nu_{em}}{c}\sqrt{\frac{2kT}{m_a}}}$$

And the LPF is

$$\Phi(\nu) = \left(\Delta\nu_D\sqrt{\pi}\right)^{-1}\exp\left(-\frac{(\nu_{obs}-\nu_{em})^2}{(\Delta\nu_D)^2}\right)$$

Valid also in case of turbulence, once modified the Doppler width by introducing ξ, the rms of turbulent velocities (with Gaussian distribution)

$$\Delta\nu_D = \frac{\nu_{em}}{c}\sqrt{\frac{2kT}{m_a} + \xi^2}$$

FYI,
Computations
never asked

Spectral line broadening (4)

The LPF for natural broadening is

$$\Phi(\nu) = \frac{\gamma/4\pi^2}{(\nu_{obs}-\nu_{em})^2+(\gamma/4\pi)^2} \qquad \text{where} \qquad \gamma = \sum_L A_{UL}$$

or $\gamma = \gamma_U + \gamma_L$, in case there are transitions from a lower level too (inclusive of radiation field and appropriate B_{UL})

Collisional broadening

FYI, Computations never asked

Collisions introduce random changes to the phase of E/B field

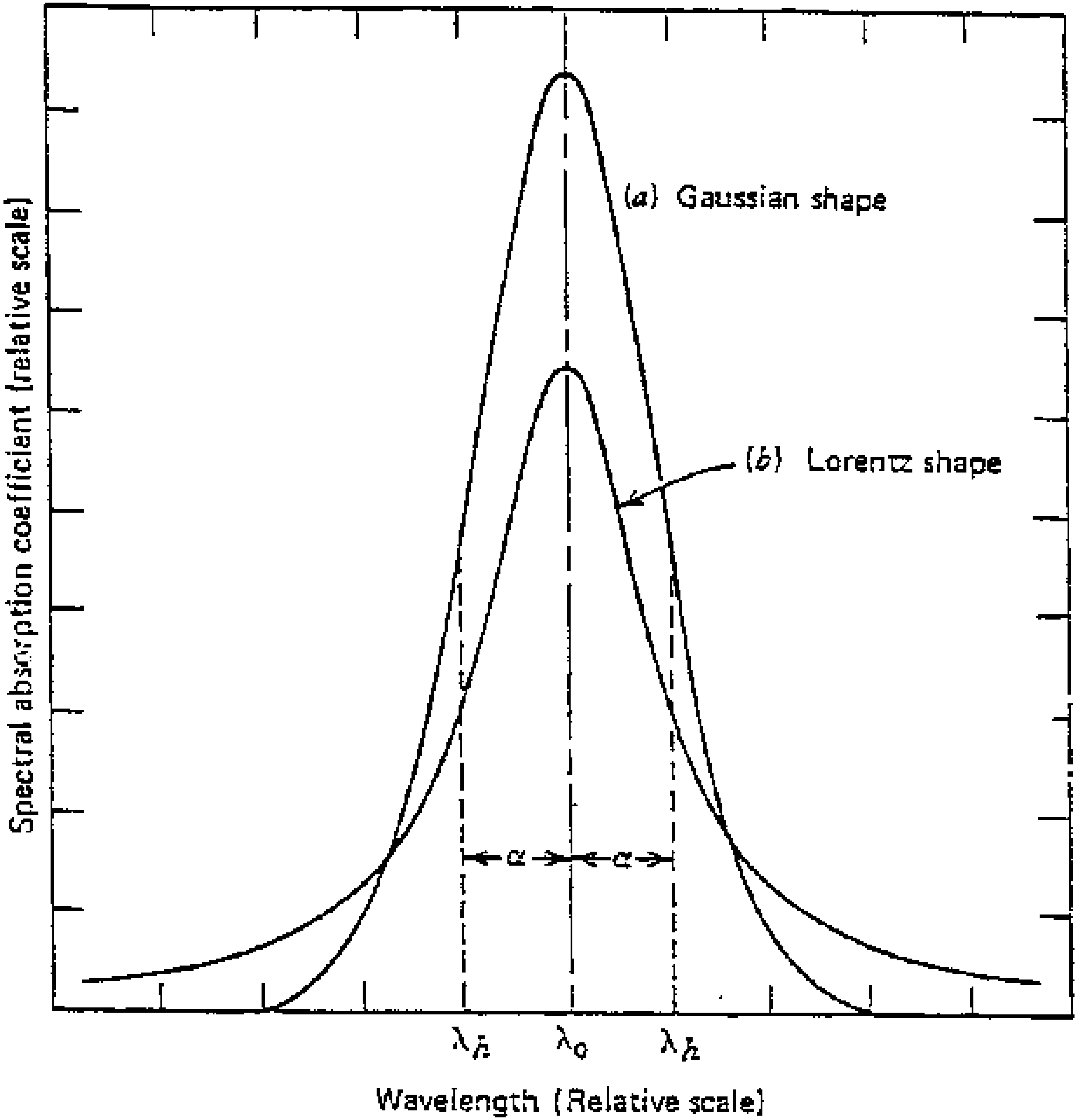
$$\Phi(\nu) = \frac{\Gamma/4\pi^2}{(\nu_{obs}-\nu_{em})^2+(\Gamma/4\pi)^2}$$

where $\Gamma = \gamma + 2\nu_{coll}$

ν_{coll} is the frequency of collisions per unit time an atom experiences.

Atoms hit other particles during emission (absorption). All broadening mechanisms coexist, with Doppler and Lorentz broadenings being dominant.

Spectral line broadening (5)

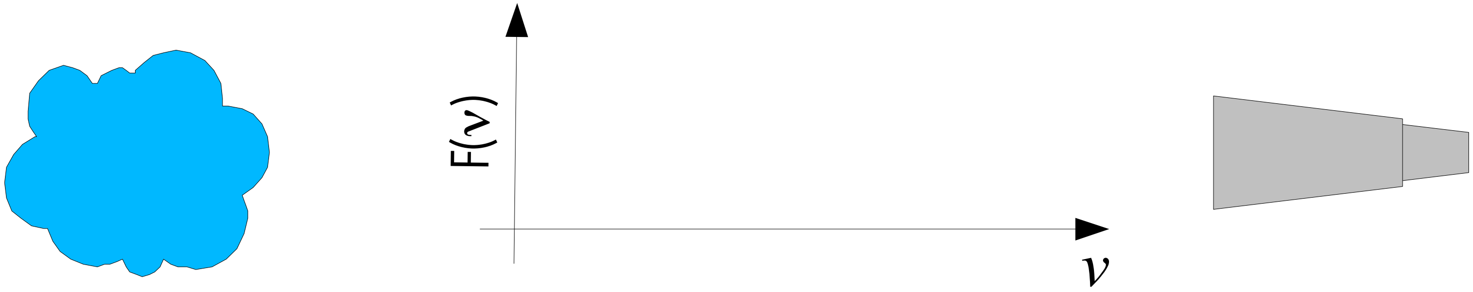


Spectral line shape produced by: (a) Doppler broadening and (b) natural and collision broadening (taken from Levi (1968)).

Test (1) : Do we understand how it works?

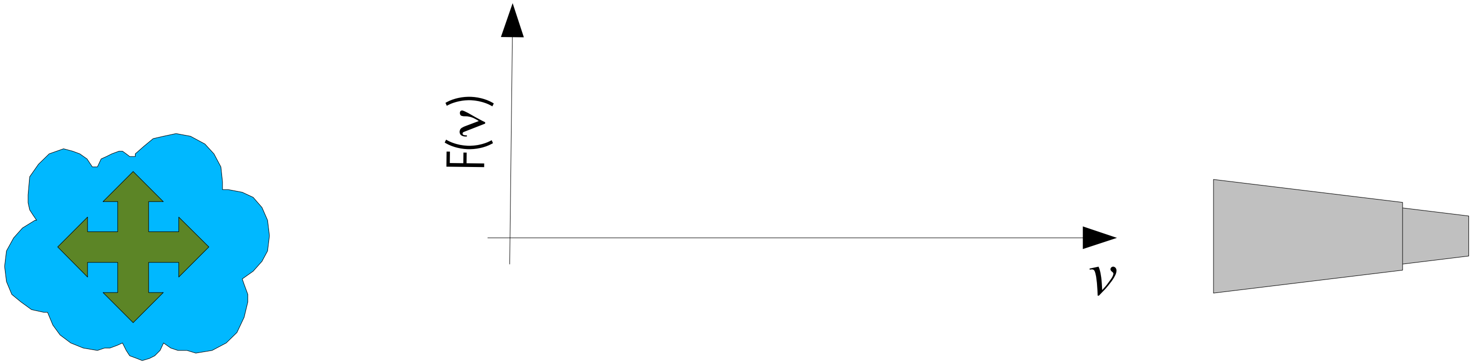
question 1:

(e.g. a standing cloud)



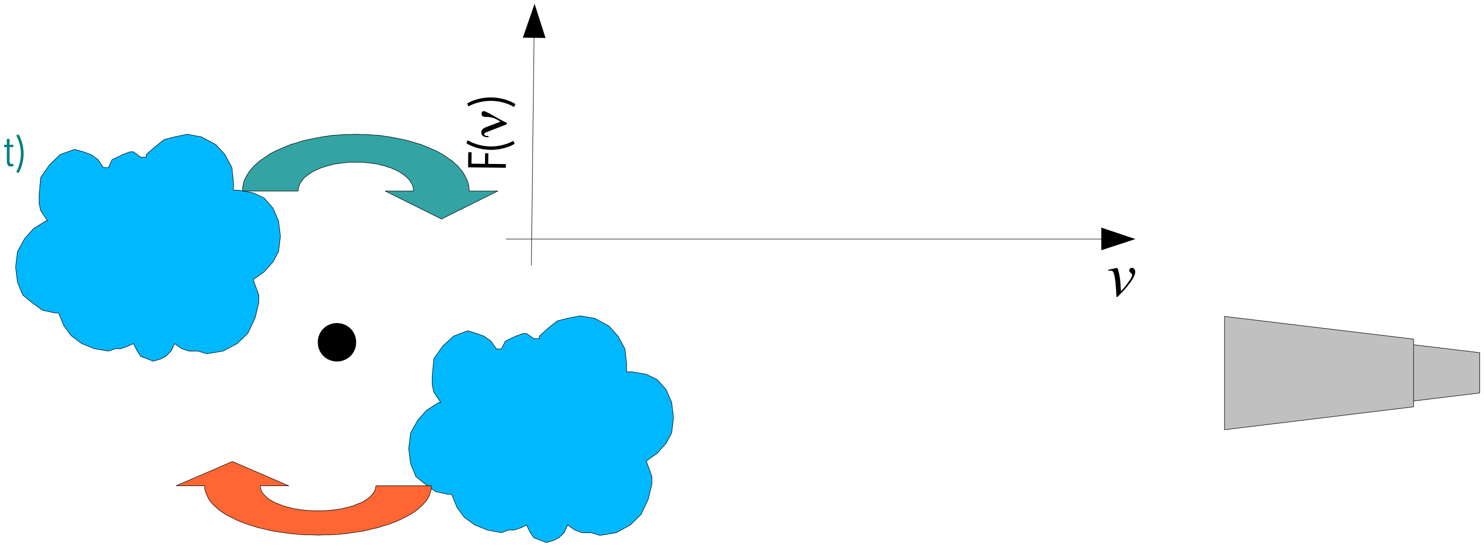
question 2:

(e.g. an expanding cloud)



question 3:

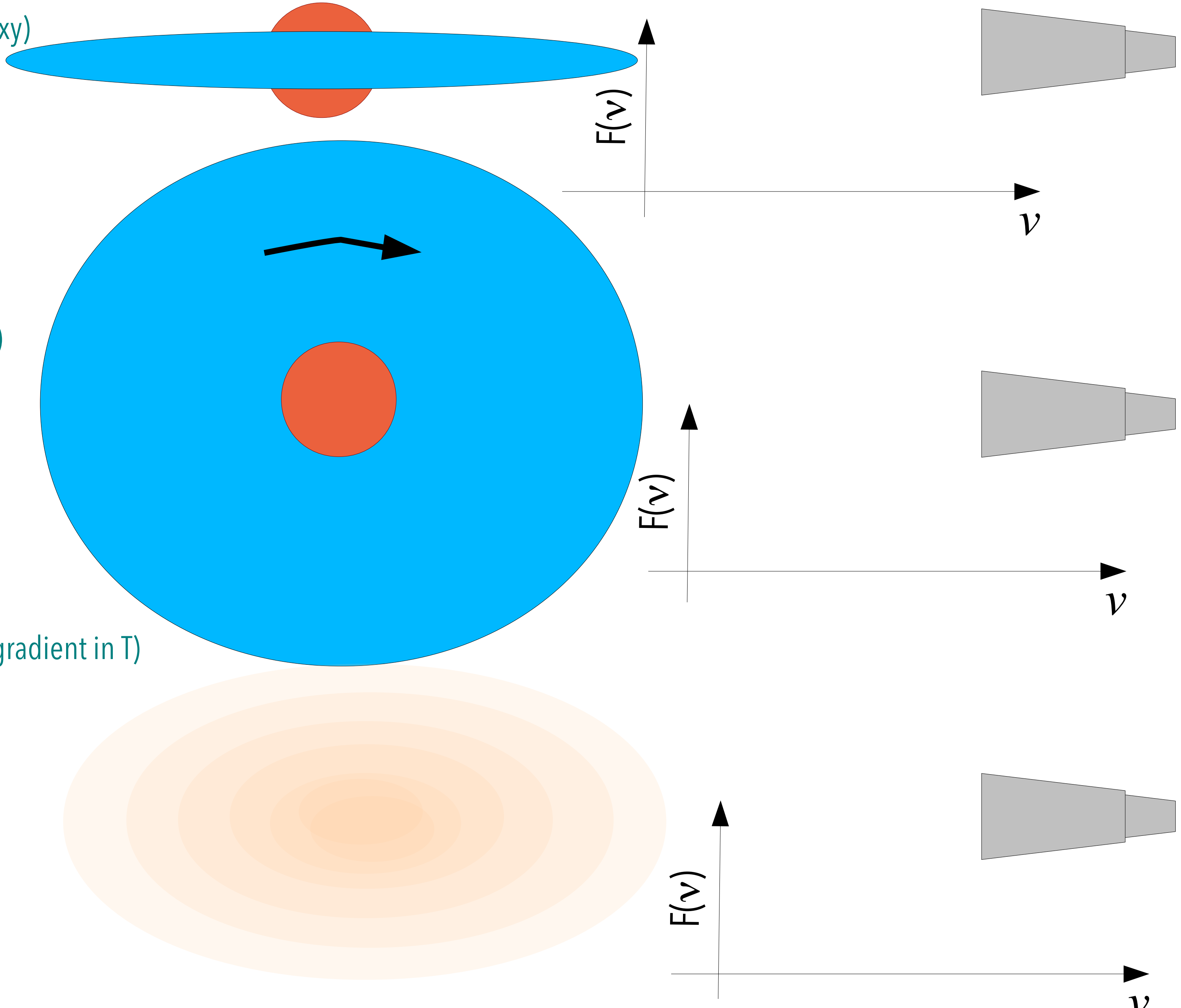
(2 clouds orbiting around a point)



Test (2) : Do we really understand how it works?

question 4:

(e.g. an edge-on spiral galaxy)

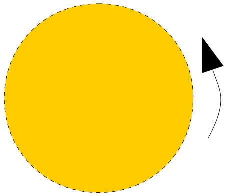


question 5:

(e.g. a face-on spiral galaxy)

question 6:

(e.g. a stratified gas with a gradient in T)



question 7:

(e.g. a rotating star)

Test (+) : Answers

[the layout of this page stands as it is to leave room for individual answers]

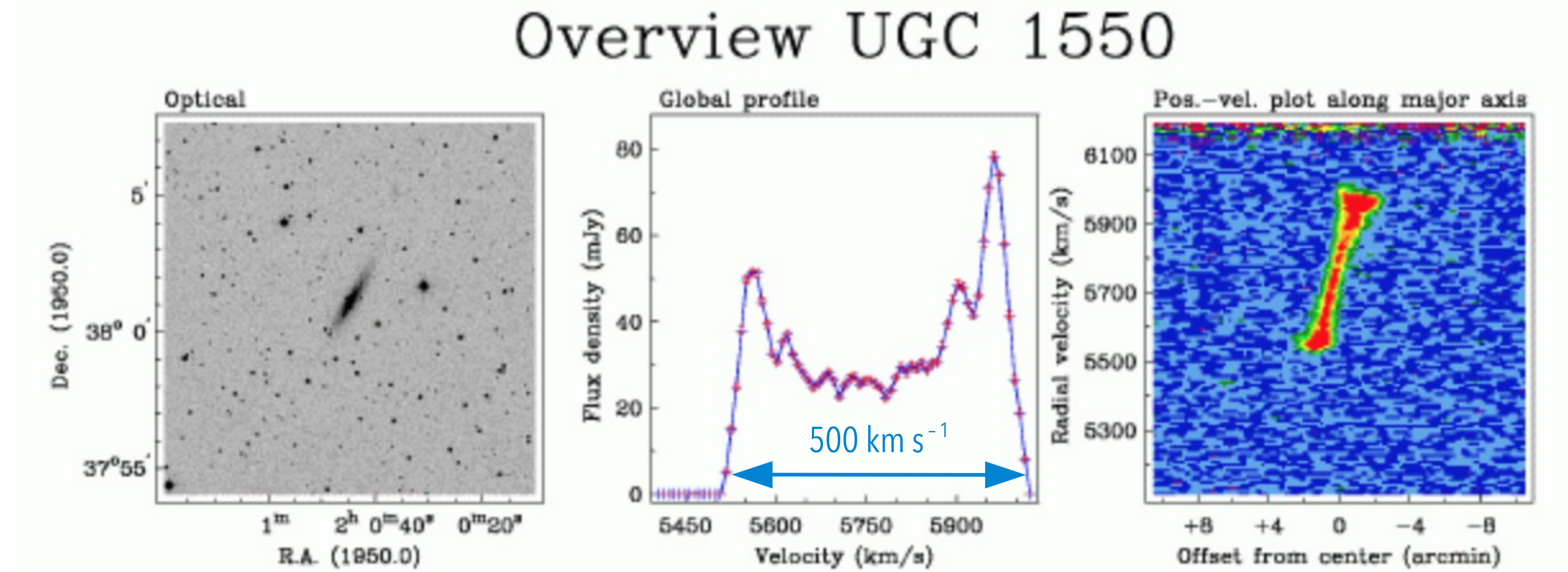
Question 1/4:

Question 2/5:

Question 3/6:

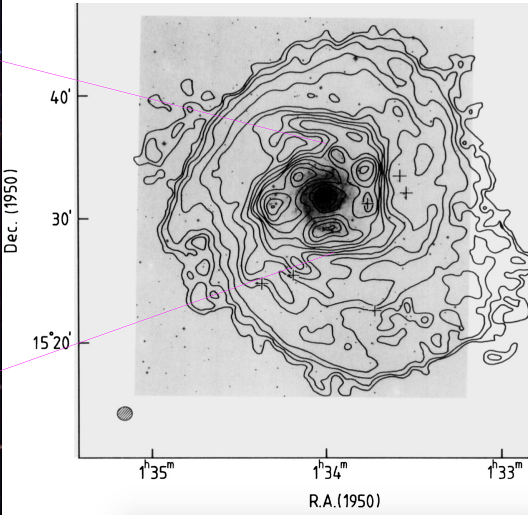
Question 7: What are the key factors? (rotation velocity + inclination angle)

Examples of edge–on and face–on spiral galaxies




Messier 74 (NGC 628)

Messier 74 (NGC 628) is a Grand Design spiral galaxy located at 32 million light-years from Earth, 1.5° east-northeast of Eta Piscium, the brightest star in the constellation Pisces. It is the brightest member of the M74 Group, a group of 5-7 galaxies.



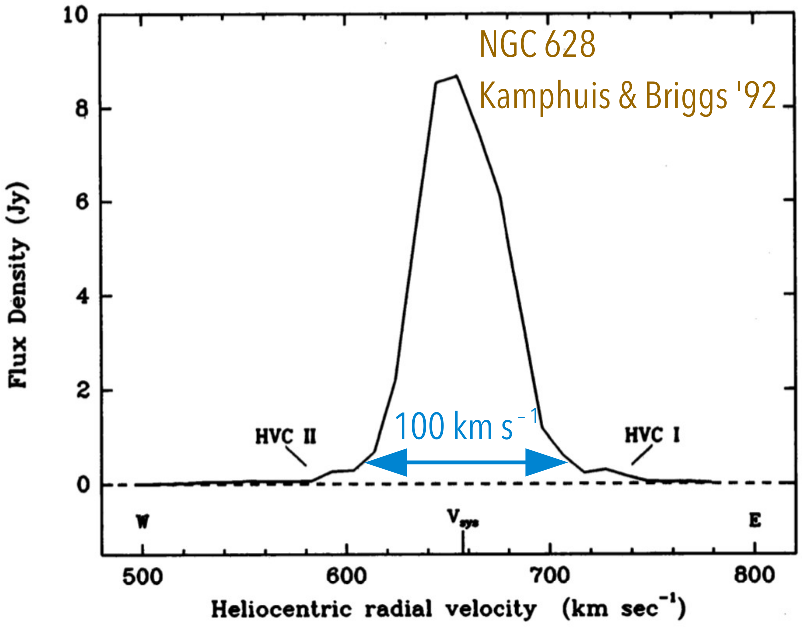


Fig. 4. Global HI profile obtained by integrating the "continuum subtracted" channel maps. Indicated are the systemic velocity V_{sys} and the high velocity gas complexes

Color coded image of the M81 Group

De Blok et al. 2018

The galactic disk is interpreted as the sum of many clouds, each with the same emission.

The M81/M82/NGC3077 group

Color image: gas emission

The centroid is shifted according to their v_r

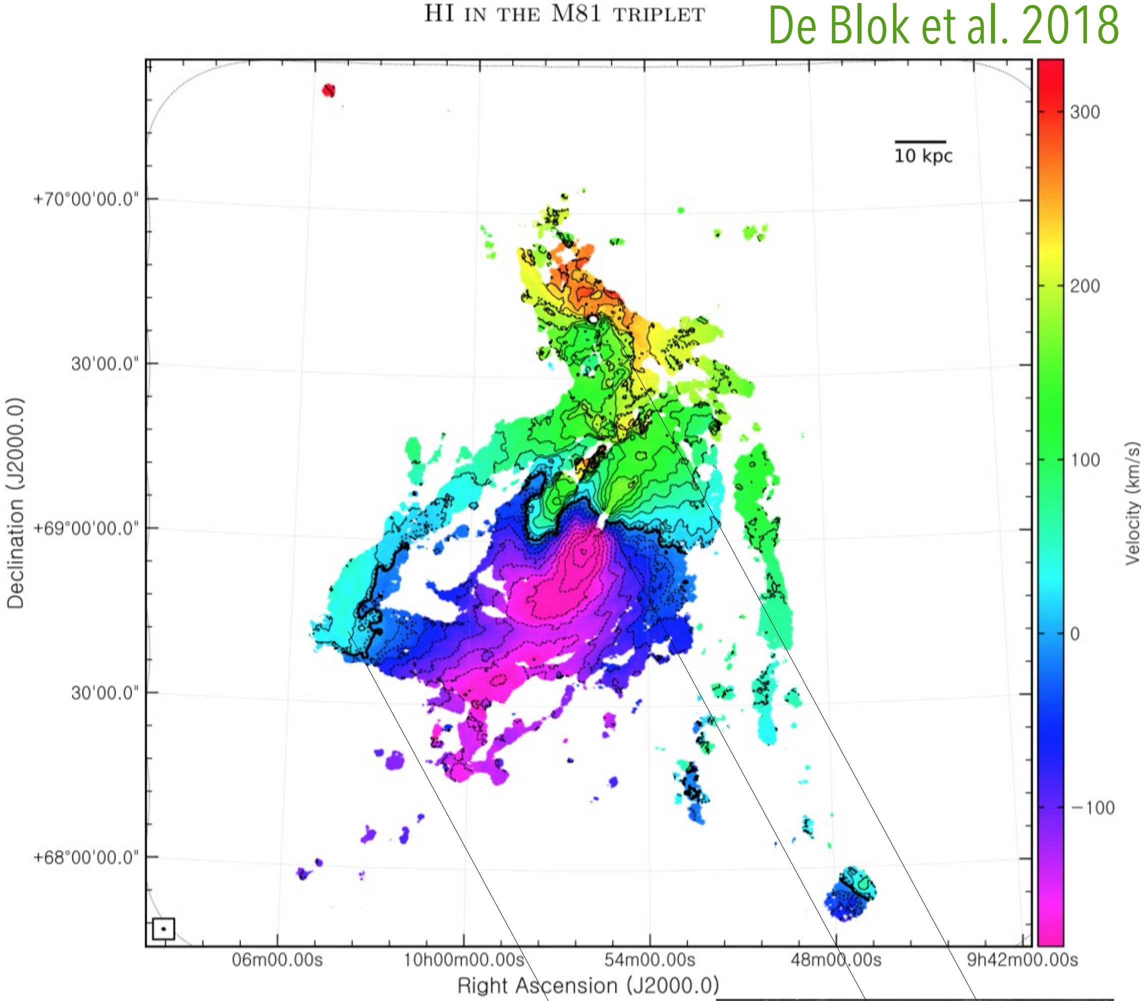
Magenta & Blue regions are approaching

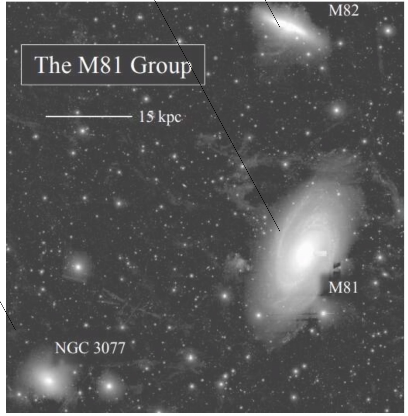
Cyan, Green & Yellow/Orange regions are receeding.

Bridges of gas are connecting the 3 galaxies

Bottom right:

optical image (stars) with the same scale as the color image





A deep, wide-field g-band mosaic of the M81 Group, taken with Subaru HSC.

Balmer JUMP/ Discontinuity:

Visible in continuum from stars

- Origin:

  bound-free transition, electrons from n=2 are ionised

- Effect:

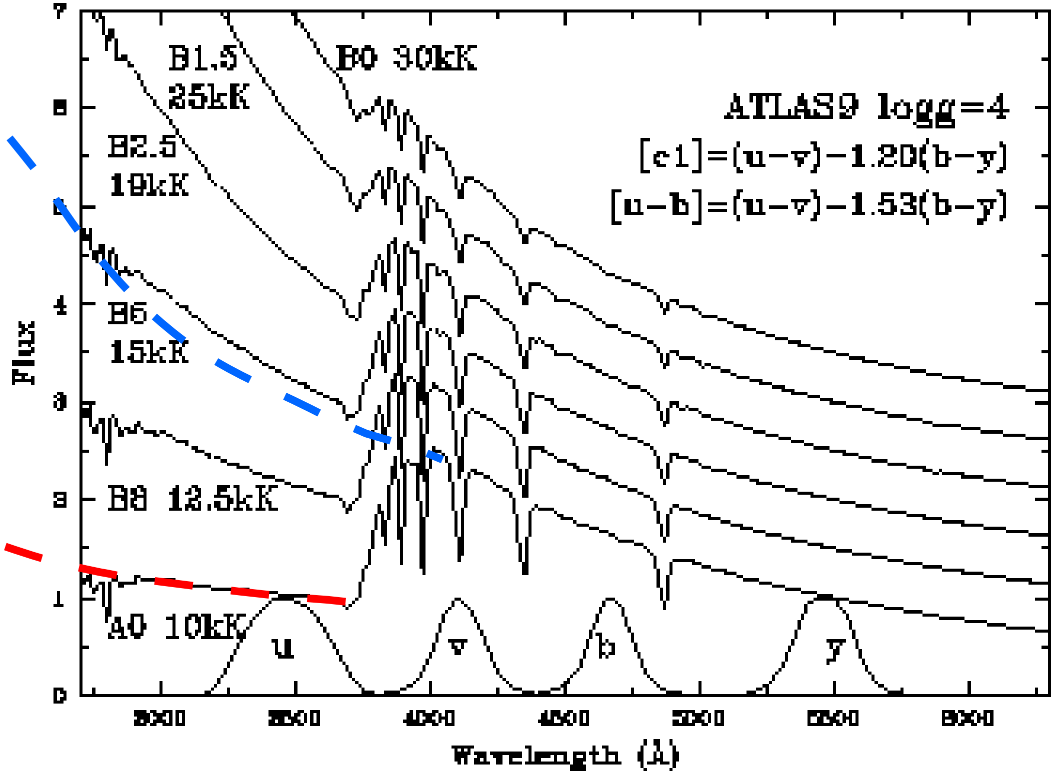
  depression of the continuum

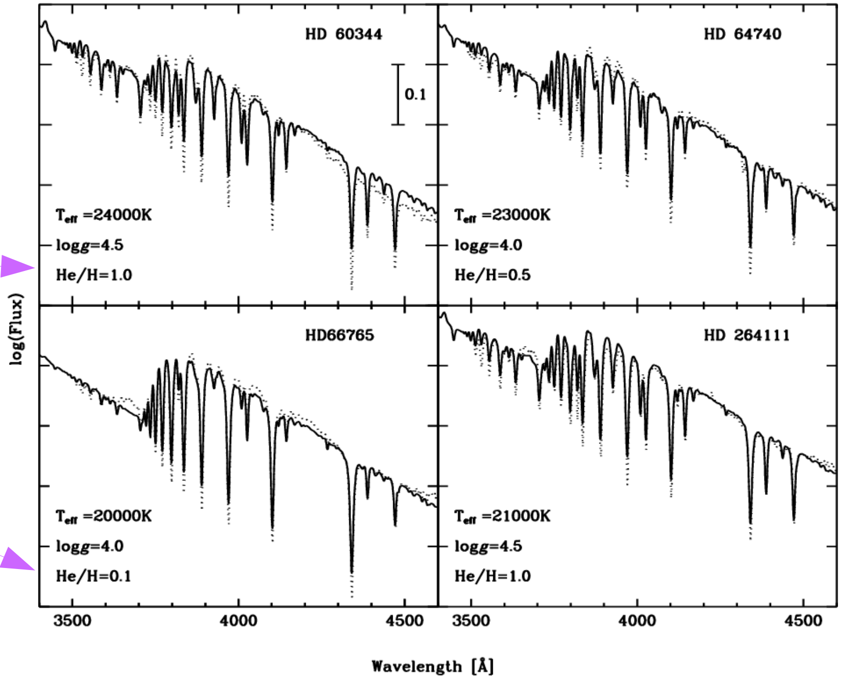
- Depends on:

  Density (composition) & Temperature of the region responsible for the absorption (largest in A-type stars)

- Located at:

  The Balmer series limit and higher energies





Atoms as oscillators: electronic transitions

Basic concept: e-m waves are radiated at the same frequency of an oscillating charge

$$d(t) = q \cdot x_o \cos(\omega t) \qquad [= e \cdot x_o \cos(\omega t)]$$

In terms of quantum mechanics, we have the **wave function** Ψ (probability density)

$$\Psi(\vec{r},t) = \psi(x,y,z)\; e^{-2\pi i (E/h) t}$$

space / time dependent

In turn, $\psi(x,y,z) \equiv \psi(r,\theta,\phi)$ in case of central potential

$$\psi(r,\theta,\phi) = \frac{R(r)}{r}\, Y(\theta,\phi)$$

(spherical harmonics)

$$Y(\theta,\phi) = Y_{lm}(\theta,\phi) = \left[\frac{(l-|m|)!}{(l+|m|)!}\,\frac{2l+1}{4\pi}\right]^{1/2} (-1)^{(m+|m|)/2} P_l^{|m|} \cos\theta\, e^{im\phi}$$

$P_l^{|m|}$ Legendre function, l & m integers

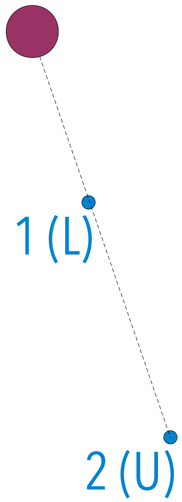
$Y_{lm}(\theta,\phi) \rightarrow$ eigenfunctions of the orbital angular momementum

FYI,
Computations
never asked

Atoms as oscillators: electric dipole transitions (1)

Basic concept:the dipole (i.e. nucleus + electron) may be written as

$$d_x(t) = \int e\cdot\mathbf{x}\,\Psi\,\Psi^*\,d\tau \qquad (\text{the same also for } y\,,z)$$



and more in general for a generic transition from $U \rightarrow L$

$$d_x^{UL}(t) = \int e\cdot\mathbf{x}\,\Psi_U\,\Psi_L^*\,d\tau = \int e\cdot\mathbf{x}\,\psi_U\,\psi_L^*\;e^{-2\pi i t(E_U-E_L)/h}\,d\tau$$

(the same also for y,z)

Using 3-D notation

$$\vec{d}^{UL}(t) = e\cdot\vec{R}^{UL}(t)\;e^{-2\pi i t(E_U-E_L)/h}$$

where: $R_x^{UL}(t) = \int \mathbf{x}\,\psi_U\,\psi_L^*\,d\tau$ [the same for $R_y^{UL}(t), R_z^{UL}(t)$]

i.e. $\vec{R}^{UL}(t) = \int \vec{\mathbf{r}}\,\psi_U\,\psi_L^*\,d\tau$

FYI,
Computations
never asked

$\vec{R}_{UL}$ provides the amplitude of the vibration/variation of $\vec{d}_{UL}$ in the transition $U \rightarrow L$

Atoms as oscillators: electric dipole transitions (2)

Emitted power & **the meaning of A_{UL}**

In classical physics, during dipole transitions, the electron "makes an oscillation" with a given ω:

$$d(t) = x_0 \cos(\omega t) \quad \rightarrow \quad \ddot{d}(t) = -x_0 \omega^2 \cos(\omega t) \quad \Leftrightarrow \quad a(t)$$

$$P(t) = \frac{2e^2}{3c^3} a^2(t) = \frac{2e^2}{3c^3} \omega^4 x_0^2 \cos^2(\omega t)$$

$$\boxed{\langle P(t) \rangle} = \frac{2e^2}{3c^3}\frac{\omega^4 x_0^2}{2} = \frac{32\pi^4}{3c^3} \nu^4 \left(\frac{e^2 x_0^2}{2} \right) = \frac{32\pi^4}{3c^3} \nu^4 \langle \ddot{d}_x^2(t) \rangle$$

$$\boxed{= A_{UL} \cdot h\nu_{UL}}$$

(i.e. number of transitions per unit time $\times$ $h\nu_{UL}$)

The line power/luminosity can be interpreted as the result of spontaneous emission processes in case it is the only effective mechanism (multiplied by the number density n_e and the volume V)

Atoms as oscillators: electric dipole transitions (3)

Then, we can derive the expression of the Einstein coefficient for spontaneous emission paying the due tribute to quantum mechanics:

$$A_{UL} = \frac{32\pi^4\nu^3}{3hc^3}\langle \ddot{d}_x^2(t)\rangle$$

Going to 3-D

$$A_{UL} = \frac{64e^2\pi^4\nu^3}{3hc^3}\vec{R}^{UL}\vec{R}^{UL} = \frac{64\pi^4\nu^3}{3hc^3}\mid P_{UL}\mid^2$$

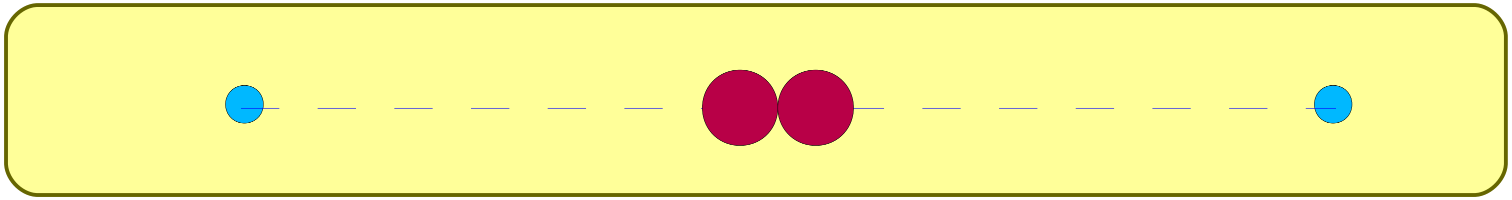
where $\mid P_{UL} \mid$ is the dimensionless transition matrix element (averaged over angular momentum) for $U \rightarrow L$ transitions

Once QM provides expressions for wave functions, A_{UL} can be determined

FYI,
Computations
never asked

Atoms as oscillators: electric quadrupole transitions

The quadrupole term can be non zero when the dipole is 0 (semi – prohibited transition, second term of expansion of potential vector A);



in this case the integral becomes

$$q_x(t) = \int e \cdot \mathbf{x}^2 \Psi_U \Psi_L^* \, d\tau \qquad \left(\text{also} \quad q_y(t), \;\; q_z(t)\right)$$

A similar expression for A_{UL} can be derived as in the case of the dipole;
all these transitions are termed (semi–) prohibited, but their probabilities (A_{UL}) although much smaller than in the dipole case, may be relevant

Selection rules: Δn arbitrary, $\Delta l = 0 \pm 2$, $\Delta J = 0, \pm 1, \pm 2$, $\Delta L = 0, \pm 1, \pm 2$
$\Delta S = 0$, $\Delta m = 0, \pm 1, \pm 2$

FYI,
Computations
never asked

Atoms as oscillators: Magnetic dipole

The magnetic dipole has to be considered and refers to hyperfine structure transitions, where energy levels differ by very small quantities

Selection rules: $\Delta n = \Delta l = \Delta L = 0,\ \Delta J = 0, \pm 1,\ \Delta m = 0, \pm 1\ \Delta S = 0\ \pm 1$

$$m(t) = m_0 \cos(\omega t)$$

$$\langle P(t) \rangle = \frac{2}{3c^3} \omega^4 \langle m^2(t) \rangle = \frac{32\pi^4}{3c^3} \nu^4 \langle m^2(t) \rangle$$

$$A_{UL} = \frac{64\pi^4}{3h} \frac{\nu^3}{c^3} |\ddot{\mu}_{UL}|^2$$

typical ratios for transitions:

$$\frac{A_Q}{A_D} \approx 5 \cdot 10^{-5} \qquad \frac{A_M}{A_D} \approx 3 \cdot 10^{-8} \quad (\textit{gross estimate})$$

for Einstein B coefficients we need a bit more patience....

The meaning of A_{UL}

example:

$$x_o = r_o = 5.3\cdot 10^{-9} \quad \text{cm} \quad \text{(Bohr radius)}$$

$$\nu_{UL} = 3.3\,10^{15} \quad \text{Hz} \quad \text{(Lya limit)}$$

$$d = e\frac{r_o}{2} = 1.3\,10^{-18}\,\text{ues cm}$$

FYI,
Computations
never asked

we get: $A_{\infty 1} = 3.5\cdot 10^{8} \quad s^{-1}$

Vectors $\vec{R}_{UL}$ can be arranged into a (symmetric) matrix.

Some elements are 0 meaning that the probability of the transition is 0, namely **really prohibited.**

(for that kind of transition)

Each element $\vec{R}_{UL}$ in the matrix may be intrepreted as oscillator strength for the transition $U \rightarrow L$

Selection rules for electric dipole transitions

Δn arbitrary (but not 0 for H and hydrogenoid ions)

$\Delta l = \pm 1$ (parity change) $\quad \Delta L = 0, \pm 1, \Delta S = 0, \Delta J = 0, \pm 1$

FYI,
Computations
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(for reference to notation see Rohlf, 1994 ''Modern physics from α to Z_0'')

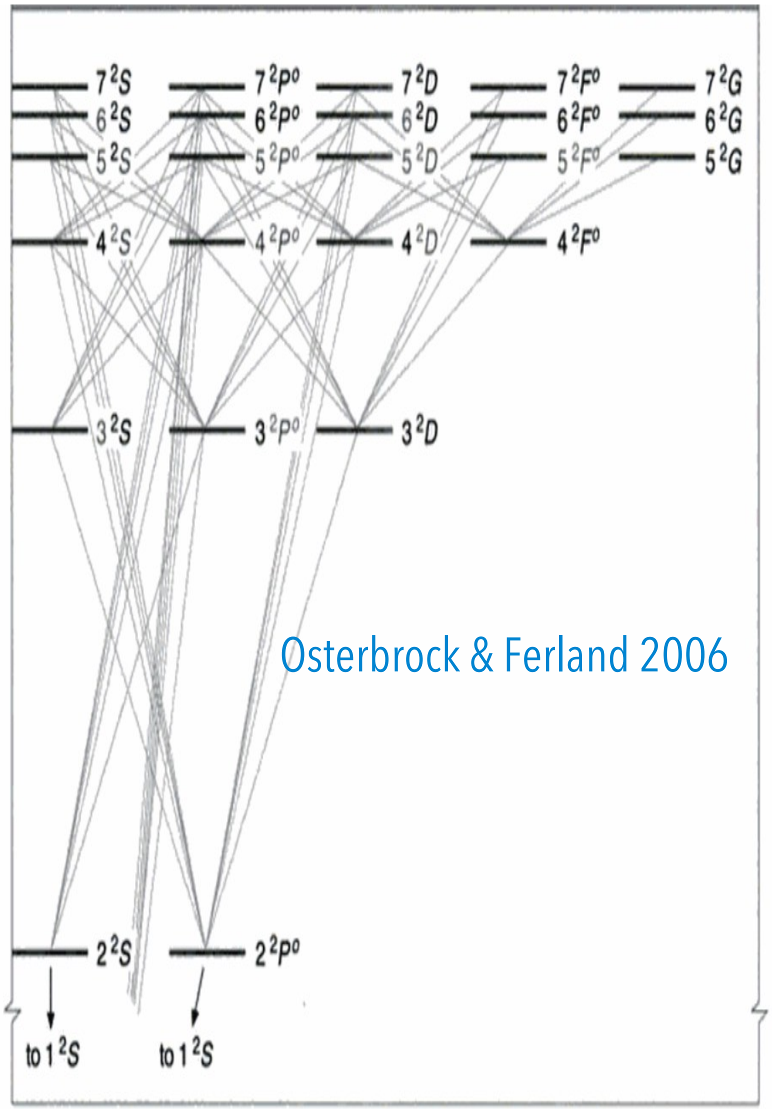
Some examples of A_{mn} coefficients for electric dipole transitions

Line	wavelength (A)	oscillator strength	A_{UL} (s^{-1})
Lyman α	1215.67	0.41620	4.70E+008
Lyman β	1025.72	0.07910	5.58E+007
Lyman γ	972.54	0.02899	1.28E+007
Lyman limit	911.80		
H α	6562.80	0.64070	4.41E+007
H β	4861.32	0.11930	8.42E+006
H γ	4340.46	0.04467	2.53E+006
H δ	4101.73	0.02209	9.73E+005
H ε	3970.07	0.01270	4.39E+005
H limit	3646.00		
P α	18751.00	0.84210	8.99E+006
P β	12818.10	0.15060	2.20E+006
P γ	10938.10	0.05584	7.78E+005
P limit	8204.00		
B α	40512.00	1.03800	2.70E+006
B β	26252.00	0.17930	7.71E+005
B γ	21655.00	0.06549	3.04E+005
Blimit	14584.00		

*From Allen's Astronomical quantities (p 70, 71) – **warning!***

A_{UL} different from Dopita & Sutherland "Astrophysics of the Diffuse Universe", p 19

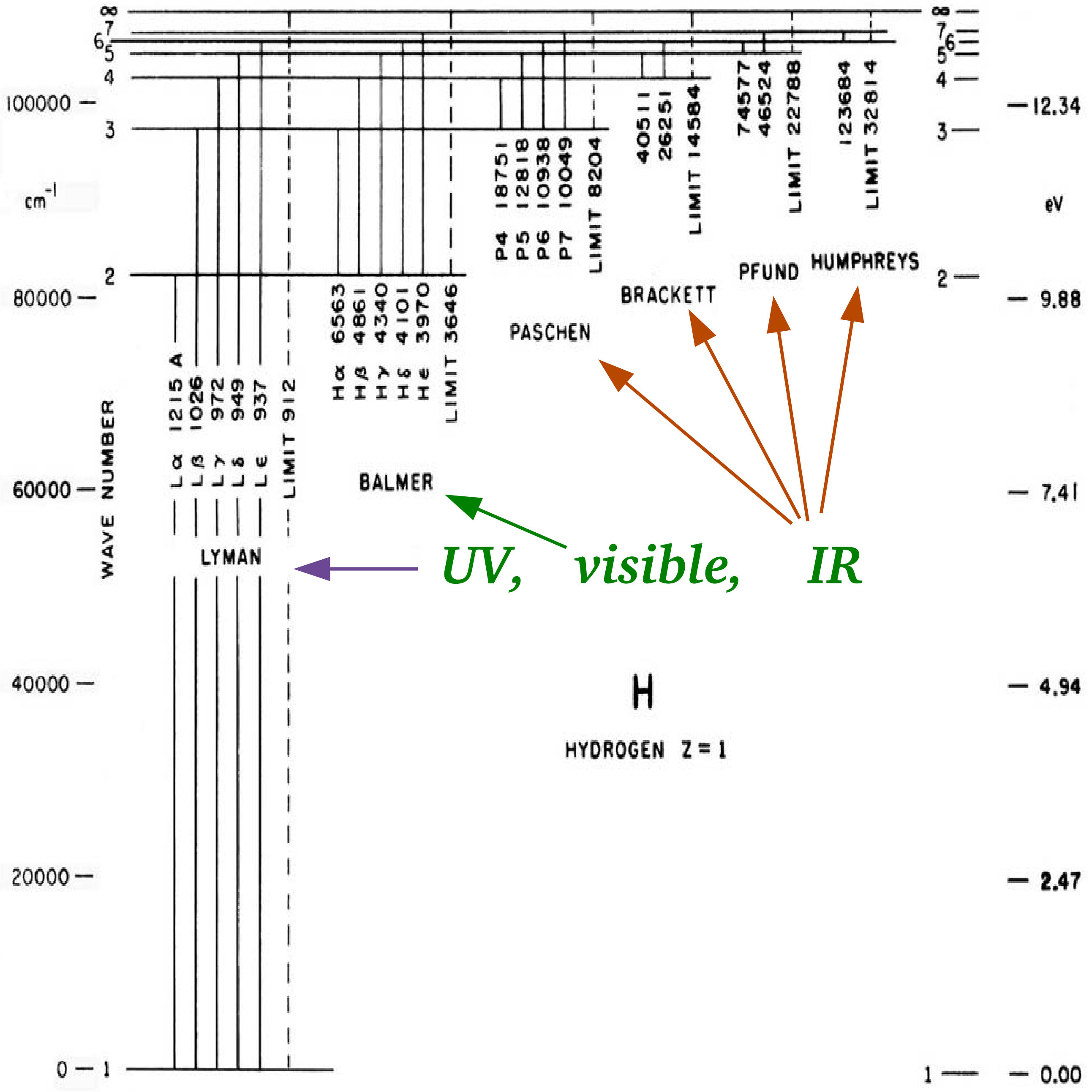
Hydrogen: Grotrian diagrams



Osterbrock & Ferland 2006

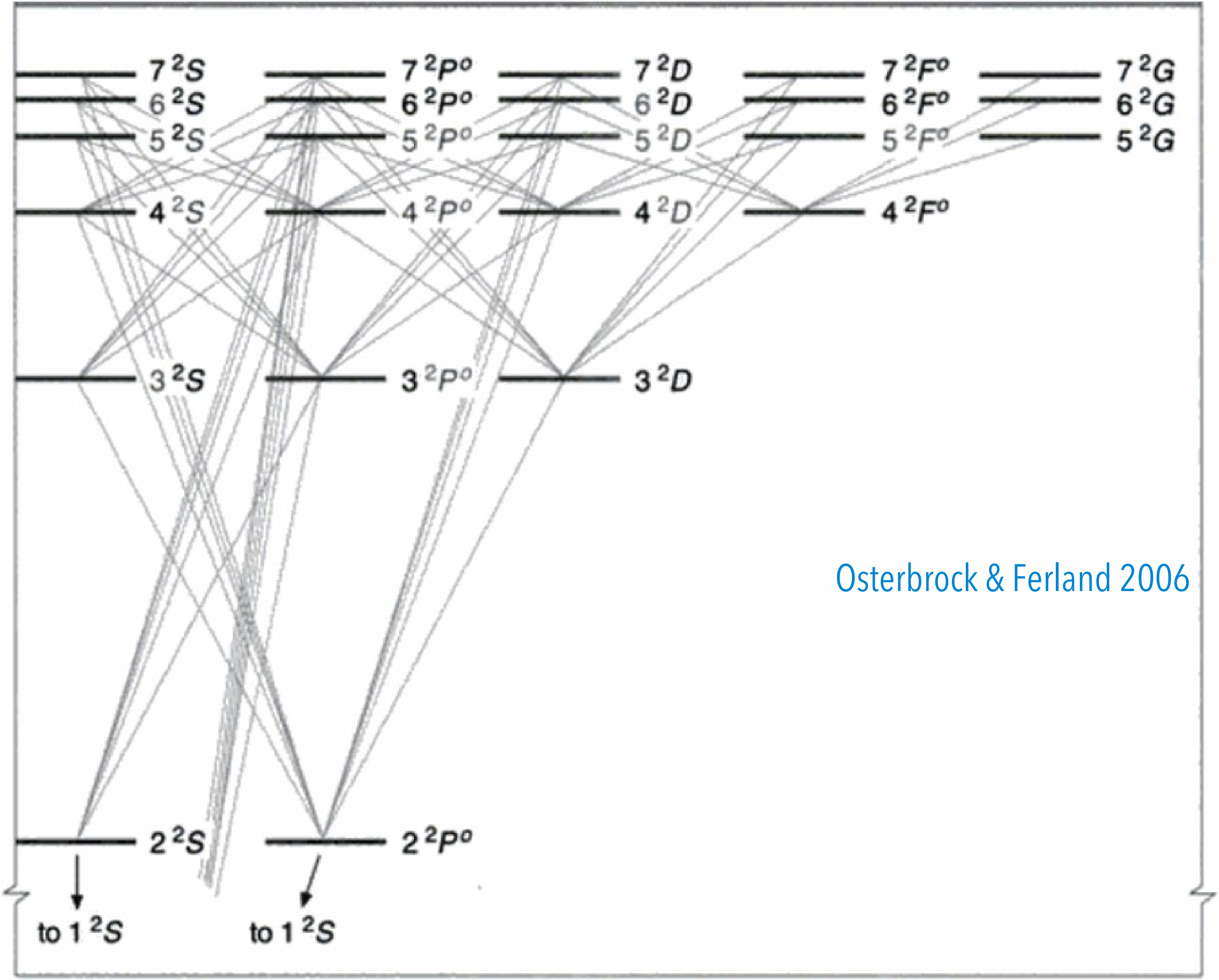
Figure 2.1

Partial energy-level diagram of H I, limited to $n \leq 7$ and $L \leq G$. Permitted radiative transitions to levels $n < 4$ are indicated by solid lines.



UV, visible, IR

Hydrogen: Grotrian diagrams



Osterbrock & Ferland 2006

Figure 2.1

Partial energy-level diagram of H I, limited to $n \leq 7$ and $L \leq G$. Permitted radiative transitions to levels $n < 4$ are indicated by solid lines.

Determining electronic transitions: Spectroscopic notation

General notation for (many) bound electrons in atoms:

All electrons are considered, closed shells do not play a role

$$ns^i np^j nd^k \quad {}^{2S+1}L_J^{(o)}$$

where

n = principal quantum number

S = total spin (2S+1 = multiplicity)

l_i = i-th electron angular momentum (=0,...n-1)

$L = \sum (l_i)$, total orbital angular momentum (inner full shells sum to 0)

J = L+S total angular momentum

L	Letter
0	S
1	P
2	D
3	F

Example : C_{III} transitions are resonance , intercombination , and forbidden

C_{III}: $A(2s2p\ {}^1P_1 \rightarrow 2s^2\ {}^1S_0) = 1.7\cdot10^9\, s^{-1}$

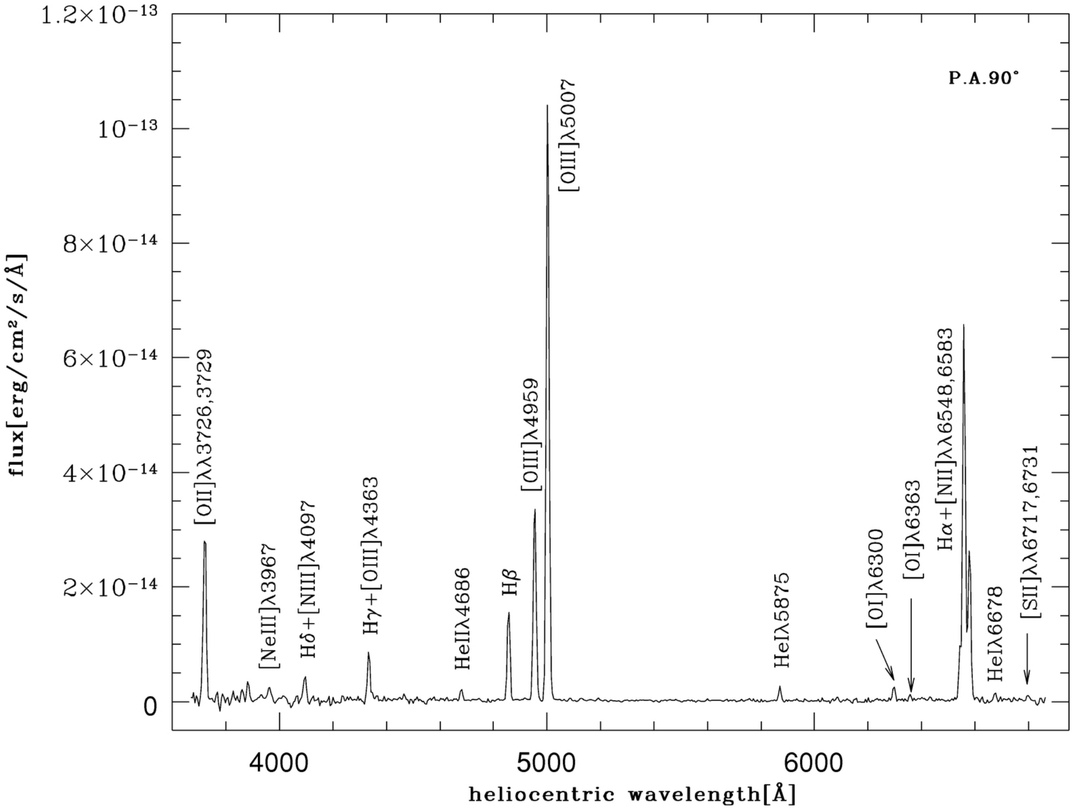
$C_{III}]$: $A(2s2p\ {}^3P_1 \rightarrow 2s^2\ {}^1S_0) = 97\, s^{-1}$

$[C_{III}]$: $A(2s2p\ {}^3P_2 \rightarrow 2s^2\ {}^1S_0) = 5.2\cdot10^{-3}\, s^{-1}$

FYI,
Computations
never asked

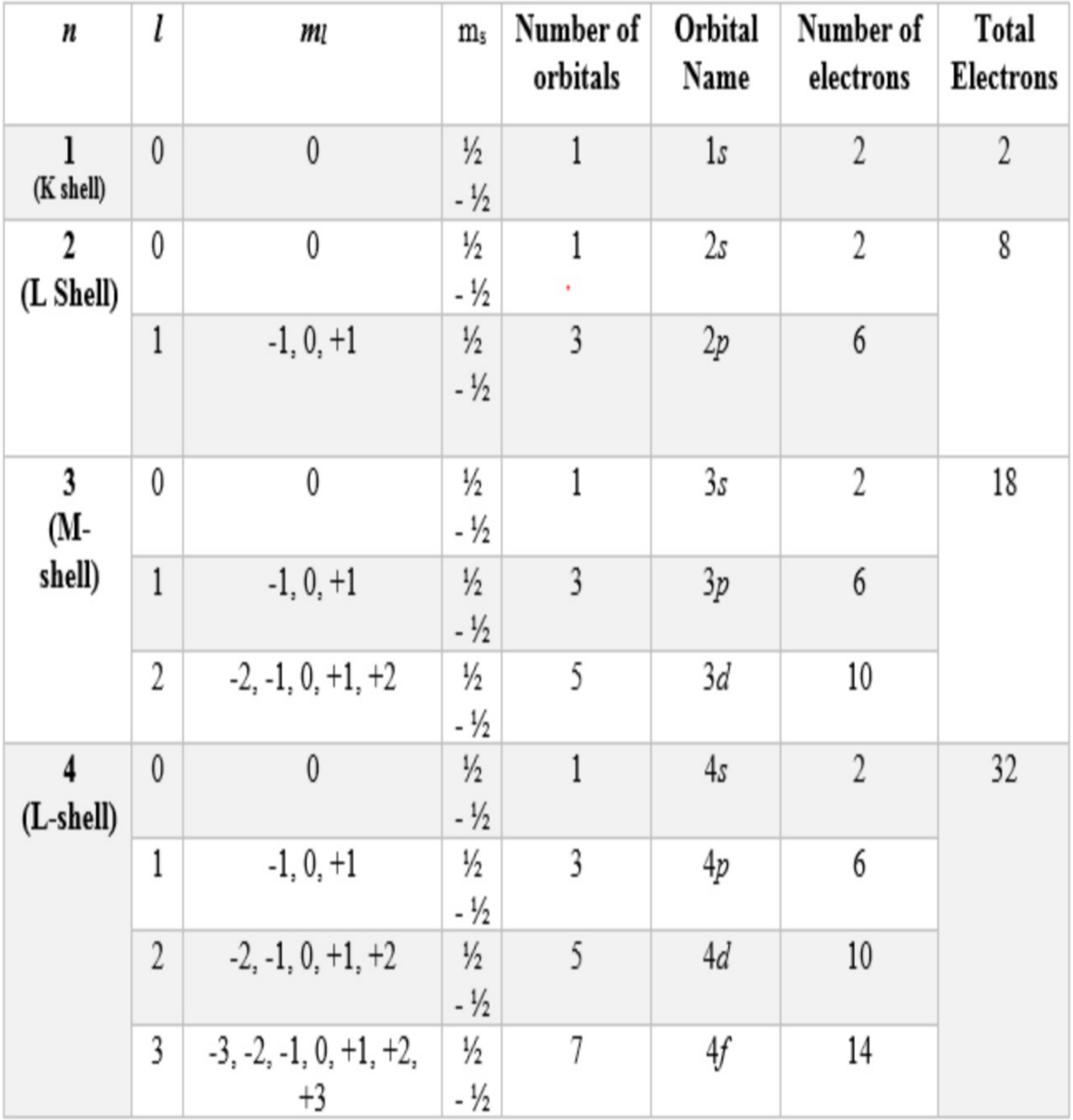
A digression… Some line are termed "collisional"

	Ion	Transition	A_{UL} (sec^{-1})
RESONANCE	CIII	$2s2p\ ^1P_1 - 2s^2\ ^1S_0$	1.7×10^9
INTERCOMBINATION	CIII]	$2s2p\ ^3P_1 - 2s^2\ ^1S_0$	97
FORBIDDEN	[CIII]	$2s2p\ ^3P_2 - 2s^2\ ^1S_0$	5.2×10^{-3}



Lowest energy levels of an atom

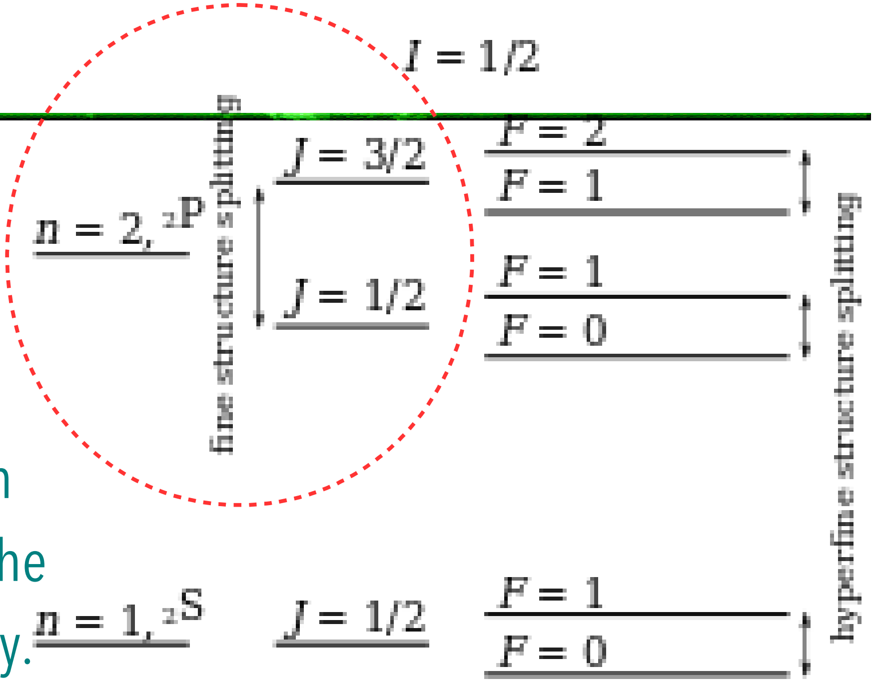
n	l	m	state	$n^{2S+1} L$
1	0	0	1s	1^2S
2	0	0	2s	2^2S
	1	0	$2p_0$	2^2P
		±1	$2p_{\pm1}$	
3	0	0	3s	3^2S
	1	0	$3p_0$	3^2P
		±1	$3p_{\pm1}$	
	2	0	$3d_0$	3^2D
		±1	$3d_{\pm1}$	
		±2	$3d_{\pm2}$	



n	*l*	*ml*	m_s	Number of orbitals	Orbital Name	Number of electrons	Total Electrons
1 (K shell)	0	0	½ - ½	1	1*s*	2	2
2 (L Shell)	0	0	½ - ½	1	2*s*	2	8
	1	-1, 0, +1	½ - ½	3	2*p*	6	
3 (M-shell)	0	0	½ - ½	1	3*s*	2	18
	1	-1, 0, +1	½ - ½	3	3*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	3*d*	10	
4 (L-shell)	0	0	½ - ½	1	4*s*	2	32
	1	-1, 0, +1	½ - ½	3	4*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	4*d*	10	
	3	-3, -2, -1, 0, +1, +2, +3	½ - ½	7	4*f*	14	

FYI,
Information
never asked

Fine structure of Energy levels



For an electron the electric potential within an atom is not simply that from the Coulomb's law.

Atoms with many e– (Li,…C,N,O,…): the interaction between orbiting electrons and their spins raises the degeneracy of the "n" states so that each "l" level has a slightly different energy.

$$E_{nJ}^{exact} = mc^2\left[\left(1 + Z\alpha\left(n - J - 1/2 + \sqrt{(J+1/2)^2 - Z^2\alpha^2}\right)^{-1}\right)^{-1/2} - 1\right]$$

where $J = L + S$

FYI,
Computations
never asked

→ The binding energy does not depend on the main quantum number alone anymore!!!!!

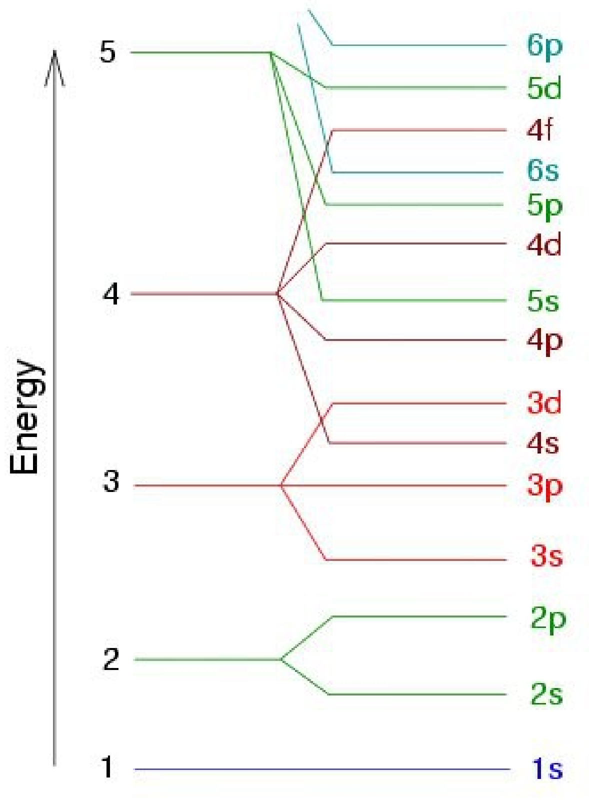
→ This spin-orbit coupling provides further energy structure.

Some atoms may have double, triple, multiple lines closely packed (see CaII, [OIII] doublet).

The "m" levels remain undistiguishable unless an external strong magnetic field is applied to the atom (Zeeman splitting).

(Different values of m have not been considered in the expression of E_{nJ}^{exact})

Fine structure in Hydrogen



3 levels for n =2

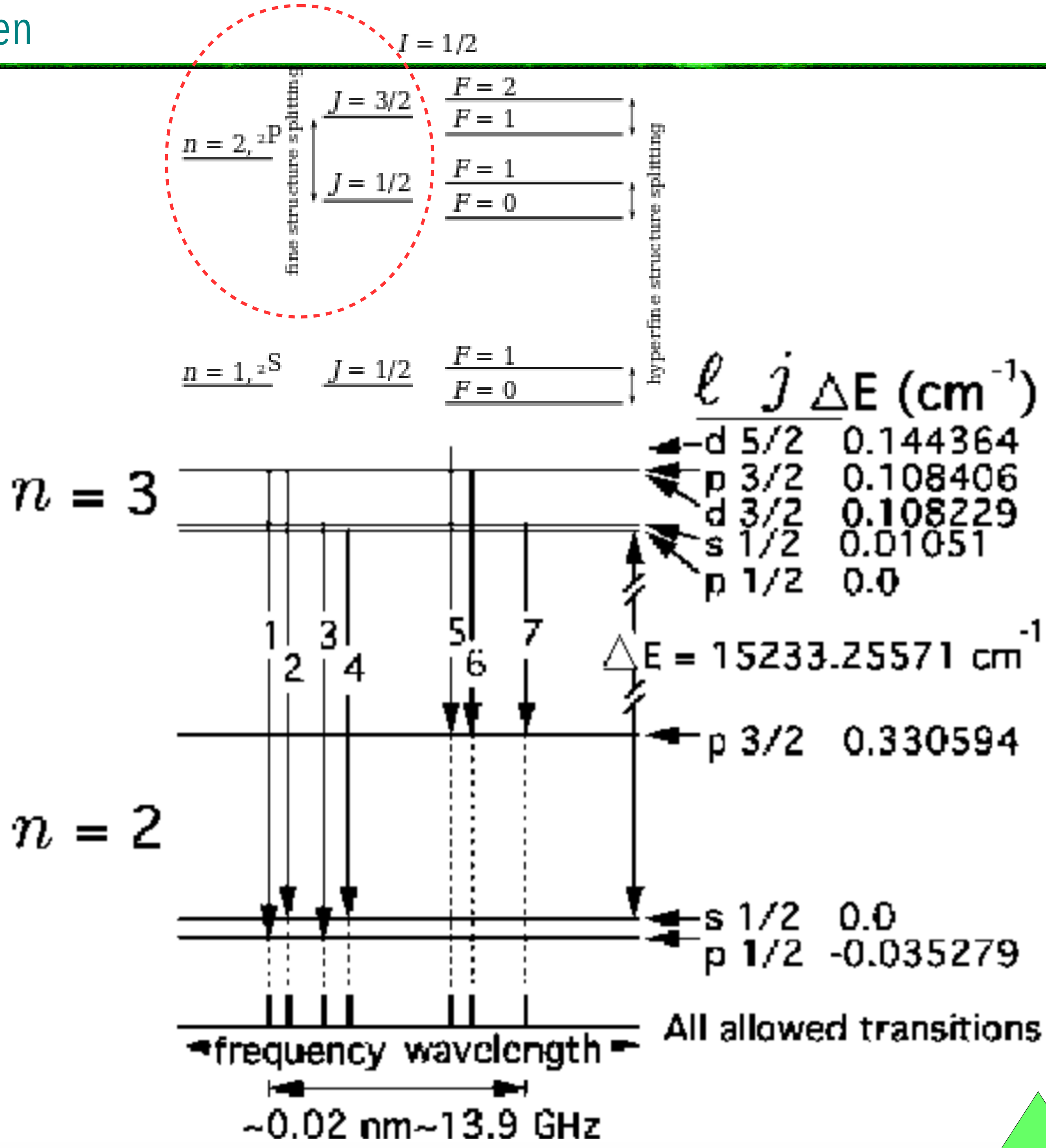


Figure 1. Diagram showing fine structure and allowed transitions for hydrogen H-alpha line.

FYI,
never asked

Fine structure lines (examples)

Result from transitions within each configuration. Example: Oxygen

Ground configuration : $1s^2 2s^2 2p^4 \quad \rightarrow \quad 3P \quad$ (the total spin is 1)

Spin - orbit coupling $\rightarrow \quad \approx \alpha^2 \sim \dfrac{1}{137^2} \times$ electron bindind energy

Fine structure lines are in the far - IR $(10 - 300 \ \mu\text{m})$

$$\text{e.g.} \quad \text{O} \qquad {}^3P_1 \rightarrow {}^3P_2 \quad \rightarrow \quad 63 \ \mu\text{m}$$

$$\qquad\qquad\quad {}^3P_0 \rightarrow {}^3P_1 \quad \rightarrow \quad 145 \ \mu\text{m}$$

The number of fine structure levels depends on the total angular momentum of the electronic configuration of the outermost shell

Multiplicity for ground state fine structure lines

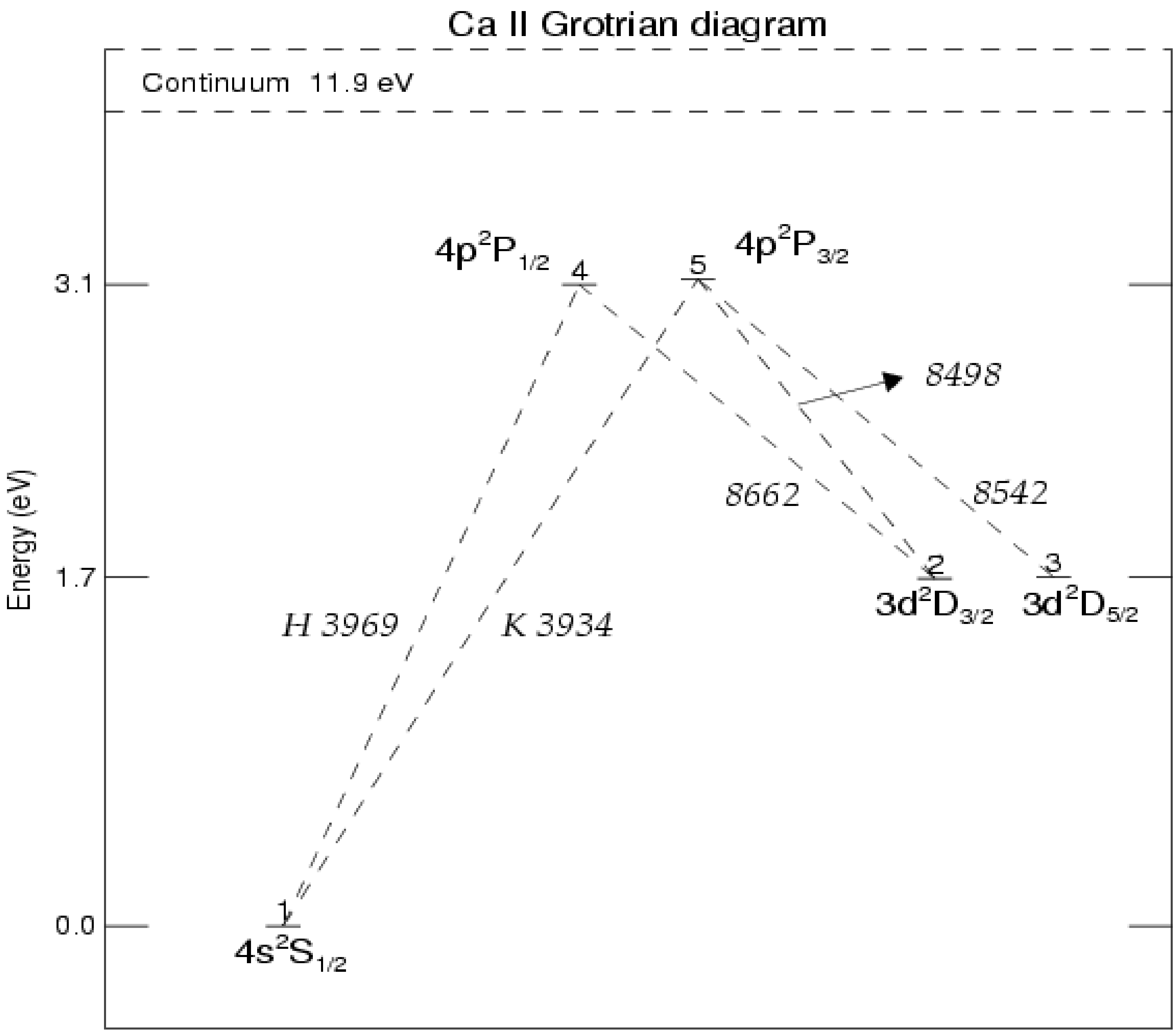
Atoms with p^1 or p^5 have fine structure doublets → single fine structure line in the ground state

Atoms with p^2 or p^4 have fine structure triplets → two fine structure lines

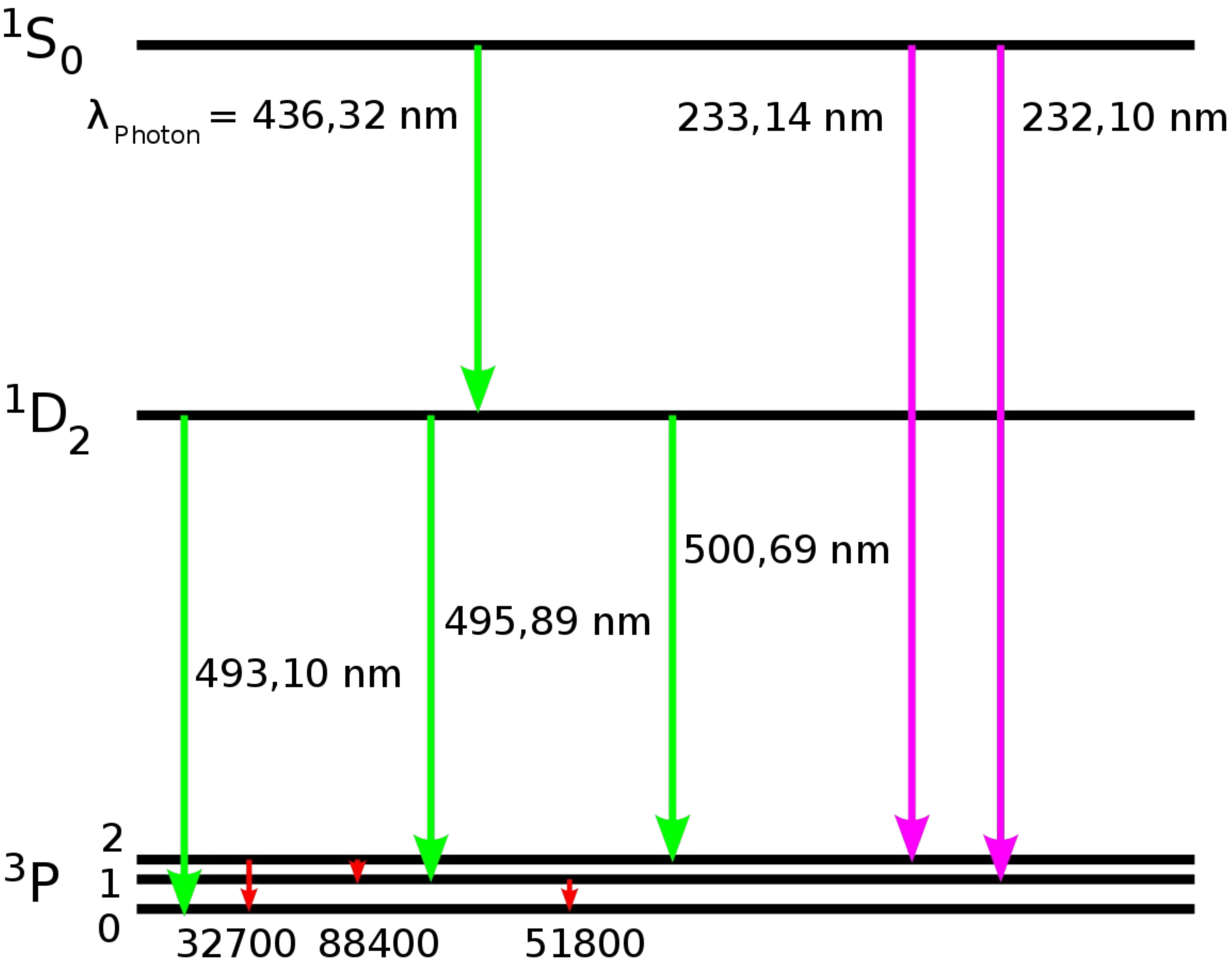
Atoms with p^3 electrons of filled shells do not have fine structure lines

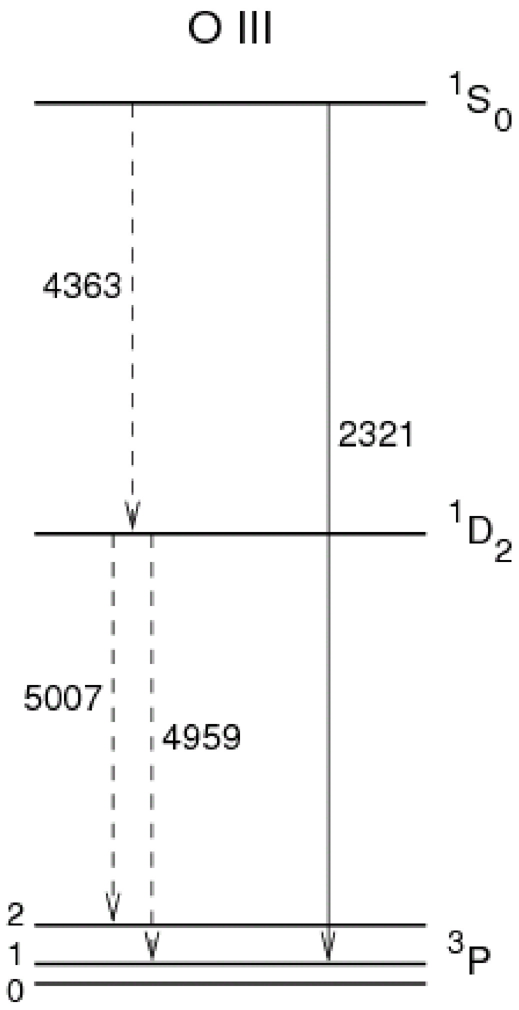
FYI,
Computations
never asked

Exercise/understanding: Fine structure of Energy levels: CaII lines

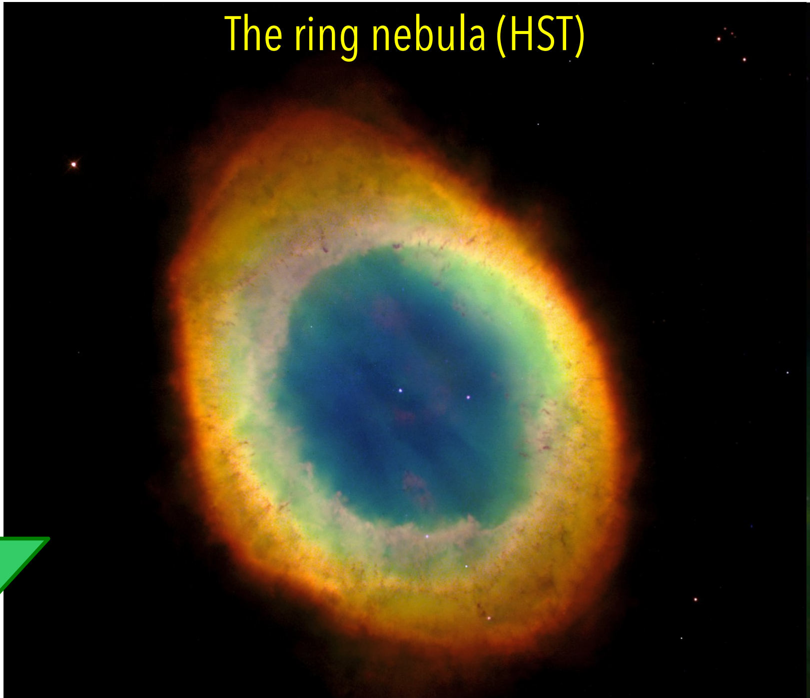


Examples: [OIII] lines

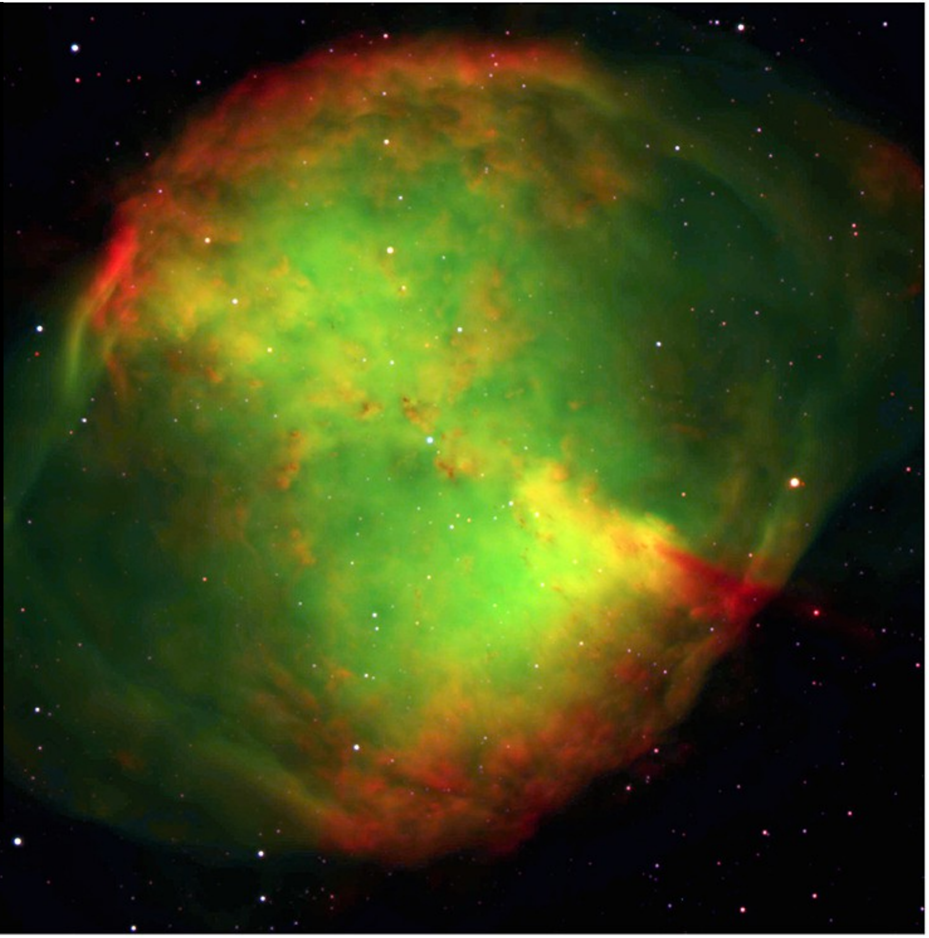




Forbidden lines: Nebulium (alias [OIII]) (note color stratification!)



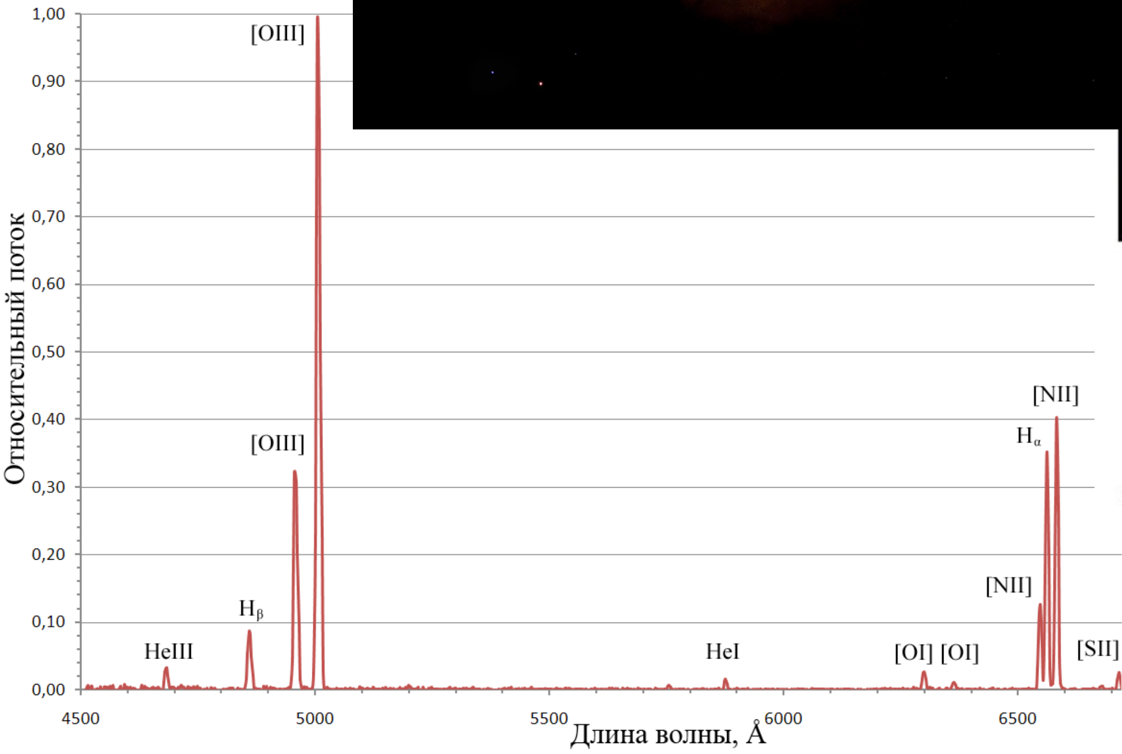
The ring nebula (HST)



blue= broad band blue filter; green: OIII; red=Hα

Planetary Nebula NGC 6853 (M 27) - VLT UT1+FORS1

ESO PR Photo 38a/98 (7 October 1998)



Four Statistical laws (for thermal equilibrium)

Maxwell – Boltzmann (velocities .aka. energy for particles)

$$\frac{dN}{dv} \propto f(v) \propto v^2 e^{-mv^2/2kT_k} \approx v^2 e^{-v^2/2\sigma^2} \quad \text{where} \quad \sigma = \frac{kT_k}{m}$$

Planck (spectral distribution for radiation)

$$U(\nu) = \frac{4\pi}{c} B_\nu(T_P) = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h\nu/kT_P} - 1}$$

Boltzmann (energy level occupation in atoms, molecules)

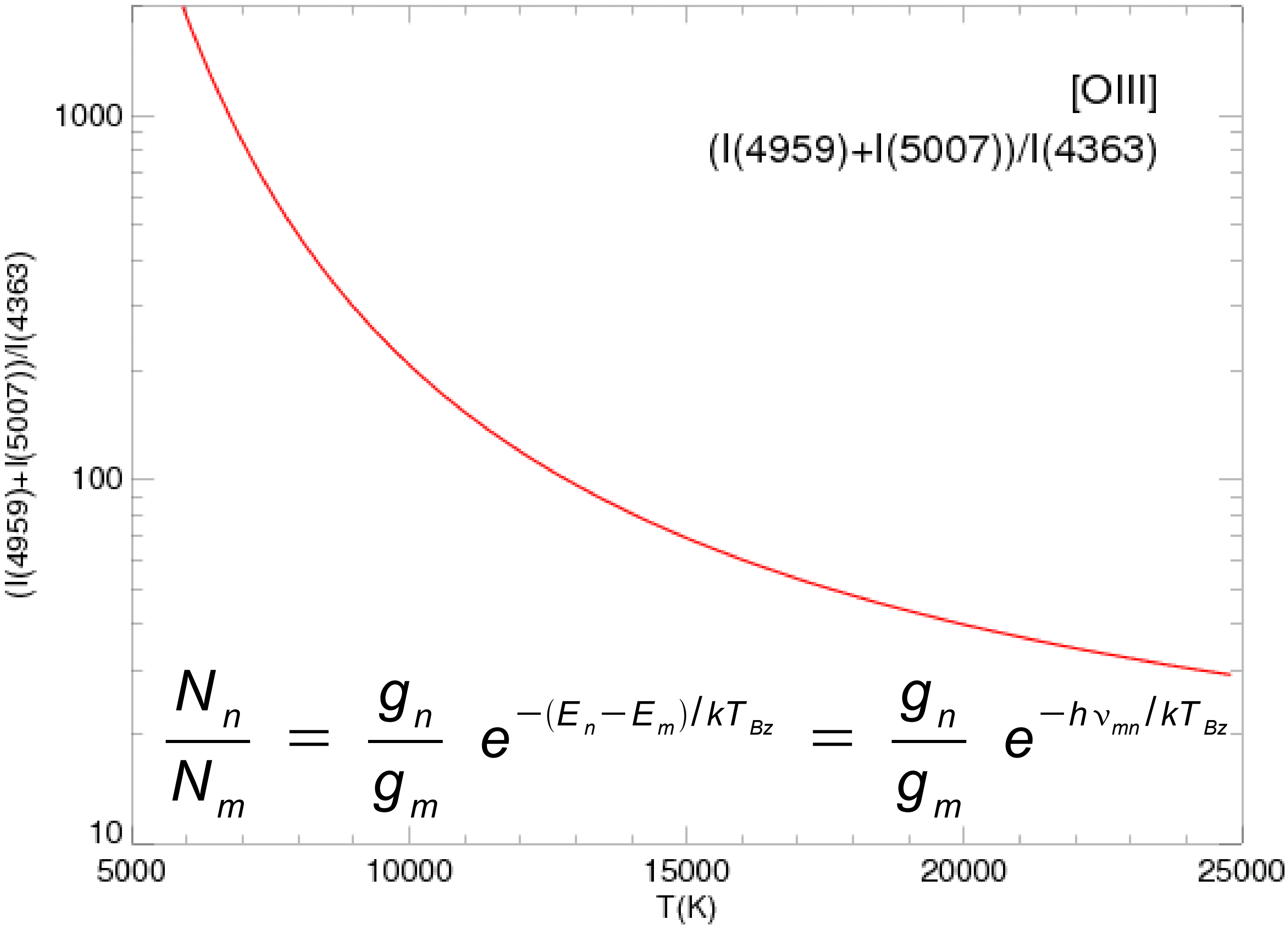
$$\frac{N_U}{N_L} = \frac{g_U}{g_L} e^{-(E_U - E_L)/kT_{Bz}} = \frac{g_U}{g_L} e^{-h\nu_{UL}/kT_{Bz}}$$

Saha (ionization states)

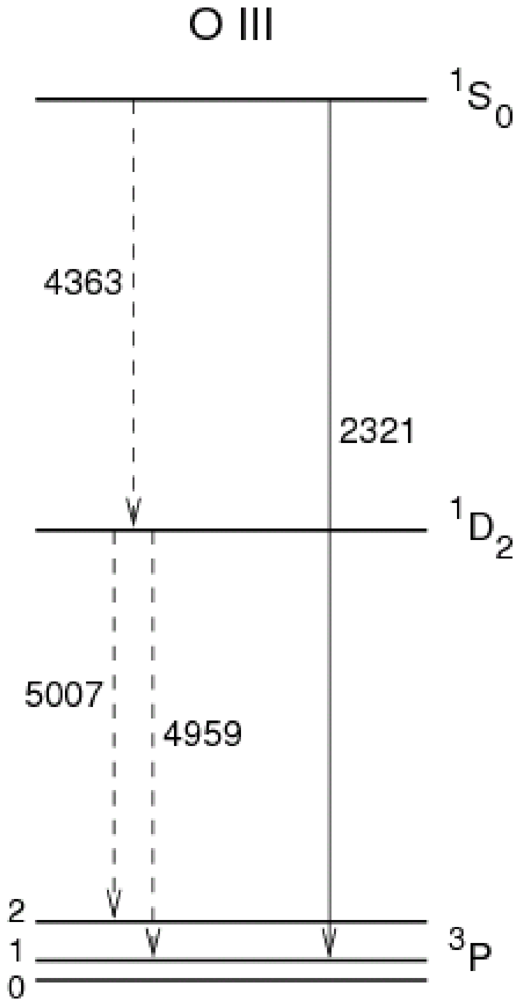
$$\frac{N_{i+1}}{N_i} = 2 \frac{u_{i+1}}{u_i} \frac{1}{N_e} \sqrt{\left(\frac{2\pi m_e kT_S}{h^2}\right)^3} e^{-(E_{i+1} - E_i)/kT_S}$$

where $\left(\sqrt{\frac{2\pi m_e kT_S}{h^2}}\right)^{-1} = \Lambda_{th}$ de Broglie thermal wavelength, and $u_i = \sum_n g_{i,n} e^{-\chi_{i,n}/kT}$

[OIII] lines diagnostics



$$\frac{N_n}{N_m} = \frac{g_n}{g_m} e^{-(E_n - E_m)/kT_{Bz}} = \frac{g_n}{g_m} e^{-h\nu_{mn}/kT_{Bz}}$$



Line ratios provide information on the temperature (note that these values are typical of HII regions!)

Line Diagnostics

TABLE 4C

IONIC ABUNDANCES, TEMPERATURES, AND DENSITIES

Parameter	NGC 1535	NGC 2022	NGC 2242	NGC 2371	NGC 2438	NGC 2440	NGC 7027
He^{+}/H^{+}	7.38E−02[a]	1.15E−02	…	2.55E−02	7.40E−02[a]	5.76E−02	6.09E−02
He^{+2}/H^{+}	9.79E−03	8.07E−02	0.10	7.72E−02	2.04E−02	4.73E−02	4.26E−02
ICF(He)	1.00	1.00	1.00	1.00	1.00	1.00	1.00
O^{o}/H^{+}	…	…	…	1.06E−05	2.52E−05	2.93E−05	4.50E−06
O^{+}/H^{+}	3.07E−07	2.29E−06	…	3.33E−05	9.34E−05	5.35E−05	1.89E−05
O^{+2}/H^{+}	2.34E−04	9.15E−05	1.16E−05	1.58E−04	3.18E−04	2.32E−04	2.25E−04
ICF(O)	1.13	8.00	1.00	4.02	1.28	1.82	1.70
N^{+}/H^{+}	6.17E−08	2.65E−07	…	1.31E−05	3.98E−05	1.10E−04	1.06E−05
ICF(N)	867.45	327.35	1.00	23.17	5.62	9.71	21.92
Ne^{+2}/H^{+}	6.30E−05	1.72E−05	1.32E−06	3.66E−05	1.02E−04	4.78E−05	3.85E−05
ICF(Ne)	1.13	8.20	1.00	4.87	1.65	2.24	1.84
S^{+}/H^{+}	9.83E−10	2.74E−08	…	5.76E−07	9.27E−07	4.92E−07	6.37E−07
S^{+2}/H^{+}_{NIR}	2.93E−07[c]	1.06E−06	2.29E−07	4.15E−06	4.50E−06	1.64E−06	2.92E−06
S^{+2}/H^{+}_{6312}	1.16E−07[b]	2.99E−06	1.90E−06	1.67E−05	3.95E−06[b]	3.69E−06[a]	1.43E−06
ICF(S)	22.22	7.16	…	1.58	1.21	1.31	1.55
Cl^{+2}/H^{+}	…	…	…	…	…	1.13E−07[a]	5.77E−08
Cl^{+3}/H^{+}	3.76E−08	5.70E−08[a]	2.81E−08	1.17E−07	…	3.81E−08	4.23E−08
ICF(Cl)	1.13	8.00	1.00	4.02	1.28	1.82	1.70
Ar^{+2}/H^{+}	4.14E−07	3.26E−07	7.73E−08	1.12E−06	1.43E−06	1.34E−06	9.43E−07
Ar^{+3}/H^{+}	4.19E−07	8.29E−07	1.94E−07	1.30E−06	…	6.64E−07	5.75E−07
ICF(Ar)	1.13	8.02	…	4.21	1.55	2.03	1.78
T_{O3} (K)	11400	13600	21300	12100	10300		
T_{N2} (K)	(30500)	10300	10300	8600[e]	10400[e]		
T_{O2} (K)	7400	7500	…	6800	13100		
T_{S2} (K)	…	…	…	11400[f]	9700[f]		
T_{S3} (K)	17900[f]	19600	(284000)	13300	10000[f]		
$N_{e,S2}$ (cm^{-3})	300	800	1300[d]	1000	200		

NOTE.—Unless otherwise noted, uncertainties in ion abundances, electron temperatures, and e ±10%, and ±10%, respectively.

[a] ±50%.

[b] ±75%.

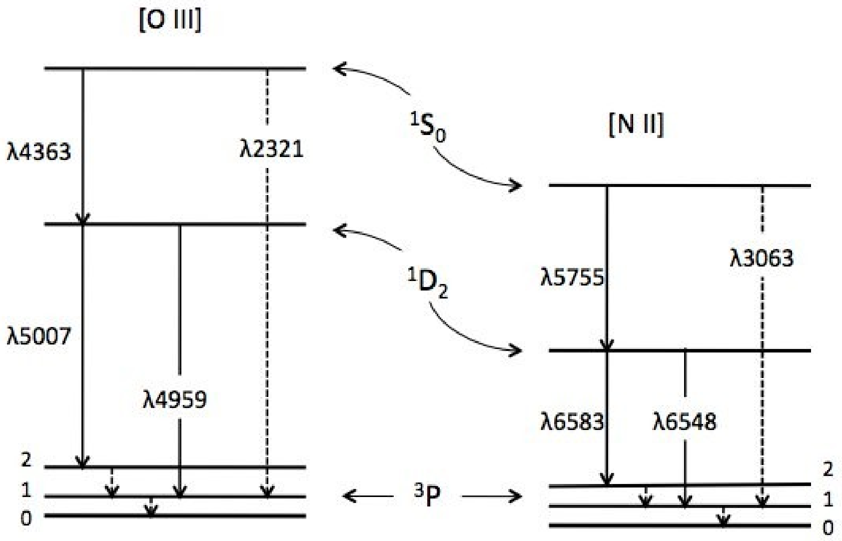
[c] [O III] temperature used to calculate this abundance.

[d] [S II] electron density from Howard, Henry, & McCartney 1997 was used, since the line at 67

[e] ±20%.

[f] ±30%.

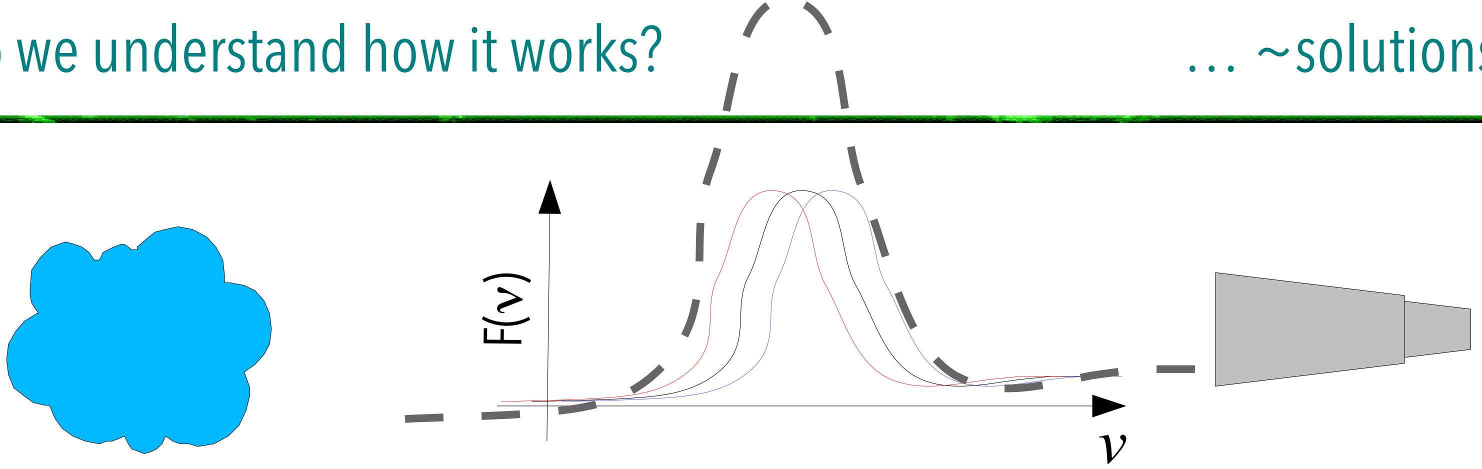
Kwitter + 2003



Test (1) : Do we understand how it works? … ~solutions!

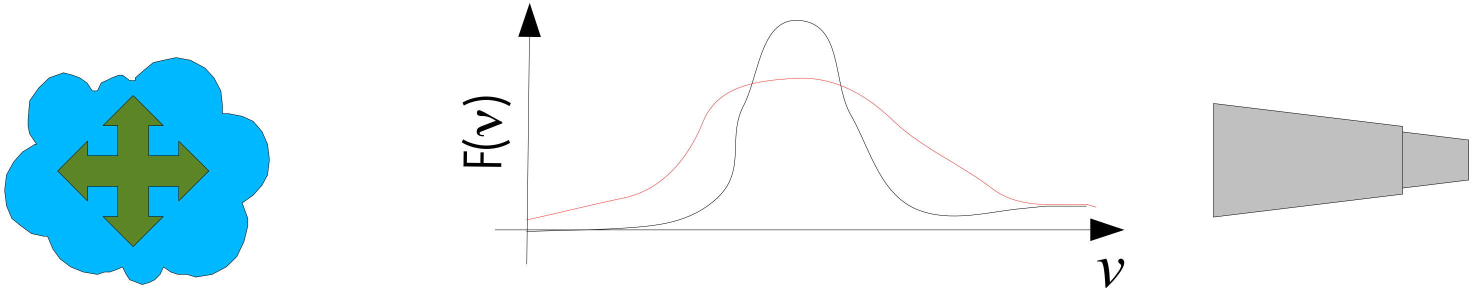
question 1:

(e.g. a standing cloud)



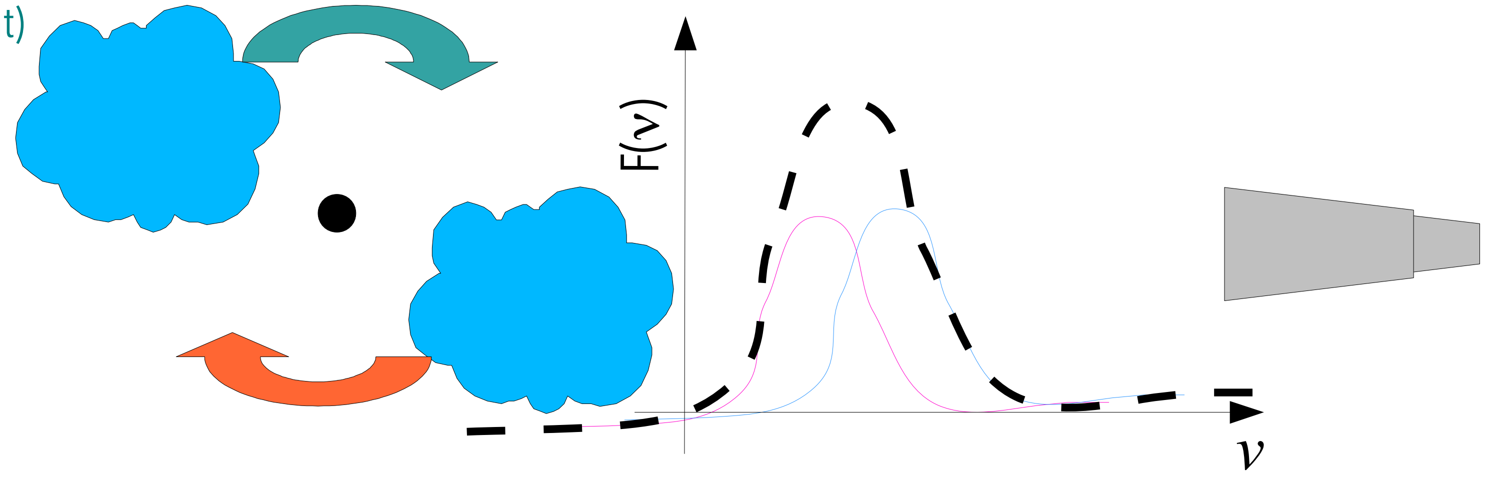
question 2:

(e.g. an expanding cloud)



question 3:

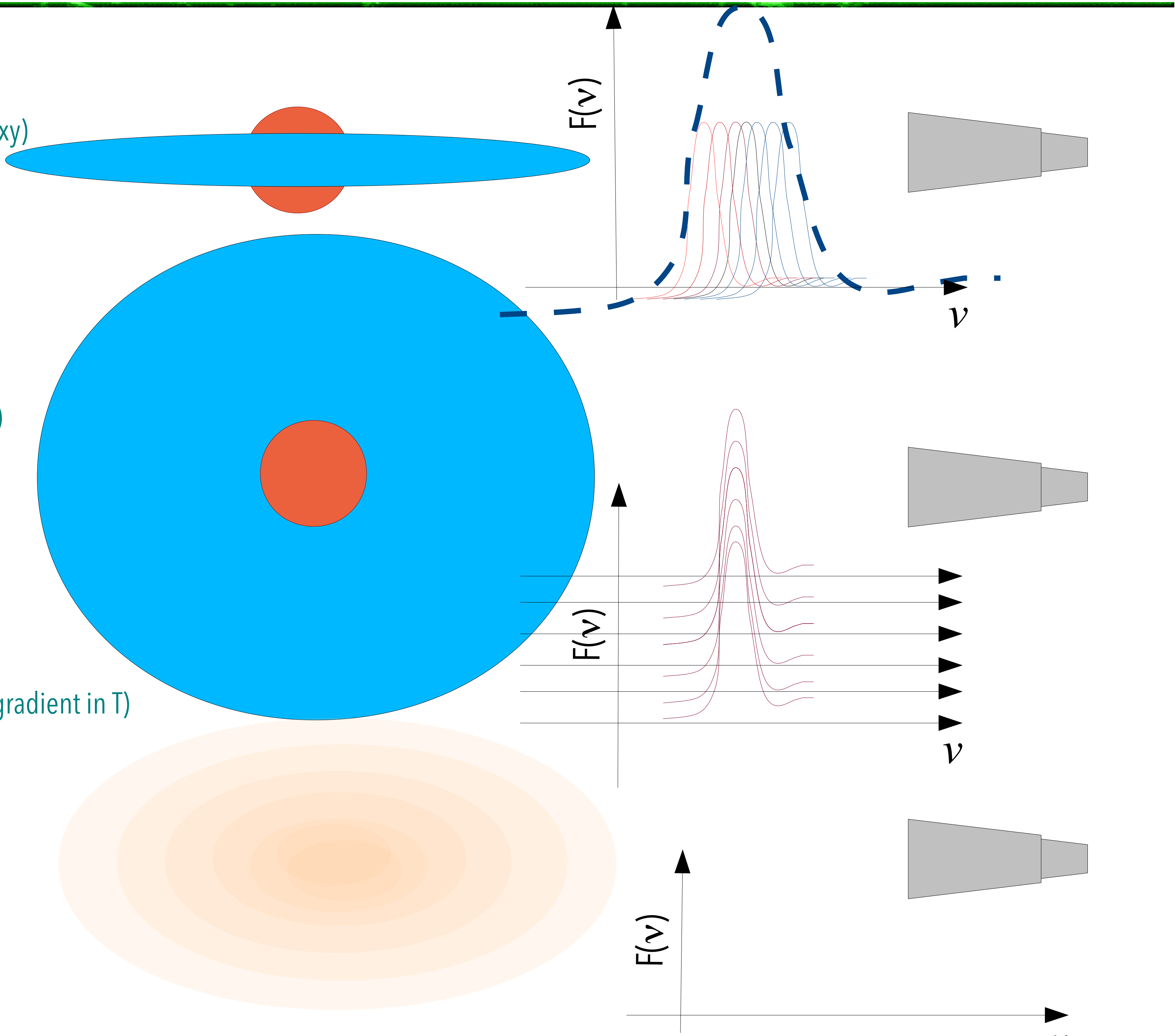
(2 clouds orbiting around a point)



Test (2) : Do we really understand how it works?

question 4:

(e.g. an edge-on spiral galaxy)

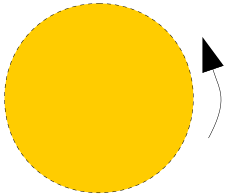


question 5:

(e.g. a face-on spiral galaxy)

question 6:

(e.g. a stratified gas with a gradient in T)



question 7:

(e.g. a rotating star)

Selection rules for electronic transitions (but some of them may be violated)

Electric Dipole:

⍰ n= any (no 0 for H and hydogenoid atoms)

⍰ l =±1 (parity change)

⍰ J = 0,±1 J=0 → J = 0 forbidden

⍰ L =0, ±1 L=0 → L = 0 forbidden ⍰ S = 0 (Permitted)

Electric Quadrupole:

⍰ n= arbitrary

⍰ l = 0± 2 (no parity change)

⍰ J = 0,±1, ±2 J=0 → J = 0 forbidden

⍰ L =0, ±1, ±2 L=0 → L = 0 forbidden ⍰ S = 0 (intercombination)

Magnetic Dipole:

⍰ n= ⍰ l = 0

⍰ J = 0,±1 J=0 → J = 0 forbidden

⍰ L = 0 ⍰ S = 0 ? (forbidden)

n, l=electron angular momentum (=0,…n-1), S= total spin, L= orbital angular momentum, J = L+S total angular momentum

Further….. there is a coupling between nuclear and electron spin ($\mathbf{F} = \mathbf{J} + \mathbf{I}$), e.g. HI

The END! Application of concepts to an astrophysical case:

Analysis of a Star forming region: Census of O, B stars, sizes, etc. https://arxiv.org/pdf/2012.14872.pdf

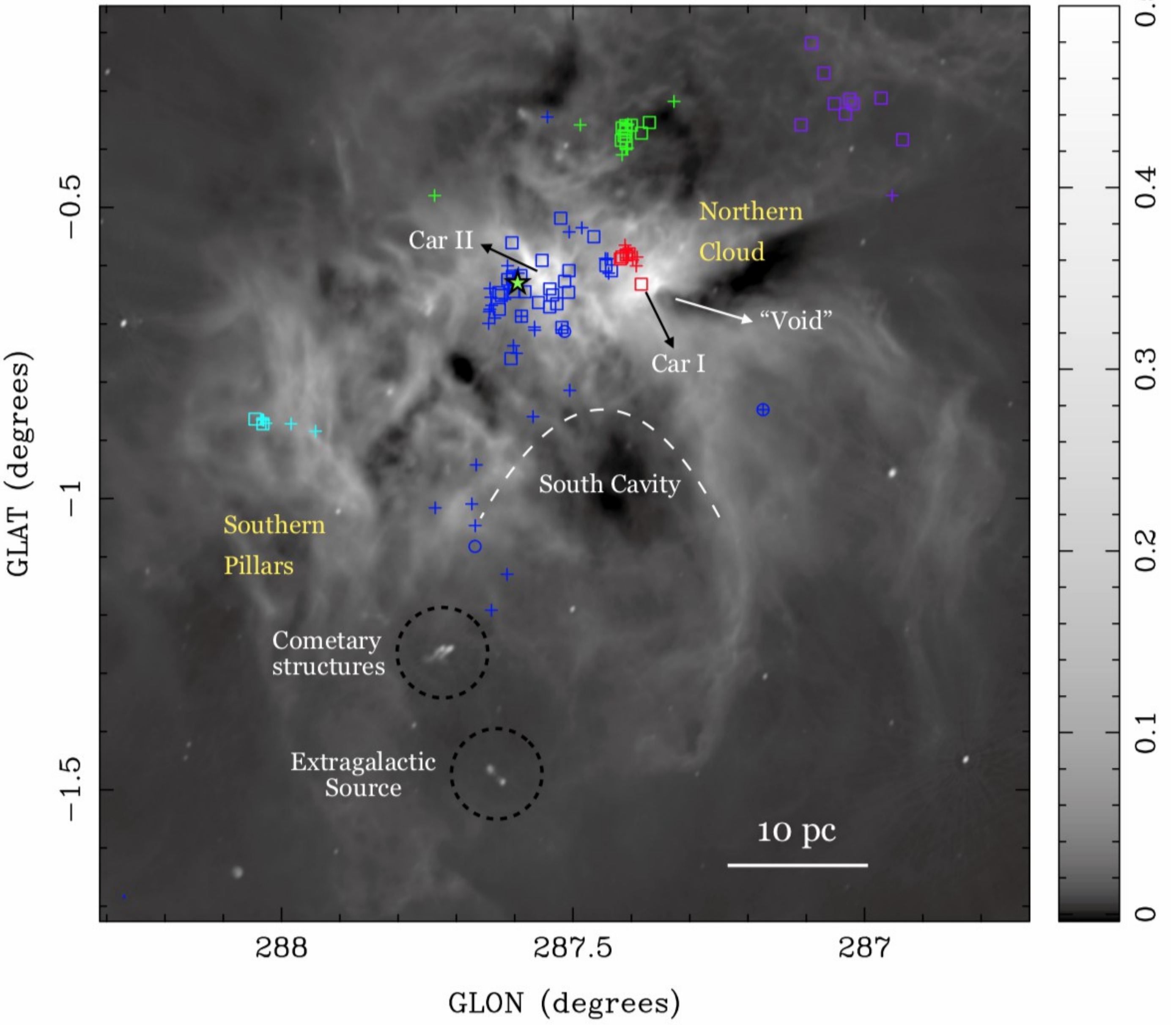


FIG. 5.— View of the radio continuum emission at 1 − 3 GHz in the central region of the CNC. Symbols show the position of the massive stars, with different colors illustrating different star clusters. Crosses show O stars, squares show B stars, and open circles show Wolf Rayet stars. Blue symbols show Trumpler 16 and Collinder 228 stellar clusters, red symbols show Trumpler 14, green show Trumpler 15, violet show Bochum 10 and cyan show Bochum 11 cluster as listed in Smith (2006). Black arrows show the position of the the two H II regions analyzed by Brooks et al. (2001), Car I and Car II. White arrow shows the "void" region where radio continuum emission seems to be absent. The curved white dashed line delineates the southern cavity discussed in the text. The black dashed circles shows the cometary objects and the extragalactic source discussed in Section 4.2.