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3. Atomic Physics

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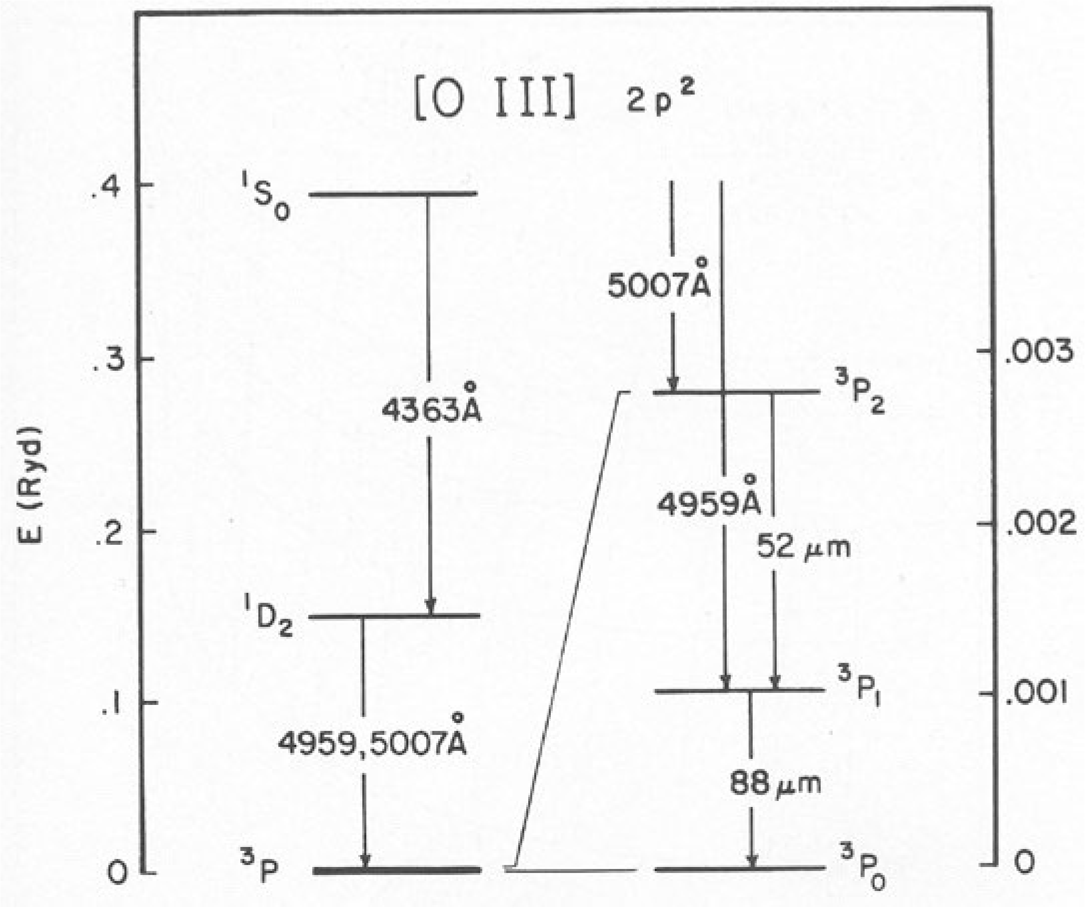
Why do we care about atomic physics in the ISM?



$$[OIII]\ 1D2 \rightarrow 3P2\ (501\ \text{nm})$$
$$1D2 \rightarrow 3P1\ (496\ \text{nm})$$
$$1\text{S}0 \rightarrow 1\text{D}2\ (436\ \text{nm})$$

Wave Equation for Atoms

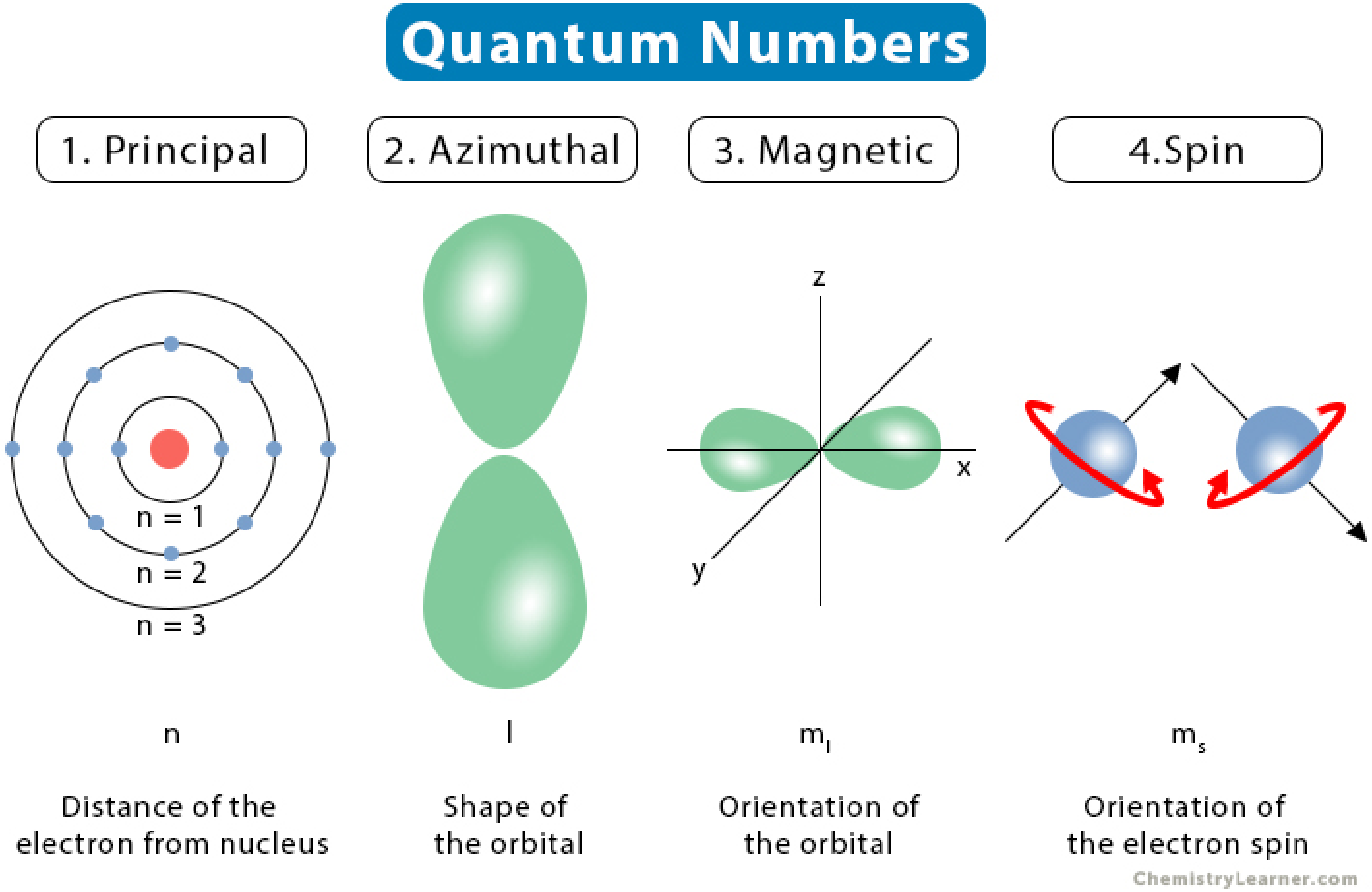
- Schrodinger equation in Spherical coordinates:

$$\left\{-\frac{\hbar^2}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]-\frac{e^2}{4\pi\epsilon_0 r}\right\}\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi)$$

- Spherical harmonic expansion solution:

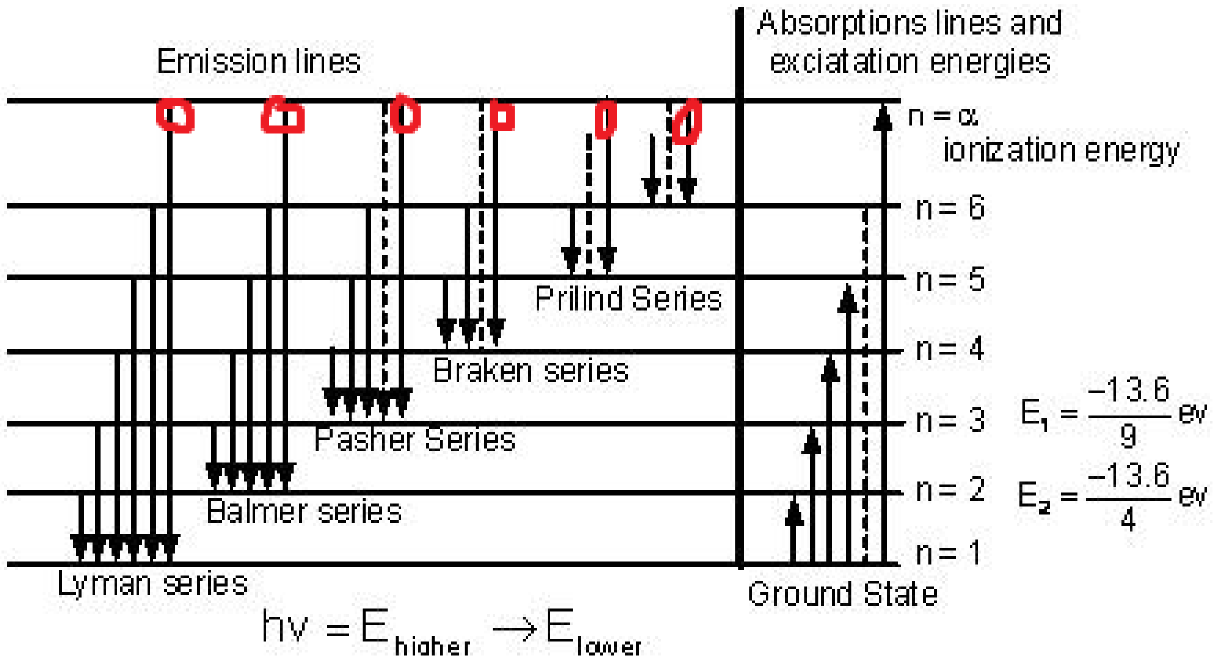
$$\psi_{(n,l,m_l)} = R_{n,l}(r) \times Y_{l,m_l}(\theta,\phi)$$

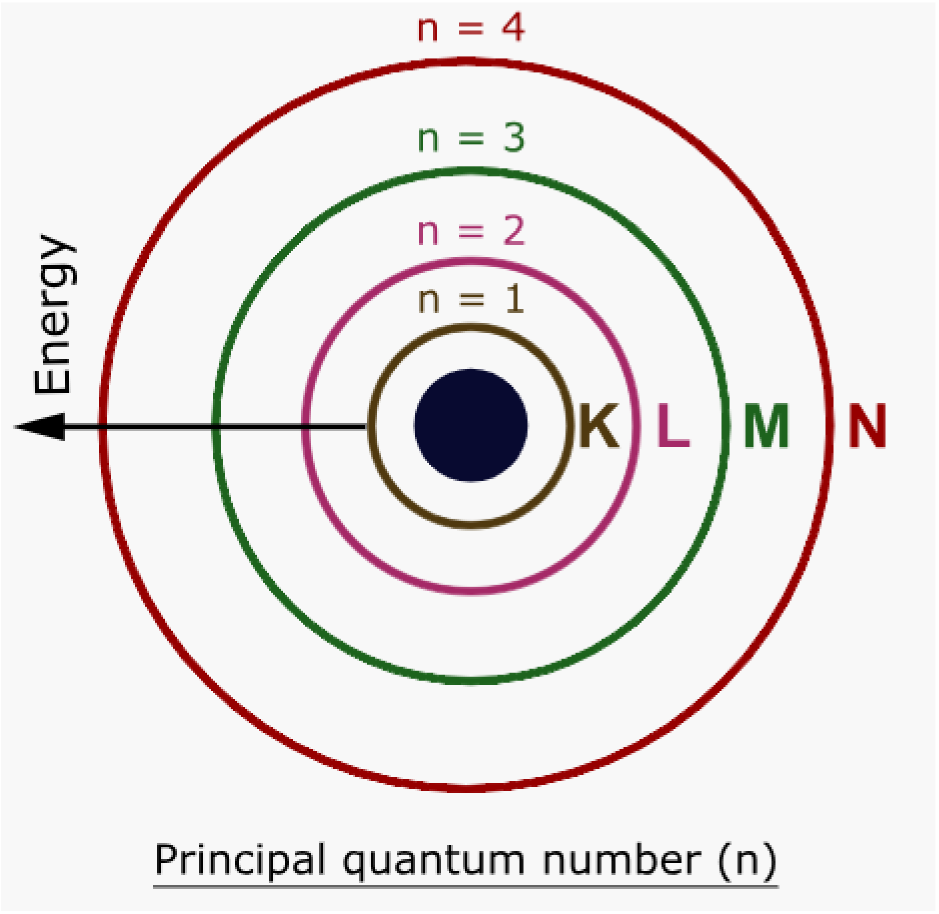
Quantum Numbers



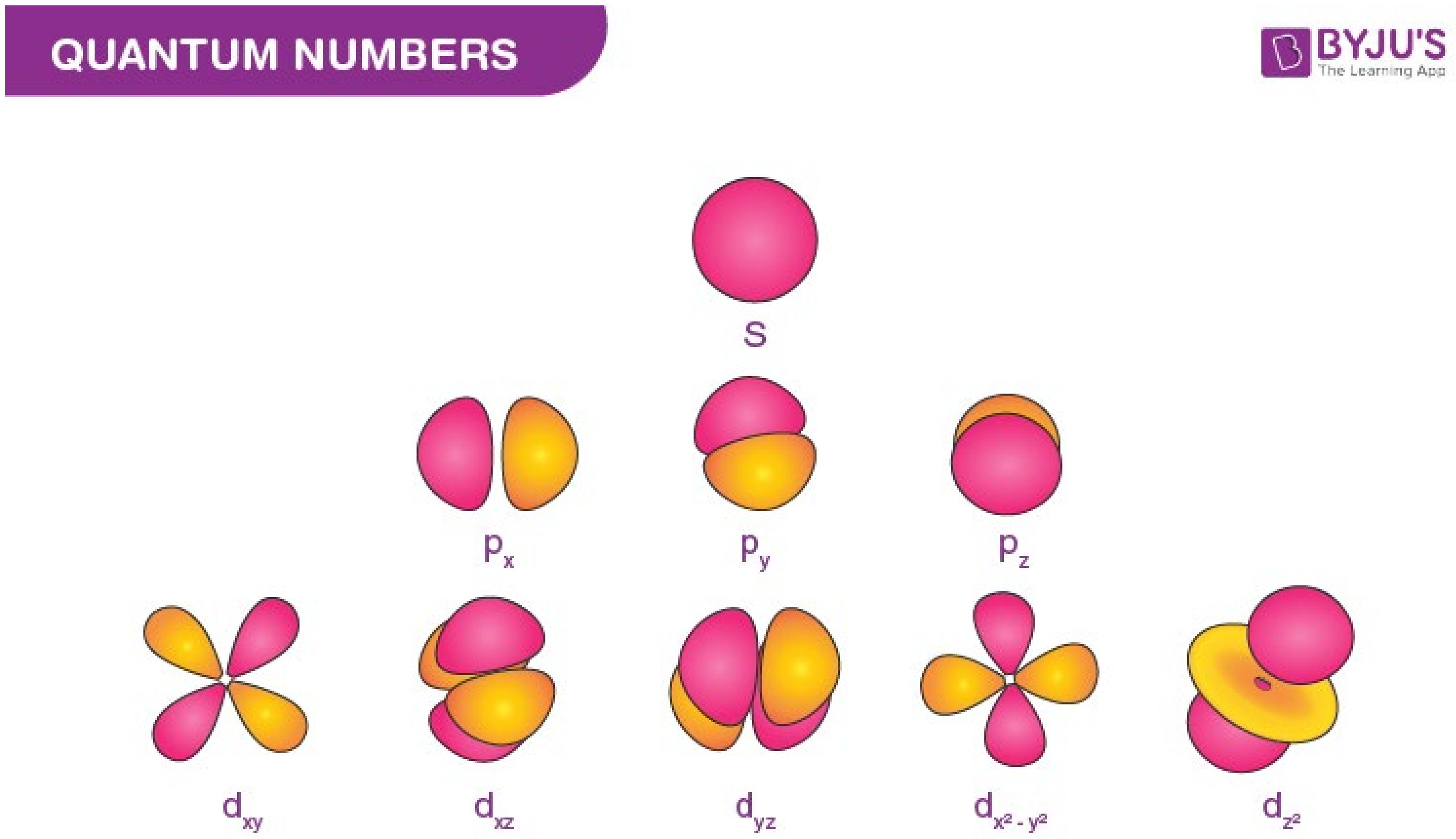
Principal Quantum Number

- N = 1, 2, 3, 4 …
- Refer as K, L, M, N … shells.
- Lines from these shells are called Lyman, Balmer, Paschen, Brakett … series.





Angular Momentum and Magnetic Quantum Numbers



Put everything together!

SYMBOL	NAME	VALUES	MEANING
n	principal	$1, 2, 3...$(any integer)	energy level, shell
l	angular momentum	$0 \rightarrow n-1$	subshell, $0 = s, 1 = p, 2 = d, 3 = f...$ this is the angular dependence of the orbital, shape of the orbital *letters have historical meaning, sharp, principle, diffuse, fundamental
m_l	magnetic	$+l \rightarrow -l$	orientation of angular momentum in space, orbital
m_s	spin	$+\frac{1}{2}, -\frac{1}{2}$	the imaginary property we call "spin", up or down

Electronic Configuration

- Pauli exclusion principle: only one electron may occupy an (n, l, ml, ms) wavefunction at a time.
- Each l subshell can contain at most ? electrons?
- Each n shell can contain at most ? electrons?
- Can we get the electron configuration of ground state of O I and S I?

Atom	# electrons	Configuration
H I	1	$1s^1$
He I	2	$1s^2$
C I	6	$1s^2\ 2s^2\ 2p^2$
N I	7	$1s^2\ 2s^2\ 2p^3$
O I	8	$1s^2\ 2s^2\ 2p^4$
Ne I	10	$1s^2\ 2s^2\ 2p^6$
Mg I	12	$1s^2\ 2s^2\ 2p^6\ 3s^2$
Si I	14	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$
S I	16	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$
Ar I	18	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

Spectroscopic Terms

- The electronic configuration gives the arrangement of electrons in the atom or ion; however, the energy levels available to form spectral lines in that configuration are the result of the interactions among the electrons in the outermost (sub-)shell.
- Three total quantum numbers associated with the collective interactions of the outermost shell electrons.

$$^{2S+1}\mathcal{L}_{J}^{p}$$

Some common configurations

Configuration	Terms	Configuration	Terms
$\ldots ns^1$	$^2S_{1/2}$	$\ldots np^3$	
$\ldots ns^2$	$^1S_0$	$\ldots np^4$	$^3P_{2,1,0}$, $^1D_2$, $^1S_0$
$\ldots np^1$	$^2P^o_{1/2,3/2}$	$\ldots np^5$	$^2P^o_{3/2,1/2}$
$\ldots np^2$		$\ldots np^6$	$^1S_0$

Energy differences between levels

- The energy differences between levels with different L quantum numbers are of order a few eV for astrophysically-interesting atomic and ionic species, and thus produce spectral lines at ultraviolet, optical, and near-infrared wavelengths.
- The energy differences between levels with different J quantum numbers within a given term (for example, between the J states in the 3PJ terms of the …np2 configuration) are a few 0.01eV, and thus produce spectral lines at far-infrared wavelengths.
- Spectral lines from transitions between different J quantum states within a term are called fine structure lines.

Selection Rules

Permitted lines arise from electric dipole transitions that obey all the dipole selection rules:

1. $\Delta L=0, \pm 1$
2. $\Delta J=0, \pm 1$, but $J=0 \rightarrow 0$ is forbidden
3. $\Delta S=0$
4. one electron $n\ell$ changes with $\Delta\ell=\pm 1$
5. parity changes

Permitted lines from transitions into or out of the ground state multiplet are called **resonance lines**.

O III lines (permitted, semi-forbidden, forbidden)

- O III 3313 A $2p^1\ 3d^1\ {}^3P_2^o$ to $2p^1\ 3p^1\ {}^3S_1$, $A_{u\ell} = 1.18 \times 10^{10}\ \mathrm{s}^{-1}$
- OIII] 1666 A $2s\ 2p^3\ {}^5S_2^o$ to $2s^2\ 2p^2\ {}^3P_2$, $A_{u\ell} = 8.06 \times 10^{2}\ \mathrm{s}^{-1}$
- [OIII] 5007 A $2s^2\ 2p^2\ {}^1D_2$ to $2s^2\ 2p^2\ {}^3P_2$, $A_{u\ell} = 2.05 \times 10^{-2}\ \mathrm{s}^{-1}$

Hyperfine Structure Lines

- If the nucleus has a non-zero magnetic moment, the interaction between the magnetic fields of the nucleus and electrons gives rise to a small energy difference of order 10-6 eV, called **hyperfine structure**. A hyperfine energy level has quantum number **F**, which is the sum of the quantized nuclear spin angular momentum **I** and the electron total angular momentum **J**: **F=I+J**.
- The most astrophysically-important hyperfine structure transition is in the hydrogen 1s 2S1/2 ground state, which has I=1/2 and J=1/2, corresponding to hyperfine quantum numbers F=0 (anti-parallel spins) and F=1 (parallel spins). The energy difference between the F=1 and F=0 states is 5.874´10-6 eV which corresponds to a radio wavelength of 21.106 cm. The transition probability is A = 2.88e-15/s. Tiny!!!