

KAIST Astrophysics

(PH481) - Part 1

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Sunyaev-Zeldovich effect

- The **Sunyaev-Zeldovich effect** is the distortion of the blackbody spectrum ($T = 2.73$ K) of the Cosmic Microwave Background (CMB) owing to the Inverse Compton (IC) scattering of the CMB photons by the energetic electrons in the galaxy clusters.
 - Thermal SZ effects, where the CMB photons interact with electrons that have high energies due to their temperature.
 - Kinematic SZ effects (Ostriker-Vishniac effect), a second-order effect where the CMB photons interact with electrons that have high energies due to their bulk motion (peculiar motion). The motions of galaxies and clusters of galaxies relative to the Hubble flow are called peculiar velocities. The plasma electrons in the cluster also have this velocity. The energies of the CMB photons that scattered by the electrons reflect this motion.
 - Determinations of the peculiar velocities of clusters enable astronomers to map out the growth of large-scale structure in the universe. This topic is fundamental importance, and the kinetic SZ effect is a promising method for approaching it.

Thermal SZ effect

- The net effect of the IC scattering on the photon spectrum is obtained by multiplying the photon number spectrum by the kernel $K(\nu/\nu_0)$ and integrating over the spectrum.

$$N_{\text{scatt}}(\nu) = \int_0^\infty N(\nu_0) K(\nu/\nu_0) d\nu_0$$

- The net effect is that the BB spectrum is shifted to the right and distorted.
- Observations of the CMB are most easily carried out in the low-frequency Rayleigh-Jeans region of the spectrum ($h\nu \ll kT_{\text{CMB}}$).
- Measurement of the CMB temperature as a function of position on the sky would thus exhibit antenna temperature dips in the directions of clusters that contain hot plasmas.
- Note that the scattered spectrum is not a BB spectrum. The effective temperature increases. But, the total number of photons detected in a given time over the entire spectrum remains constant.

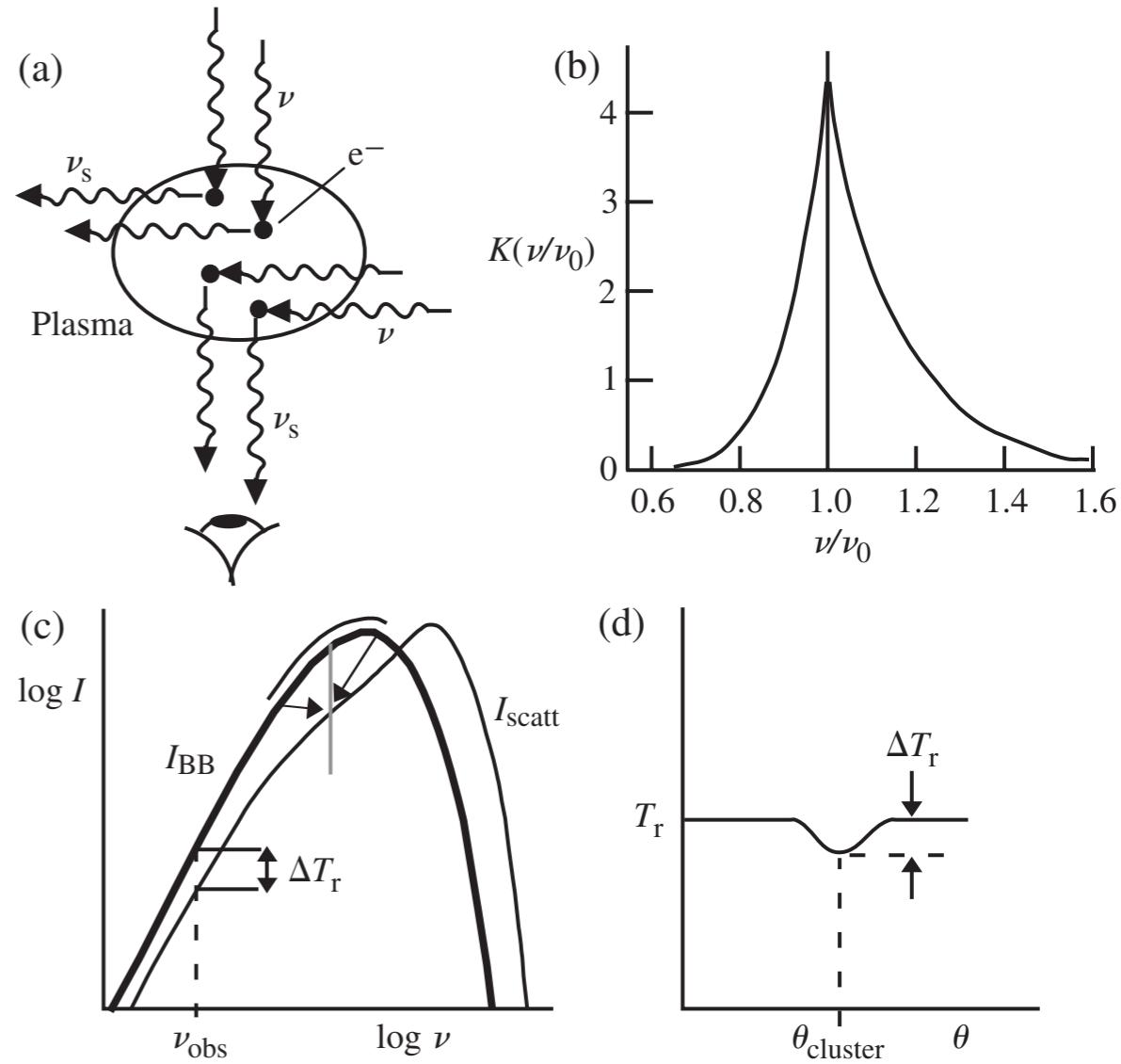
Recall that at low frequency regime, the brightness temperature is

$$T_b = \frac{c^2}{2\nu^2 k_B} I_\nu$$

But, the effective temperature: $\int F_n u d\nu = \sigma T_{\text{eff}}^4$

The result of such scatterings for an initial blackbody photon spectrum is shown in the following figure for the value:

$$\frac{kT_e}{mc^2}\tau = 0.5$$



- **Change of the BB temperature**

- In the Rayleigh-Jeans region,

$$I(\nu) = \frac{2\nu^2}{c^2} k_B T_{\text{CMB}}$$

- If the spectrum is shifted parallel to itself on a log-log plot, the fractional frequency change of a scattered photon is constant.

$$\varepsilon = \frac{\Delta\nu}{\nu} = \frac{\nu' - \nu}{\nu} = \text{constant} \quad \text{or} \quad \nu' = \nu(1 + \varepsilon) \longrightarrow d\nu' = d\nu(1 + \varepsilon)$$

- Total photon number is conserved: $N'(\nu')d\nu' = N(\nu)d\nu \rightarrow \frac{I'(\nu')}{h\nu'}d\nu' = \frac{I(\nu)}{h\nu}d\nu$

$$\therefore I'(\nu') = I(\nu) \quad I(\nu) = I\left(\frac{\nu'}{1 + \varepsilon}\right) = \frac{2\nu'^2}{c^2(1 + \varepsilon)^2} k_B T_{\text{CMB}}$$

$$\frac{\Delta I}{I} = \frac{I' - I}{I} = \frac{1}{(1 + \varepsilon)^2} - 1 \approx -2\varepsilon = -2\frac{\Delta\nu}{\nu}$$

$$\frac{\Delta T_{\text{CMB}}}{T_{\text{CMB}}} = \frac{\Delta I}{I} \approx -2\varepsilon = -2\frac{\Delta\nu}{\nu}$$

- The properly calculated result is $\varepsilon = \frac{\Delta\nu}{\nu} = \frac{k_B T_{\text{CMB}}}{mc^2} \tau$.

$$\frac{\Delta T_{\text{CMB}}}{T_{\text{CMB}}} \approx -2\frac{k_B T_{\text{CMB}}}{mc^2} \tau$$

A typical cluster have an average electron density of $\sim 2.5 \times 10^{-3} \text{ cm}^{-3}$, a core radius of $R_c \sim 10^{24} \text{ cm}$ ($\sim 320 \text{ pc}$), and an electron temperature of $k_B T_e \approx 5 \text{ keV}$.

A typical optical depth is thus

$$\tau \approx 3\sigma_T n_e R_e \approx 0.005$$

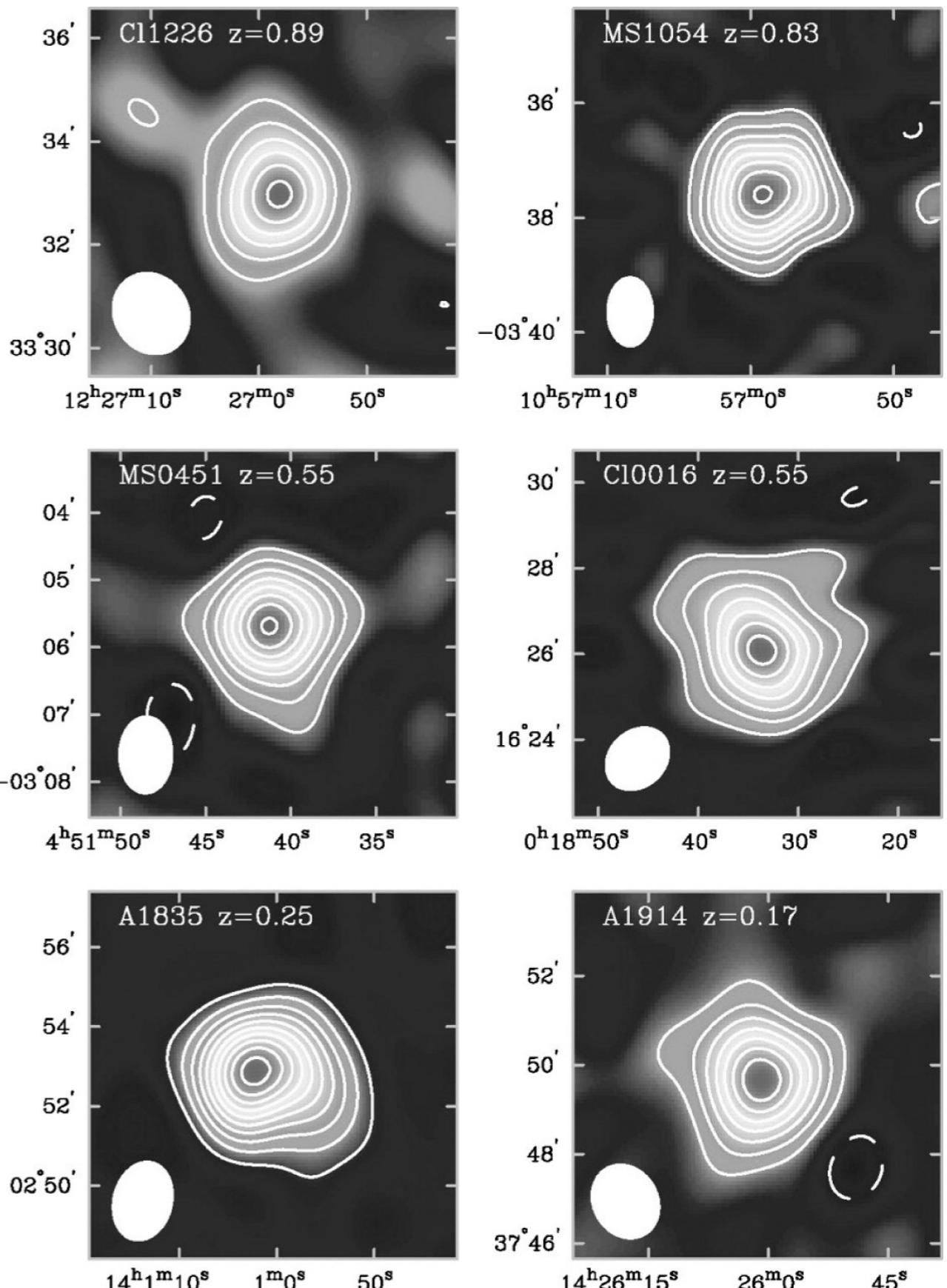
The expected antenna temperature change is

$$\frac{\Delta T_{\text{CMB}}}{T_{\text{CMB}}} \approx -1 \times 10^{-4}$$

$$\Delta T_{\text{CMB}} \approx -0.3 \text{ mK for } T_{\text{CMB}} = 2.7 \text{ K}$$

This effect has been measured in dozens of clusters.

Interferometric images at 30 GHz of six clusters of galaxies. The solid white contours indicate negative decrements to the CMB. (Carlstrom et al. 2002, ARAA, 40, 643)



Hubble Constant

- A value of the Hubble constant is obtained for a given galaxy only if one has independent measures of a recession speed v and a distance d of a galaxy.

$$H_0 = \frac{v}{d}$$

- Recession speed is readily obtained from the spectral redshift.
- Distance:

► X-ray observations: $I(\nu, T_e) = C \frac{g(\nu, T_e)}{T_e^{1/2}} \exp(-h\nu/kT_e) n_e^2 (2R)$

► S-Z CMB decrement: $\frac{\Delta T_{\text{CMB}}}{T_{\text{CMB}}} = -2 \frac{kT_e}{mc^2} \tau = -2 \frac{kT_e}{mc^2} (\sigma_T n_e 2R)$

- The radio and X-ray measurements yield absolute values of the electron density n_e and cluster radius R without a priori knowledge of the cluster distance.
- Imaging of the cluster in the radio or X-ray band yields the angular size of the cluster θ . Then the distance d to the cluster is obtained by

$$d = \frac{R}{\theta}$$

- The SZ effect (at radio frequencies) in conjunction with X-ray measurements can give distances to clusters of galaxies. This can be used to derive the Hubble constant.

Thomson Scattering (free Electron Scattering)

- Recall the Larmore's formula

$$\frac{dP}{d\Omega} = \frac{e^2 a^2}{4\pi c^3} \sin^2 \Theta, \quad P = \frac{2e^2 a^2}{3c^3}$$

- Let us consider the **process in which a free charged particle (electron) radiates in response to an incident electromagnetic wave.**

- In non-relativistic case, we may ignore magnetic force.

magnetic/electric force ratio in Lorentz force: $F_B/F_E \sim (v/c)B/E = v/c \ll 1$

- Consider a monochromatic wave with frequency ω_0 and linearly polarized in direction $\hat{\epsilon}$:

$$\mathbf{E} = \hat{\epsilon} E_0 \sin \omega_0 t$$

Lorentz force

$$\mathbf{F}_E = q\mathbf{E}$$

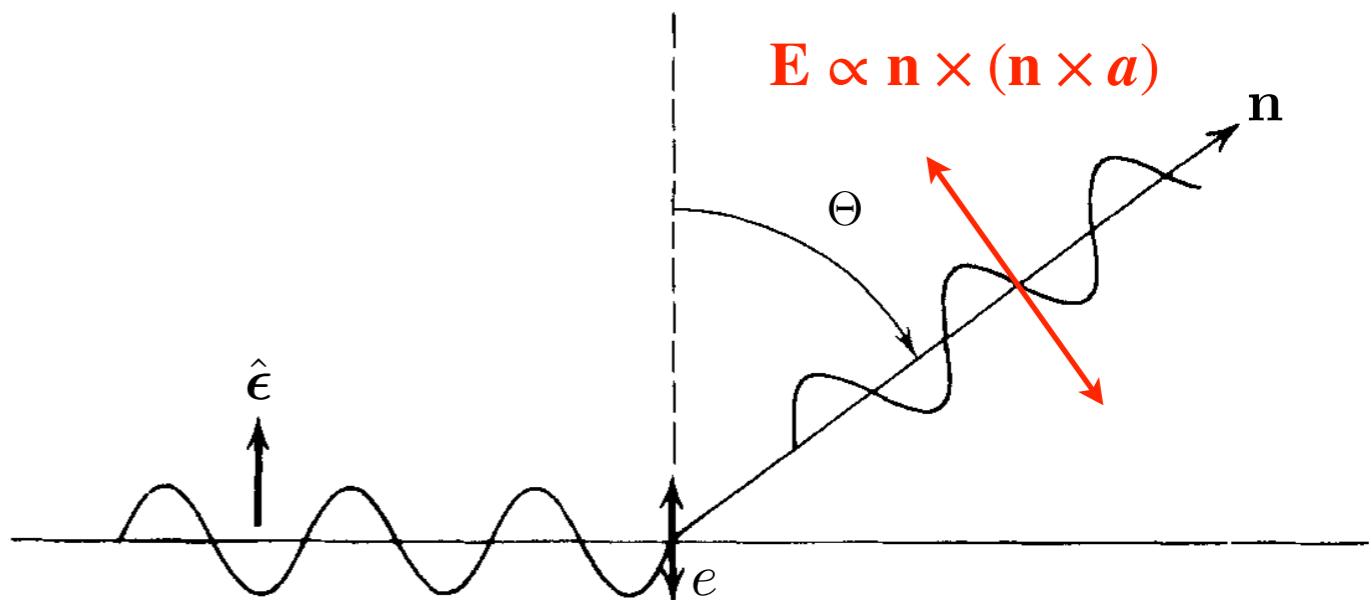
$$\mathbf{F}_B = q \frac{\mathbf{v} \times \mathbf{B}}{c}$$

Thus the force on a particle with the charge $-e$ is

$$\mathbf{F} = e\mathbf{E} = \hat{\epsilon} e E_0 \sin \omega_0 t$$

the acceleration of the electron is

$$\mathbf{a} = \hat{\epsilon} \frac{eE_0}{m} \sin \omega_0 t$$



- We obtain the time-averaged power per solid angle $\left(\langle \sin^2 \omega_0 t \rangle_t = 1/2 \right)$:

$$\left\langle \frac{dP}{d\Omega} \right\rangle_t = \frac{e^4 E_0^2}{8\pi m^2 c^3} \sin^2 \Theta, \quad \langle P \rangle_t = \frac{e^4 E_0^2}{3m^2 c^3}$$

Note that the time-averaged incident flux (Poynting flux) is $\langle S \rangle = \frac{c}{8\pi} E_0^2$.

The **differential cross section** for linearly polarized radiation is obtained by

$$\frac{d\sigma}{d\Omega} = \left\langle \frac{dP}{d\Omega} \right\rangle_t / \langle S \rangle \longrightarrow \frac{d\sigma}{d\Omega} = \frac{e^2}{m^2 c^4} \sin^2 \Theta = r_0^2 \sin^2 \Theta, \quad r_0 \equiv \frac{e^2}{mc^2}$$

where the quantity r_0 gives a measure of the “size” of the point charge. (Note electrostatic potential energy $e\phi = e^2/r_0$).

For an electron, the classical electron radius has a value $r_0 = 2.82 \times 10^{-13}$ cm.

The total cross section is found by integrating over solid angle.

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi r_0^2 \int_{-1}^1 (1 - \mu^2) d\mu = \frac{8\pi}{3} r_0^2$$

For an electron, the scattering process is then called Thomson scattering or electron scattering, and the **Thomson cross section** is

$$\sigma_T = \frac{8\pi}{3} r_0^2 = 6.652 \times 10^{-25} \text{ cm}^2$$

- Note:

The total and differential cross sections are frequency independent.

The scattered radiation is linearly polarized in the plane of the incident polarization vector $\hat{\epsilon}$ and the direction of scattering \mathbf{n} .

$\sigma \propto 1/m^2$: electron scattering is larger than ions by a factor of $(m_p/m_e)^2 = (1836)^2 \approx 3.4 \times 10^6$.

We have implicitly assumed that electron recoil is negligible. This is only valid for nonrelativistic energies. For higher energies, the (quantum-mechanical) Klein-Nishina cross section has to be used.

- What is the cross section for scattering of unpolarized radiation?

An unpolarized beam can be regarded as the independent superposition of two linear-polarized beams with perpendicular axes.

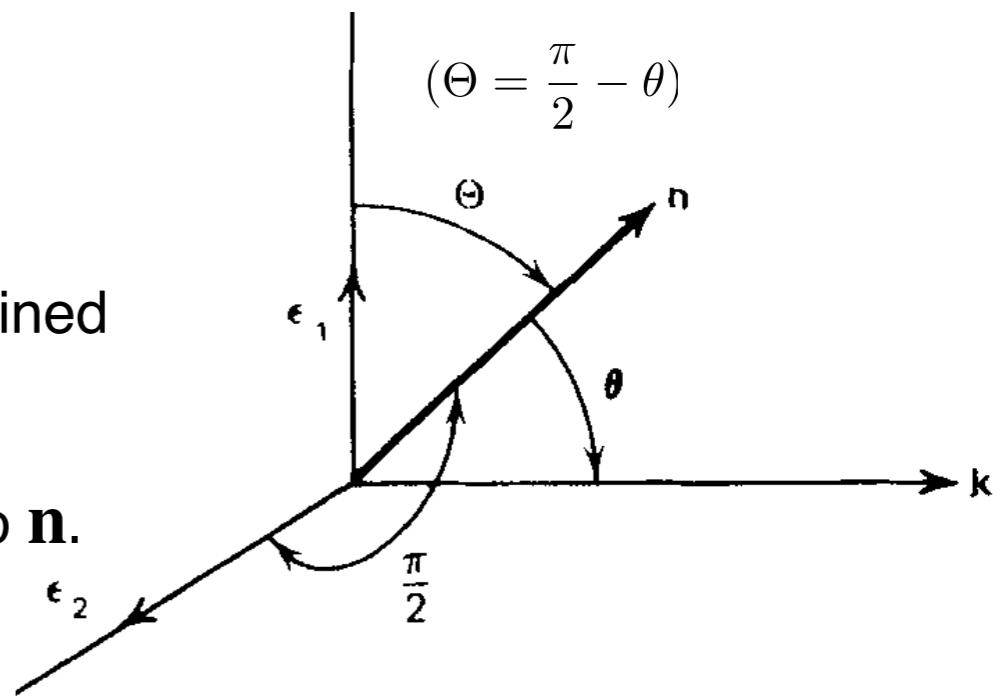
Let us assume that \mathbf{n} = direction of scattered radiation

\mathbf{k} = direction of incident radiation

Choose

- (1) the first electric field along $\hat{\epsilon}_1$, which is in the plane defined by \mathbf{n} and \mathbf{k} .

- (2) the second one along $\hat{\epsilon}_2$ orthogonal to this plane and to \mathbf{n} .



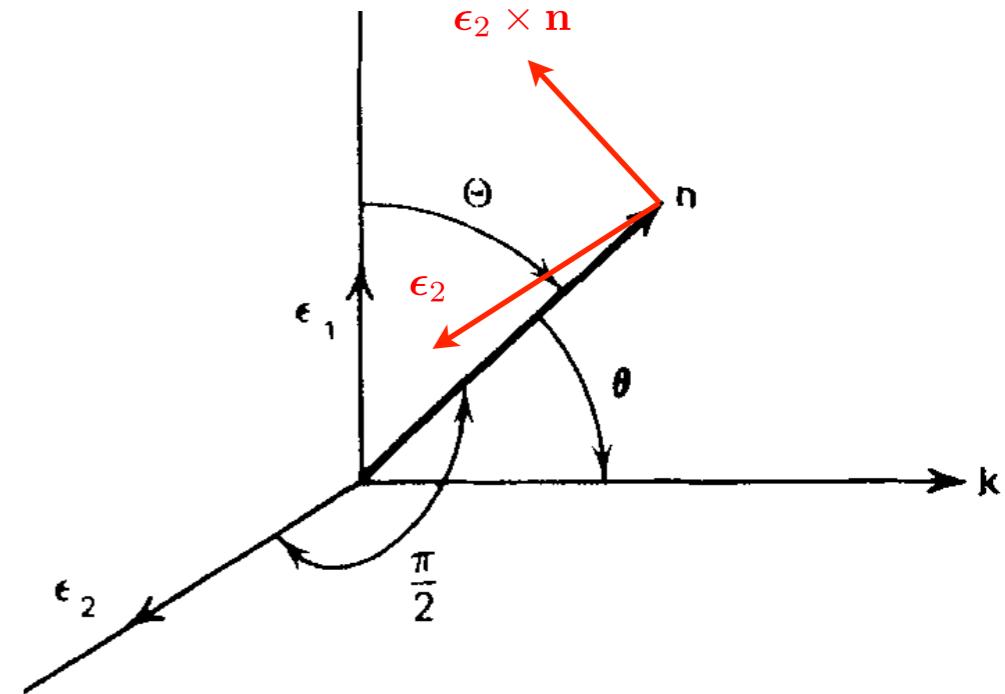
- Let Θ = angle between $\hat{\epsilon}_1$ and \mathbf{n} . Note that angle between $\hat{\epsilon}_2$ and \mathbf{n} is $\pi/2$, and $\theta = \pi/2 - \Theta$ is the angle between the scattered wave and incident wave

Then, the differential cross section for unpolarized radiation

is the average of the cross sections for scattering of two electric fields.

$$\begin{aligned}\left(\frac{d\sigma}{d\Omega}\right)_{\text{unpol}} &= \frac{1}{2} \left[\left(\frac{d\sigma}{d\Omega}\right)_{\epsilon_2} + \left(\frac{d\sigma}{d\Omega}\right)_{\epsilon_1} \right] \\ &= \frac{1}{2} \left[\left(\frac{d\sigma(\pi/2)}{d\Omega}\right)_{\text{pol}} + \left(\frac{d\sigma(\Theta)}{d\Omega}\right)_{\text{pol}} \right] \\ &= \frac{1}{2} r_0^2 (1 + \sin^2 \Theta)\end{aligned}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{unpol}} = \frac{1}{2} r_0^2 (1 + \cos^2 \theta)$$



This depends only on the angle between the incident and scattered directions, as it should for unpolarized radiation.

Total cross section:

$$\begin{aligned}\sigma_{\text{unpol}} &= \int \left(\frac{d\sigma}{d\Omega}\right)_{\text{unpol}} d\Omega = \pi r_0^2 \int_{-1}^1 (1 + \mu^2) d\mu \\ &= \frac{8\pi}{3} r_0^2 \\ &= \sigma_{\text{pol}}\end{aligned}$$

Properties of Thomson Scattering

- Forward-backward symmetry: the differential cross section is symmetric under $\theta \rightarrow -\theta$.
- Total cross section of unpolarized incident radiation = total cross section for polarized incident radiation. This is because the electron at rest has no preferred direction defined.
- **Scattering creates polarization**

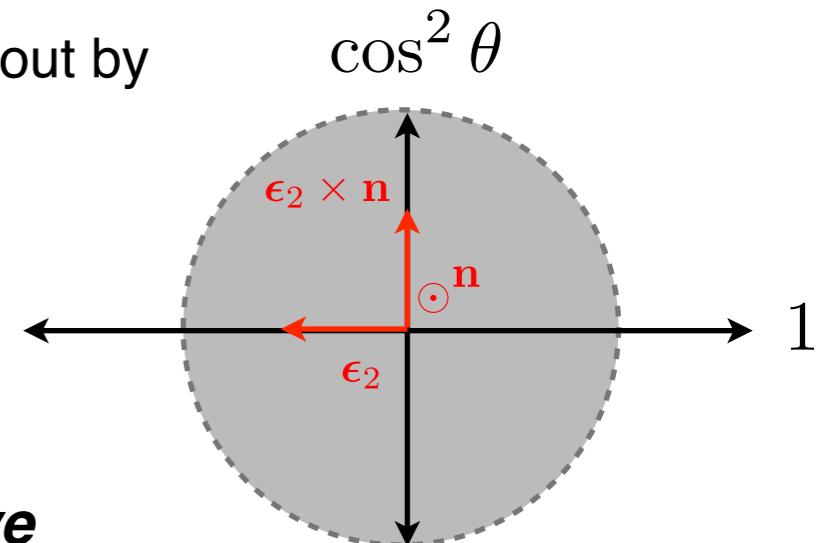
- The scattered intensity is proportional to $1 + \cos^2 \theta$, of which 1 arises from the incident electric field along $\hat{\epsilon}_2$ and $\cos^2 \theta$ from the incident electric field along $\hat{\epsilon}_1$.
- The portion of " $\cos^2 \theta$ " of the polarization along $\hat{\epsilon}_2$ will be cancelled out by the independent polarization along $\hat{\epsilon}_2 \times \mathbf{n}$.
- Therefore, the degree of polarization of the scattered wave:

$$\Pi = \frac{1 - \cos^2 \theta}{1 + \cos^2 \theta}$$

- ***Electron scattering of a completely unpolarized incident wave produces a scattered wave with some degree of polarization.***

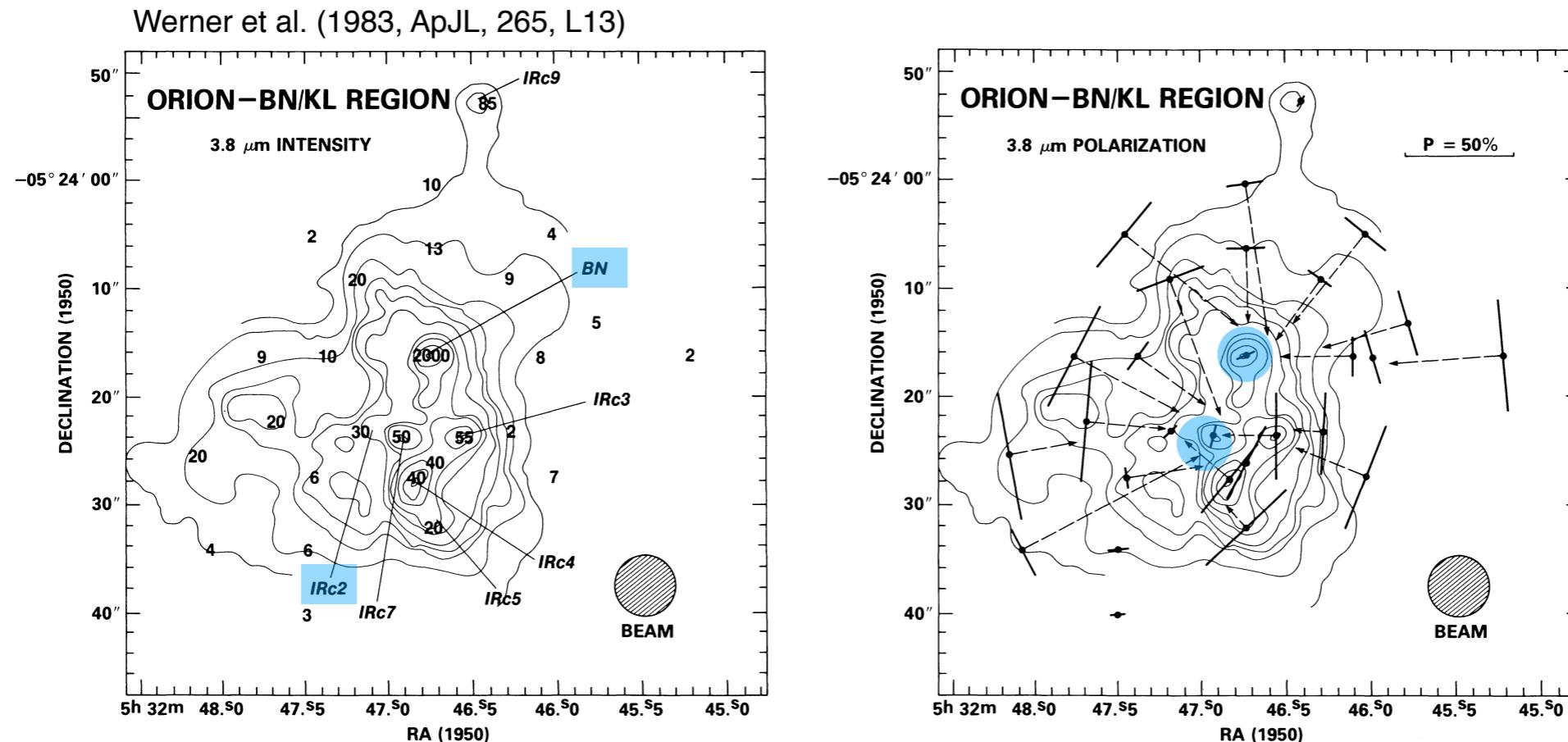
No net polarization along the incident direction ($\theta = 0$), since, by symmetry, all directions are equivalent.

100% polarization perpendicular to the incident direction ($\theta = \pi/2$), since the electron's motion is confined to a plane normal to the incident direction.



Astrophysical Applications of Polarization by Scattering

- **Detection of a concentric pattern of polarization vectors in an extended region indicates that the light comes via scattering from a central point source.**



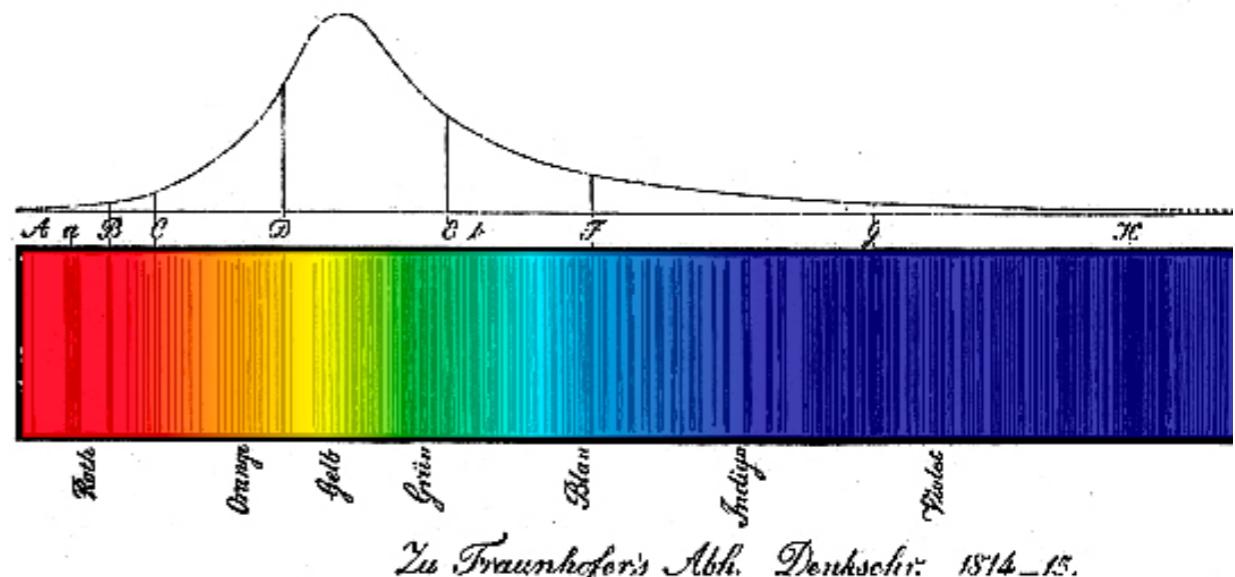
- Left map shows the IR intensity map at $3.8 \mu\text{m}$ of the Becklin-Neugebauer/Kleinmann-Low region of Orion. It is not easy to identify which bright spots correspond to locations of possible protostars.
 - However, the polarization map singles out only two positions of intrinsic luminosity: IRc2 (now known to be an intense protostellar wind) and BN (suspected to be a relatively high-mass star)
 - All the other bright spots (IRc3 through 7) correspond to IR reflection nebulae.
- The above example is not for Thompson scattering. But, dust scattering also produces polarization from unpolarized light.

Atomic Structure, Radiative Transitions

History: Fraunhofer Lines

- In 1814, Joseph von Fraunhofer (1789-1826) used one of the high-quality prisms he had manufactured to diffract a beam of sunlight onto a whitewashed wall.
 - Besides the characteristic colors of the rainbow, he saw many dark lines.
 - He catalogued the exact wavelength of each dark line and labelled the strongest of them with letters. These are still known today as Fraunhofer lines. Many of these labels, such as the sodium D lines (5896\AA , 5890\AA ; Na I D_1 , D_2) are still used today.
 - He did not know what caused the dark lines he observed.
 - However, he performed a similar experiment using light from the nearby star Betelgeuse and found that the pattern of dark lines changed significantly. He concluded correctly that most of those features were somehow related to the composition of the object.
 - The first real step in understanding Fraunhofer's observations came in the middle of the 19th century with the experiments of Gustav Kirchhoff (1824-1887) and Robert Bunsen (1811-1891). They studied the color of the light emitted when metals were burnt in flames. In certain cases, the wavelength of the emitted light gave an exact match with the Fraunhofer lines. These experiments demonstrated that the Fraunhofer lines were a direct consequence of the atomic composition of the Sun.
 - In fact, some of the lines were due to the Earth's atmosphere, the so-called telluric lines.

The solar spectrum as recorded by Fraunhofer (color overlaid).



History: Nebulium?

- In 1918, extensive studies of the emission spectra of nebulae found a series of lines which had not been observed in the laboratory.
 - Particularly strong were features at 4959Å and 5007Å. For a long time, this pair could not be identified and these lines were attributed to a new element, '**nebulium**'.
- In 1927, Ira Bown (1898-1973) discovered that the lines were not really due to a new chemical element but instead ***forbidden lines from doubly ionized oxygen*** [O III].
- He realized that in the diffuse conditions found in nebulae, atoms and ions could survive a long time without undergoing collisions. Indeed, ***under typical nebula conditions the mean time between collisions is in the range 10-10,000 secs.*** This means that there is sufficient time for excited, metastable states to decay via weak, forbidden line emissions.
- The forbidden lines could not be observed in the laboratory where it was not possible to produce collision-free conditions over this long timeframe.
- Other 'nebulium' lines turned out to be forbidden lines originating from singly ionized oxygen [O II] and nitrogen [N II].

Atomic Hydrogen

- Spectra of atomic hydrogen, H, are of paramount astronomical importance.
 - This is because ***approximately 90% of atomic matter by number is hydrogen.***
- The spectrum of atomic hydrogen also plays an important role in the theory of quantum mechanics.
 - Hydrogen is the only atom for which exact quantum mechanical solutions can be found for its energy levels and wavefunctions.
- Schrodinger equation
 - momentum operator: $\mathbf{p} = \frac{\hbar}{i}\nabla$
 - Hamiltonian operator: $H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r}$
 - Schrodinger equation: $-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{Ze^2}{r}\psi = E\psi$
 - Solution: $\psi_{n,l,m}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$

radial function:

$$R_{nl}(r) = - \left[\left(\frac{2Z}{na_0} \right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^3} \right]^{1/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho)$$

spherical harmonics:

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

$$\rho = \frac{2Z}{na_0}r, \quad a_0 \equiv \frac{\hbar^2}{m_e c^2} = 0.529\text{\AA} \text{ (Bohr radius)},$$

L_{n+l}^{2l+1} = associated Laguerre polynomial

$P_l^{|m|}$ = associated Legendre function

- Each bound state of the hydrogen atom is characterized by a set of four quantum numbers (n, l, m, m_s)

- $n = 1, 2, 3, \dots$: principal quantum number
- $l = 0, 1, 2, \dots, n - 1$: 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	...

- $m = -l, -l + 1, \dots, 0, \dots, l - 1, l$: 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 : $2 \times \sum_{l=0}^{N-1} (2l + 1) = 2n^2$

- Wavefunctions for a hydrogen-like atom

$$R_{1,0} = \left(\frac{Z}{a_0}\right)^{3/2} 2 e^{-\rho}$$

$$R_{2,0} = \left(\frac{Z}{2a_0}\right)^{3/2} 2 (1 - \rho) e^{-\rho}$$

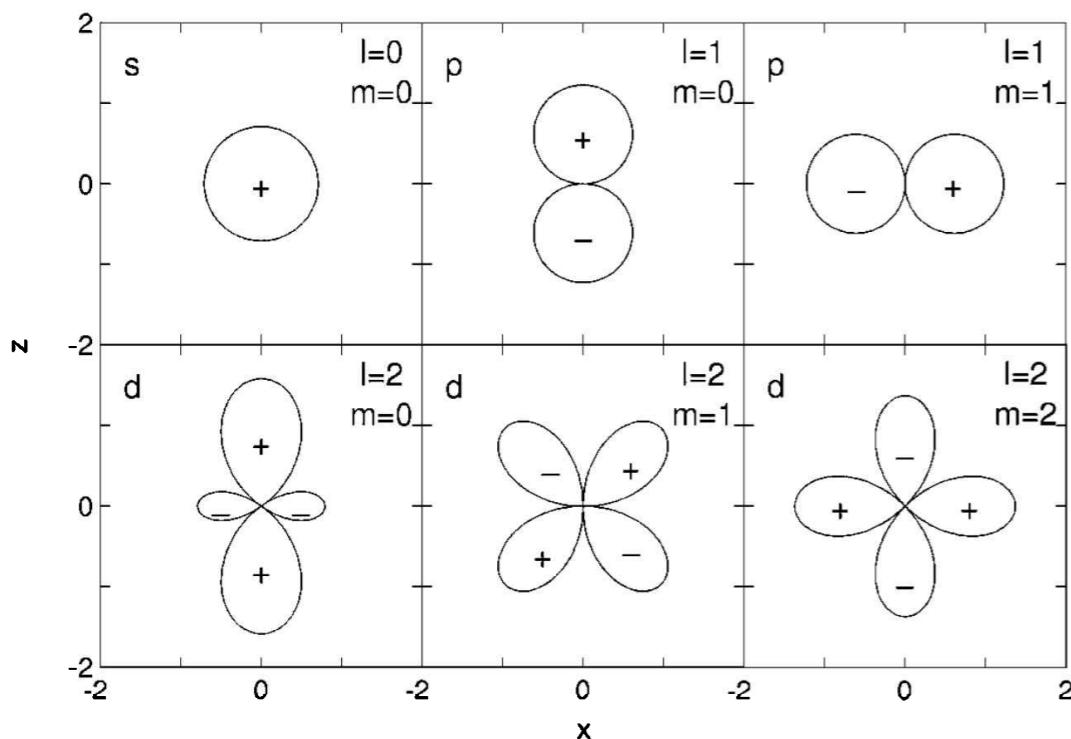
$$R_{2,1} = \left(\frac{Z}{2a_0}\right)^{3/2} \frac{2}{\sqrt{3}} \rho e^{-\rho}$$

$$R_{3,0} = \left(\frac{Z}{3a_0}\right)^{3/2} 2 \left(1 - 2\rho + \frac{2}{3}\rho^2\right) e^{-\rho}$$

$$R_{3,1} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{3} \rho \left(1 - \frac{1}{2}\rho\right) e^{-\rho}$$

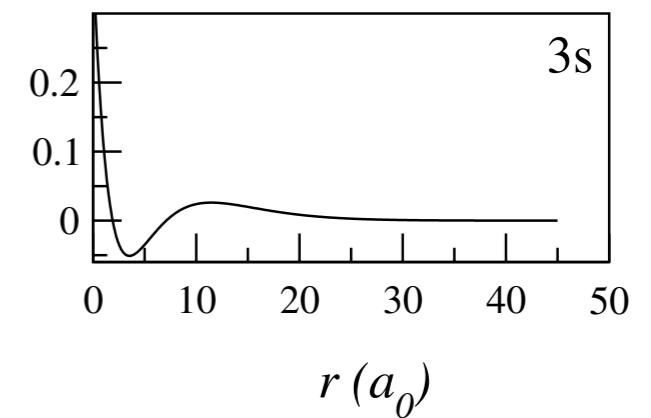
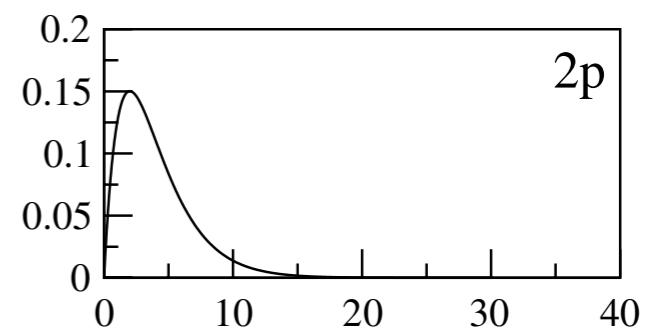
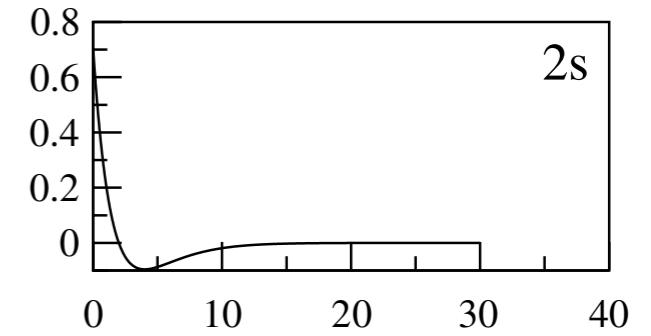
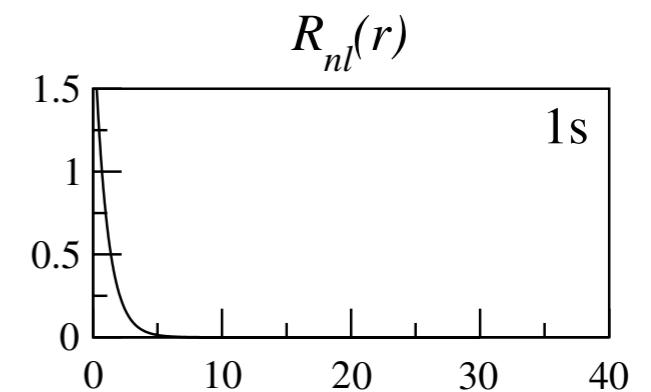
$$R_{3,2} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{2\sqrt{2}}{3\sqrt{5}} \rho^2 e^{-\rho}$$

Normalisation: $\int_0^\infty R_{n,l}^2 r^2 dr = 1$



Spherical harmonics

Radial functions



- The spherical harmonics are eigenfunctions of the orbital angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$

$$\mathbf{L}^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}, \quad L_z Y_{lm} = m\hbar Y_{lm}$$

- The sizes of the angular moment and z -component are $|\mathbf{L}| = \sqrt{l(l+1)}\hbar$, $|L_z| = m\hbar$
- Wavefunction (with $l = 0$) at $r = 0$

$$R_{10}(r) = \frac{2}{(a_0/Z)^{3/2}} e^{-r/(a_0/Z)}$$

$$R_{20}(r) = \frac{1}{(2a_0/Z)^{3/2}} \left(2 - \frac{r}{a_0/Z}\right) e^{-r/(2a_0/Z)}$$

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{1}{4\pi}}$$

$$|\psi_{n,l=0}(0)|^2 = \frac{1}{\pi} \left(\frac{Z}{na_0}\right)^3 \neq 0$$

This indicates that the electron can interact with the nucleus \rightarrow hyperfine structure!

- Probability: $|\psi(r, \theta, \phi)|^2 d^3x = R_{nl}^2(r) |Y_{lm}(\theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi$
- Properties of the spherical harmonics: $\int_0^\pi \int_0^{2\pi} |Y_{lm}(\theta, \phi)|^2 \sin \theta d\theta d\phi = 1$
- This implies that **closed shells are spherically symmetric and have very little interaction with external electrons.**

$$\sum_{m=-l}^l |Y_{lm}(\theta, \phi)|^2 = \frac{2l+1}{4\pi}$$

H-atom Spectra

- The spectrum of the hydrogen atom comes from electrons jumping between different levels in the atom.
 - If very small contributions from the electron and nuclear spins are neglected, the energy levels depend only on the principal quantum number n .*
 - The electronic spectrum of the H atom comes from changes in n .
 - The wavelength, λ , for the transition $n_2 \rightarrow n_1$ is given by the Rydberg formula:

$$\frac{1}{\lambda} = \frac{1}{1215.68 \text{\AA}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right), \quad n_2 > n_1$$

- 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	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

$$\Delta n \equiv n_2 - n_1$$

$$\Delta n = 1 \text{ is } \alpha,$$

$$\Delta n = 2 \text{ is } \beta,$$

$$\Delta n = 3 \text{ is } \gamma,$$

$$\Delta n = 4 \text{ is } \delta,$$

$$\Delta n = 5 \text{ is } \epsilon.$$

Lyman series : Ly α , Ly β , Ly γ , ...

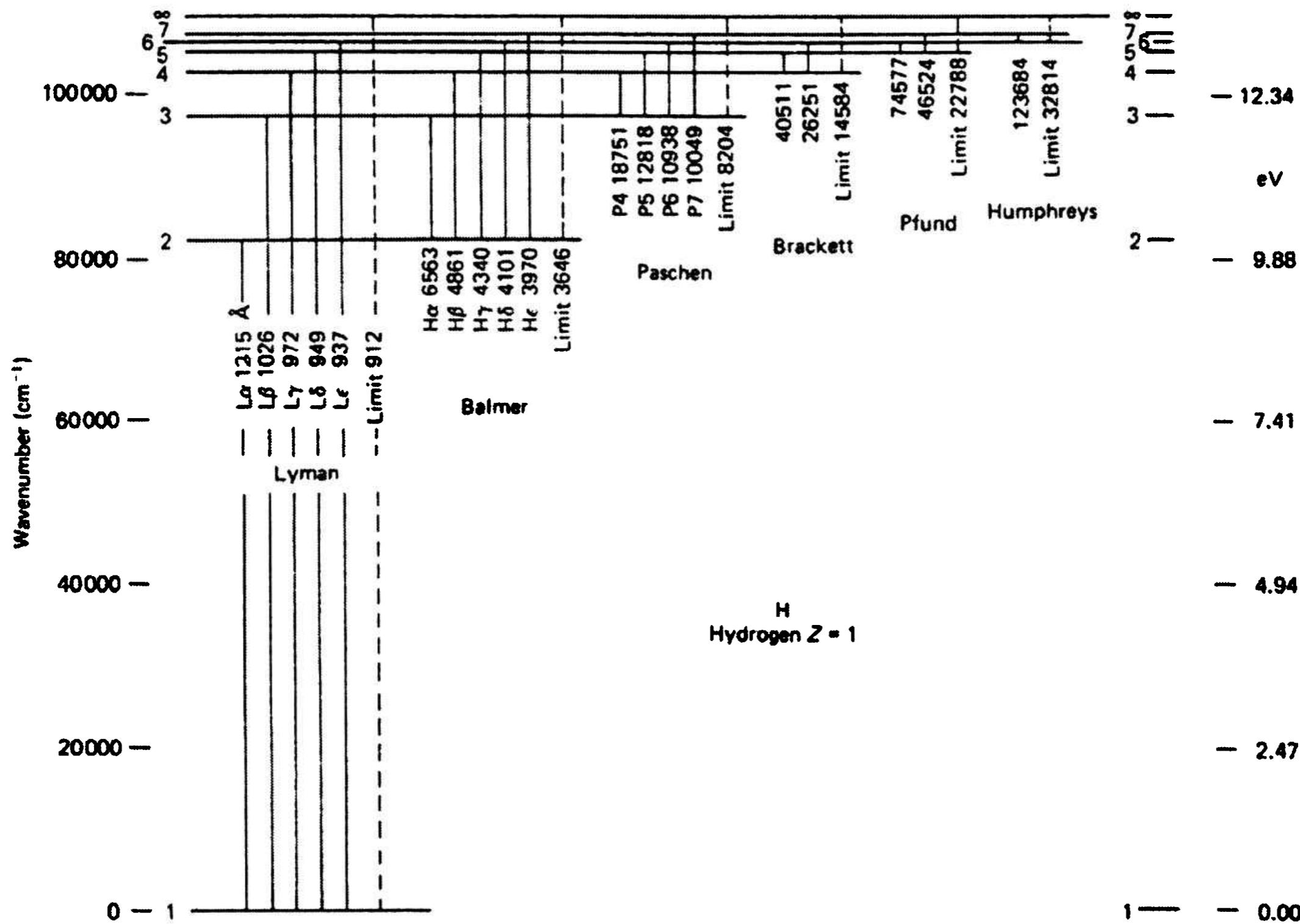
Balmer series : H α , H β , H γ , ...

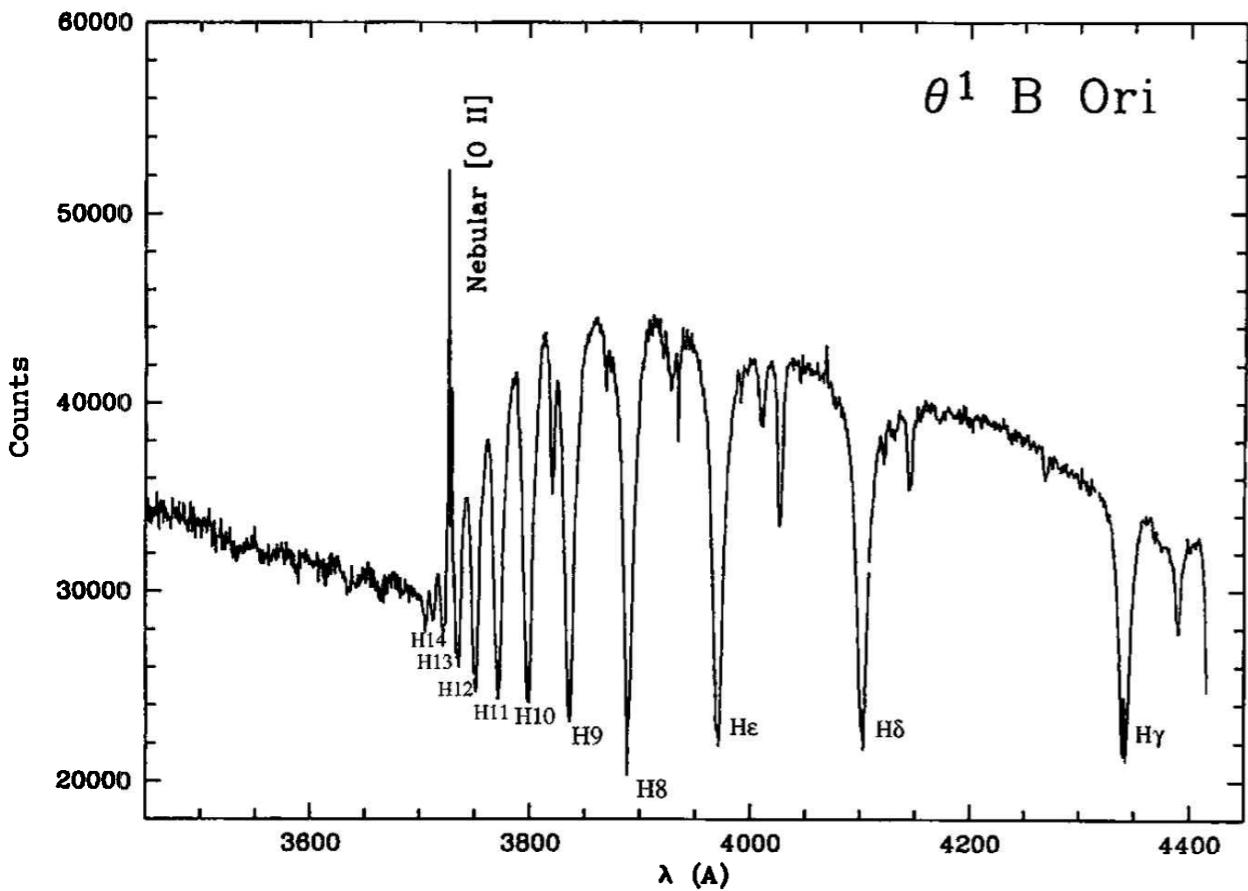
Paschen series: P α , P β , P γ , ...

Brackett series : Br α , Br β , Br γ , ...

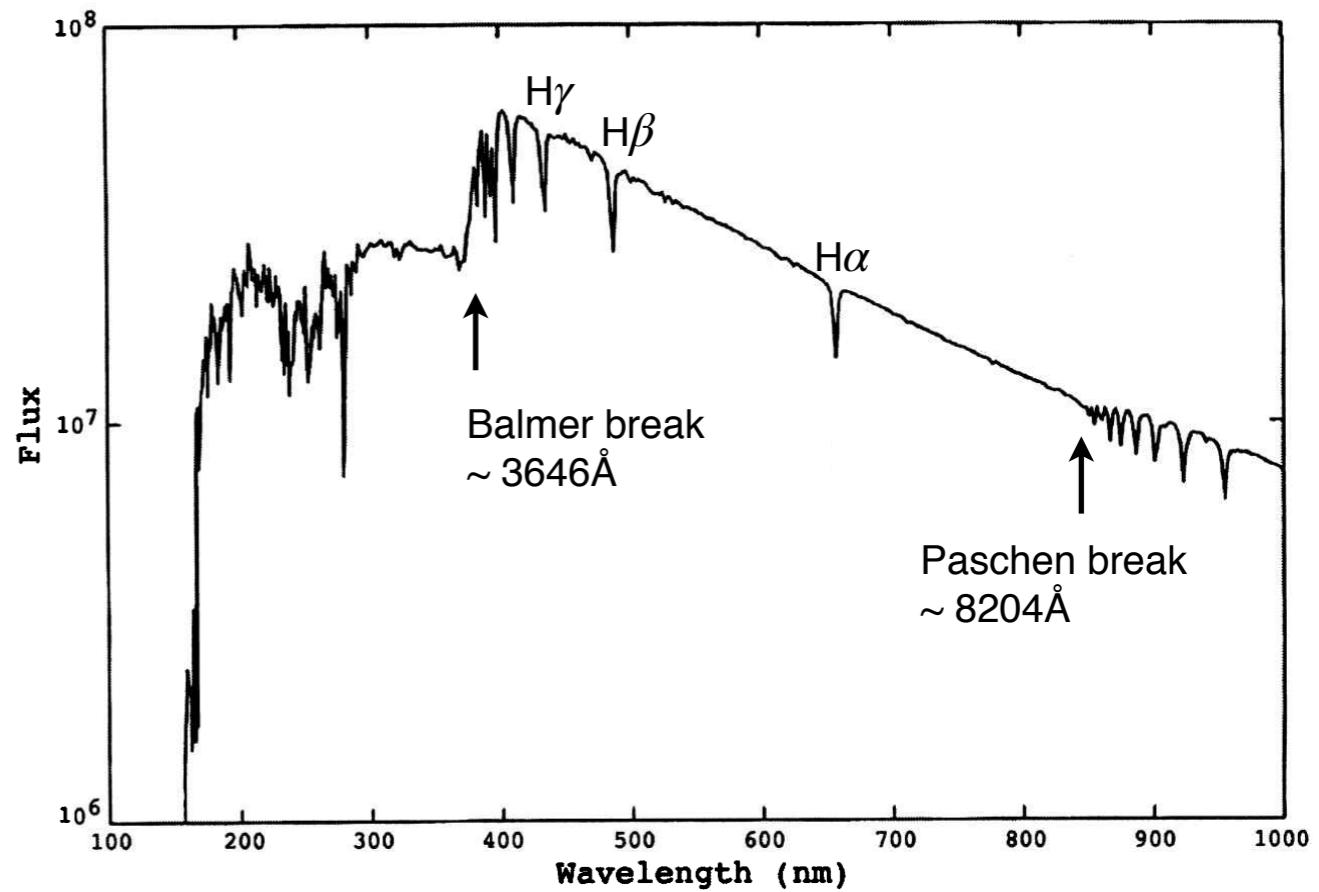
Transitions with high Δn are labelled by the n_2 . Thus, H15 is the Balmer series transition between $n_1 = 2$ and $n_2 = 15$.

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





Spectrum of B-type star Θ^1 B Ori showing Balmer series absorption lines



Model spectrum of an A5-type star showing both the Balmer and Paschen discontinuities (or jumps, breaks).

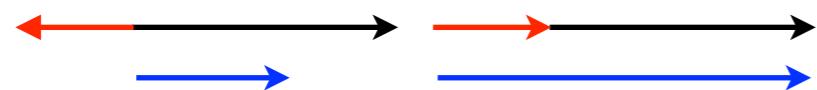
The Balmer discontinuity is prominent in A-type stars.

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 $\mathbf{F} = \mathbf{J} + \mathbf{I}$.

- In classical mechanics, adding vector a and vector b gives a vector c , whose length must lie in the range

$$|a - b| \leq c \leq a + b \quad \text{Here, } a, b, c \text{ are the lengths of their respective vectors.}$$



$$c = |a - b| \quad c = a + b$$

- In quantum mechanics, a similar rule applies except that the results are quantized. The allowed values of the quantized angular momentum, c , span the range from the sum to the difference of a and b in steps of one:

$$c = |a - b|, |a - b| + 1, \dots, a + b - 1, a + b$$

- For example, add the two angular momenta $L_1 = 2$ and $L_2 = 3$ together to give $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$. The result is

$$L = 1, 2, 3, 4, 5.$$

The Fine Structure of Hydrogen

- So far the discussion on H-atom levels has assumed that all those with the same principal quantum number, n , have the same energy.
 - However, this is not correct: inclusion of relativistic (or magnetic) effects split these levels according to the total angular momentum quantum number J . ***The splitting is called fine structure.***

- For hydrogen, $S = \frac{1}{2} \rightarrow J = L \pm \frac{1}{2}$

- Spectroscopic notation: $(2S+1)L_J$

configuration	L	S	J	term	level
ns	0	$1/2$	$1/2$	2S	$^2S_{1/2}$
np	1	$1/2$	$1/2, 3/2$	$^2P^o$	$^2P_{1/2}^o, ^2P_{3/2}^o$
nd	2	$1/2$	$3/2, 5/2$	2D	$^2D_{3/2}, ^2D_{5/2}$
nf	3	$1/2$	$5/2, 7/2$	$^2F^o$	$^2F_{5/2}^o, ^2D_{7/2}^o$

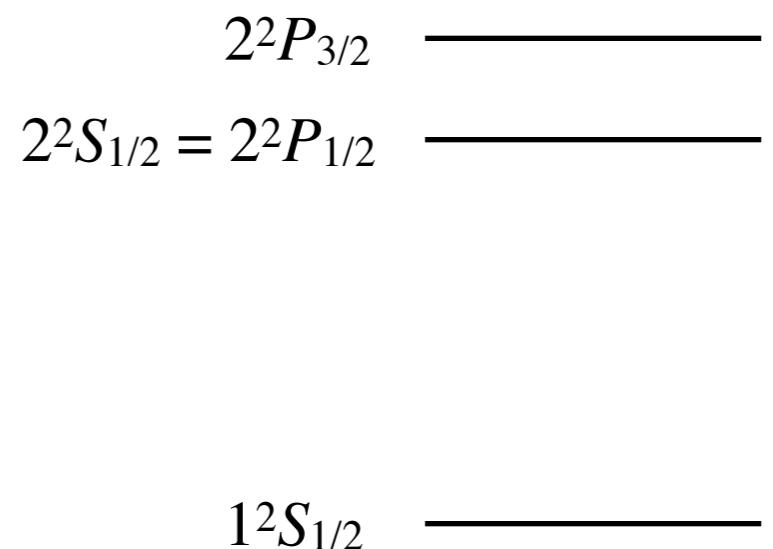
Note that the levels are called to be
 singlet if $2S+1 = 1 \quad S = 0, J = L$
 doublet if $2S+1 = 2 \quad S = 1/2, J = L \pm 1/2$
 triplet if $2S+1 = 3 \quad S = 1, J = L - 1, L, L + 1$
 (when $L > 0$)

- The above table shows the fine structure levels of the H atom.
- Note that the states with principal quantum number $n = 2$ give rise to three fine-structure levels. In spectroscopic notation, these levels are $2^2S_{1/2}$, $2^2P_{1/2}^o$ and $2^2P_{3/2}^o$.

- Fine structure of the hydrogen atom

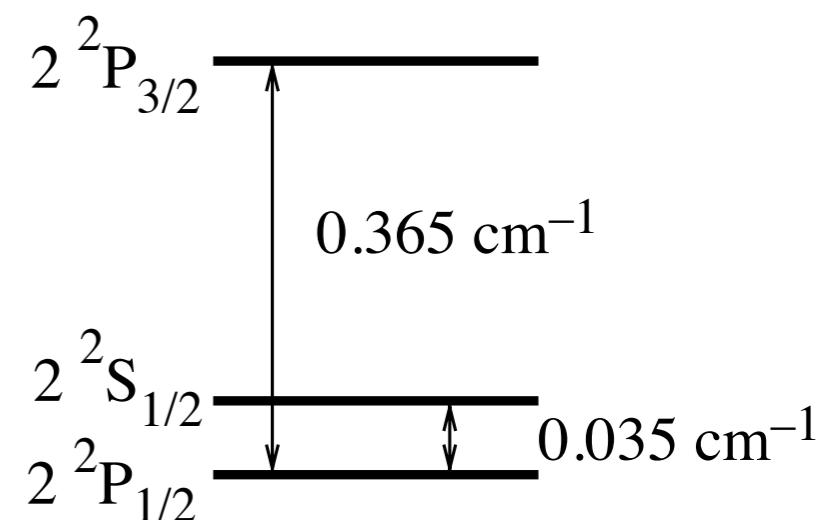
configuration	L	S	J	term	level
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np	1	$1/2$	$1/2, 3/2$	$^2P^o$	$^2P_{1/2}^o, ^2P_{3/2}^o$
nd	2	$1/2$	$3/2, 5/2$	2D	$^2D_{3/2}, ^2D_{5/2}$
nf	3	$1/2$	$5/2, 7/2$	$^2F^o$	$^2F_{5/2}^o, ^2D_{7/2}^o$

Relativistic QM (Dirac's eq)



- Splitting in the $n = 2$ levels of atomic hydrogen. The larger splitting is the fine structure and the smaller one the Lamb shift.
 - According to the Dirac equation, the $^2S_{1/2}$ and $^2P_{1/2}$ levels should have the same energies.
 - However, the interaction between the electron and the vacuum (which is not accounted for by the Dirac equation) causes a tiny energy shift on $^2S_{1/2}$. (Quantum electrodynamics effect)

Quantum Electrodynamics



What is the origin of the Spin-Orbit interaction (fine structure splitting)?

- **Fine-structure splitting:** Relativistic effects couple electron orbital angular momentum and electron spin to give the so-called fine structure in the energy levels. Inclusion of relativistic effects splits the terms into **levels** according to their J value.
- When the electron will move around the nucleus with a non relativistic velocity \mathbf{v} , the electric field exerting on the electron will be $\mathbf{E} = Ze\frac{\mathbf{r}}{r^3}$. (Note that the nucleus has a positive charge Ze .)
- In the electron rest frame, this electric field will be perceived as a magnetic field

$$\begin{aligned}\mathbf{B}' = \mathbf{B}_\perp &= \gamma(\mathbf{B}_\perp - \boldsymbol{\beta} \times \mathbf{E}) = -\frac{\mathbf{v}}{c} \times \mathbf{E} \\ &= -\frac{Ze}{c} \frac{\mathbf{v} \times \mathbf{r}}{r^3} \\ &= \frac{Ze}{m_e c r^3} \boldsymbol{\ell}\end{aligned}\quad \text{Here, the magnetic field is perpendicular to the electron's orbital plane.}$$

(where $\boldsymbol{\ell} \equiv \mathbf{r} \times \mathbf{p} = m_e \mathbf{r} \times \mathbf{v}$ is the electron's orbital angular momentum of electron)

- This magnetic field will interact with the electron's **magnetic moment**, which is

$$\boldsymbol{\mu} = -\frac{e}{m_e c} \mathbf{s}$$

- Then, the interaction energy is

$$U = -\mu \cdot \mathbf{B} = \frac{Ze^2}{m_e^2 c^2 r^3} \mathbf{s} \cdot \boldsymbol{\ell}$$

- For the sum of the interactions of all electrons will be

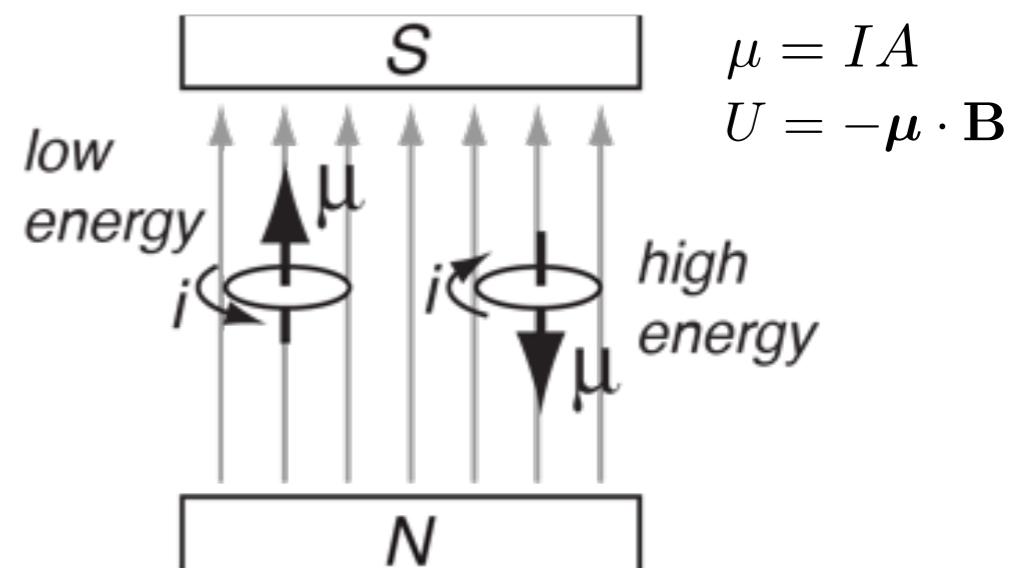
$$H_{\text{so}} = \sum_i \xi_i (\mathbf{s}_i \cdot \boldsymbol{\ell}_i)$$

- The individual spin and orbital angular momenta may be averaged over in such a way that an equivalent interaction is simply

$$H_{\text{so}} = \xi (\mathbf{S} \cdot \mathbf{L}) \quad \text{where } \mathbf{S} = \sum_i \mathbf{s}_i, \quad \mathbf{L} = \sum_i \boldsymbol{\ell}_i$$

- From the relation $\mathbf{J}^2 = |\mathbf{L} + \mathbf{S}|^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{S} \cdot \mathbf{L}$, we obtain

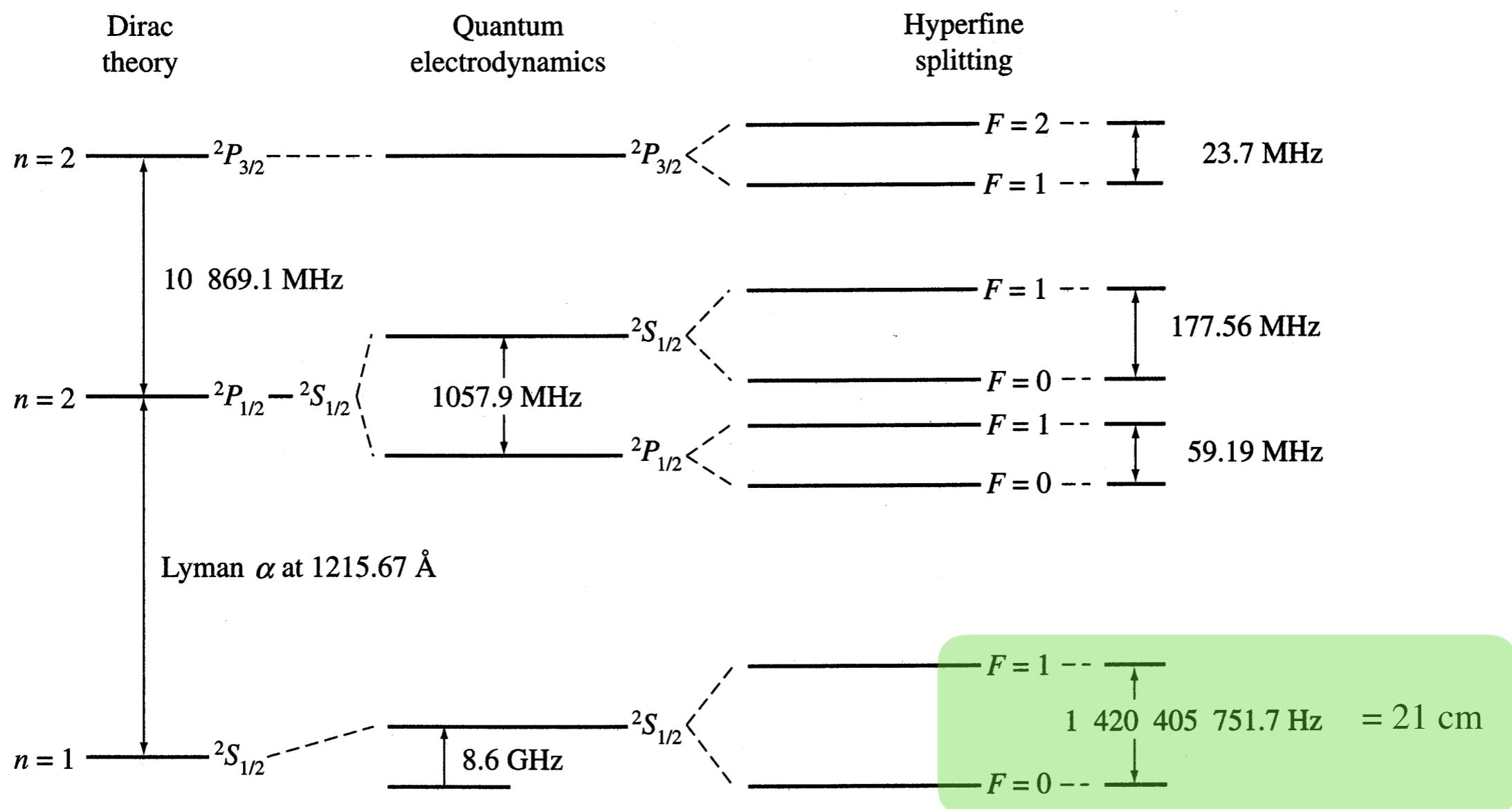
$$H_{\text{so}} = \frac{1}{2} \xi (\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2)$$



- ***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

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



Allowed Transitions in Hydrogen

- **Selection Rules**

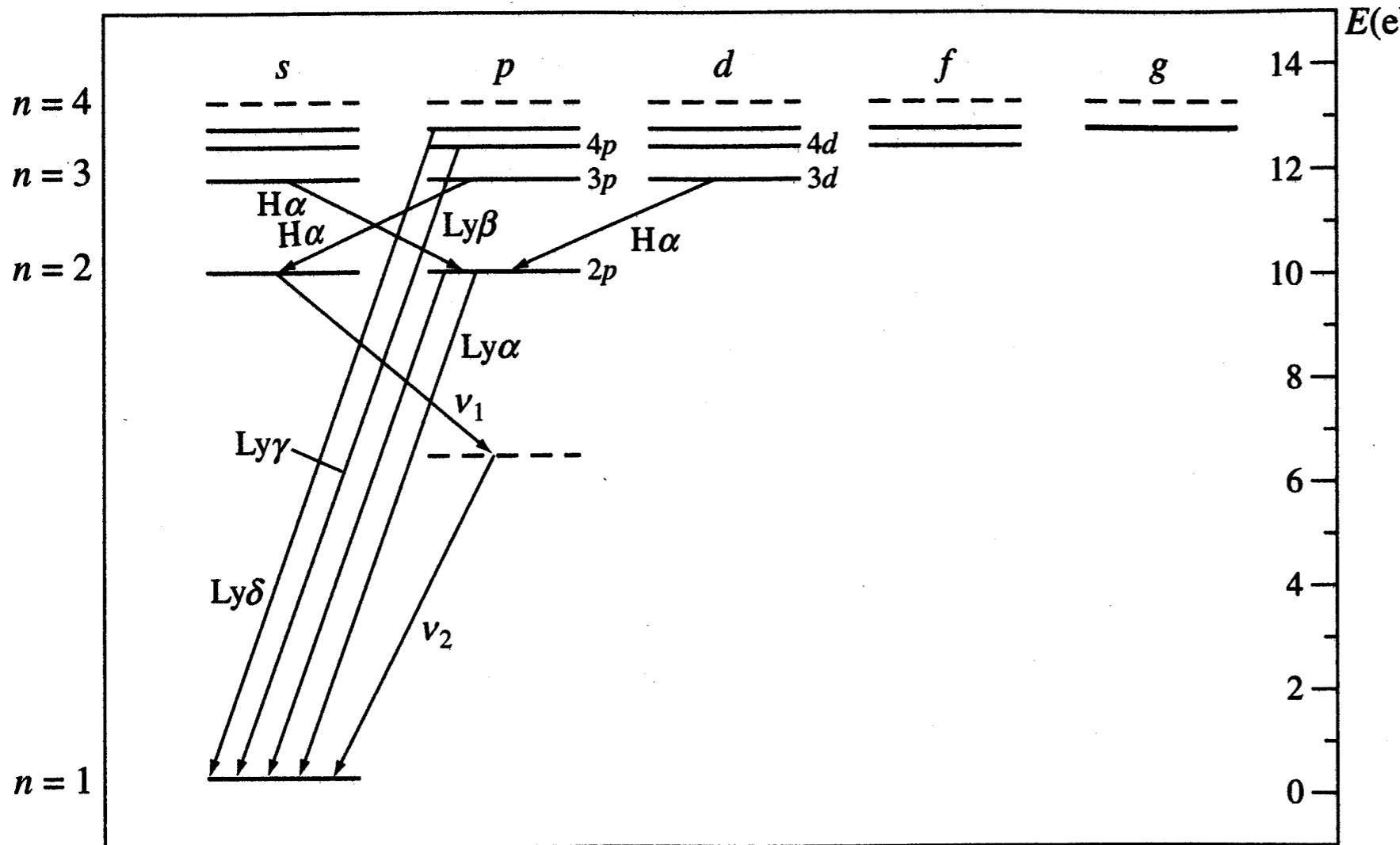
- Transitions are governed by selection rules which determine whether they can occur. The selection rules can be derived using the rules of quantum mechanics.
 - (1) For electric dipole transitions, Rules 1, 2 and 3 must always be obeyed.
 - (2) Intercombination lines violate rule 4.
 - (3) Forbidden lines violate rule 5 and/or 6. Electric quadrupole and magnetic dipole transitions are also described as forbidden.
- **Resonance line:** denote the longest wavelength, dipole-allowed transition arising from the ground state of a particular atom or ion. Ly α line is a resonance line.

Electric dipole	Electric quadrupole	Magnetic dipole
1. $\Delta J = 0, \pm 1$ Not $J = 0 - 0$	$\Delta J = 0, \pm 1, \pm 2$ Not $J = 0 - 0, \frac{1}{2} - \frac{1}{2}, 0 - 1$	$\Delta J = 0, \pm 1$ Not $J = 0 - 0$
2. $\Delta M_J = 0, \pm 1$	$\Delta M_J = 0, \pm 1, \pm 2$	$\Delta M_J = 0, \pm 1$
3. Parity changes	Parity unchanged	Parity unchanged
4. $\Delta S = 0$	$\Delta S = 0$	$\Delta S = 0$
5. One electron jumps Δn any $\Delta l = \pm 1$	One or no electron jumps Δn any $\Delta l = 0, \pm 2$	No electron jumps $\Delta n = 0$ $\Delta l = 0$
6. $\Delta L = 0, \pm 1$ Not $L = 0 - 0$	$\Delta L = 0, \pm 1, \pm 2$ Not $L = 0 - 0, 0 - 1$	$\Delta L = 0$

parity = $(-1)^L$ for hydrogen

parity = $(-1)^{\sum_i L_i}$ for many-electron system

- Hydrogen



$H\alpha$ transitions

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

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

$2p_{\frac{1}{2}} - 3d_{\frac{5}{2}}$ is not allowed;

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

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

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

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

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

The transition between $2s - 1s$ is not allowed.

Lyman series: $n' = 2 \rightarrow n < 2$ $\alpha : n' - n = 1$

Balmer series: $n' = 3 \rightarrow n < 3$ $\beta : n' - n = 2$

Paschen series: $n' = 4 \rightarrow n < 4$ $\gamma : n' - n = 3$

Brackett series: $n' = 5 \rightarrow n < 5$ $\delta : n' - n = 4$

Pfund series: $n' = 6 \rightarrow n < 6$ $\epsilon : n' - n = 5$

Humphreys series: $n' = 7 \rightarrow n < 7$

- Hydrogen: ***lifetime of excited states***

$$\tau_i = \left(\sum_j A_{ij} \right)^{-1} \quad \text{where } A_{ij} \text{ is the Einstein A coefficient}$$

Level	2s	2p	3s	3p	3d
τ/s	0.14	1.6×10^{-9}	1.6×10^{-7}	5.4×10^{-9}	2.3×10^{-7}

- Lifetimes for allowed transitions are shown, a few times 10^{-9} s.
- However, the lifetime for the (2s) $2^2S_{1/2}$ level is ~ 0.14 s, which is 10^8 times longer than the 2p states. (***The level is called to be metastable.***)

- Two-photon continuum radiation***

- In low-density environments, an electron in the $2^2S_{1/2}$ level can jump to a virtual p state, which lies between $n = 1$ and $n = 2$ levels. The electron then jumps from this virtual state to the ground state, in the process emitting two photons with total frequency $\nu_1 + \nu_2 = \nu_{\text{Ly}\alpha}$.
- Since this virtual p state can occur anywhere between $n = 1$ and $n = 2$, continuum emission longward of Ly α will result.

