

Interstellar Medium (ISM)

Week 3

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[Draine, Physics of the ISM and IGM]

Table 4.1 Terms for ns and np Subshells

Ground configuration	Terms / Levels (in order of increasing energy)	Examples
$\dots ns^1$	$^2S_{1/2}$	HI, He II, C IV, N V, O VI
$\dots ns^2$	1S_0	He I, C III, N IV, O V
$\dots np^1$	$^2P_{1/2,3/2}^o$	C II, N III, O IV
$\dots np^2$	$^3P_{0,1,2}^o, ^1D_2, ^1S_0$	CI, N II, O III, Ne V, S III
$\dots np^3$	$^4S_{3/2}^o, ^2D_{3/2,5/2}^o, ^2P_{1/2,3/2}^o$	NI, O II, Ne IV, S II, Ar IV
$\dots np^4$	$^3P_{2,1,0}, ^1D_2, ^1S_0$	O I, Ne III, Mg V, Ar III
$\dots np^5$	$^2P_{3/2,1/2}^o$	Ne II, Na III, Mg IV, Ar IV
$\dots np^6$	1S_0	Ne I, Na II, Mg III, Ar III

[Kowk, Physics and Chemistry of the ISM]

Atomic terms arising from p^n and d^n configurations

Electron configuration	Terms
p^1, p^5	2P
p^2, p^4	$^1S, ^1D, ^3P$
p^3	$^2P, ^2D, ^4S$
d^1, d^9	2D
d^2, d^8	$^1S, ^1D, ^1G, ^3P, ^3F$
d^3, d^7	$^2P, ^2D, ^2F, ^2G, ^2H, ^4P, ^4F$
d^4, d^6	$^1S, ^1D, ^1F, ^1G, ^1I, ^3P, ^3D, ^3F, ^3G, ^3H, ^5D$
d^5	$^2S, ^2P, ^2D, ^2F, ^2G, ^2H, ^2I, ^4P, ^4D, ^4F, ^4G, ^6S$

Source: Bernath 1995, *Spectra of Atoms and Molecules*, Table 5.6.

Atom	K	L	M	N	O	Ground level
	$1s$	$2s\ 2p$	$3s\ 3p\ 3d$	$4s\ 4p\ 4d$	$5s$	
H	1	1				$^2S_{1/2}$
He	2	2				1S_0
Li	3	2	1			$^2S_{1/2}$
Be	4	2	2			1S_0
B	5	2	2	1		$^2P_{1/2}^o$
C	6	2	2	2		3P_0
N	7	2	2	3		$^4S_{1/2}^o$
O	8	2	2	4		3P_1
F	9	2	2	5		$^2P_{3/2}^o$
Ne	10	2	2	6		1S_0
Na	11	2	2	6	1	$^2S_{1/2}$
Mg	12			2		1S_0
Al	13			2	1	$^2P_{1/2}^o$
Si	14		10	2	2	3P_0
P	15			2	3	$^4S_{1/2}^o$
S	16	Ne core		2	4	3P_2
Cl	17			2	5	$^2P_{3/2}^o$
Ar	18			2	6	1S_0
K	19	2	2	6	2	$^2S_{1/2}$
Ca	20				2	1S_0
Sc	21				1	2
Ti	22				2	2
V	23		18		3	2
Cr	24				5	1
Mn	25	A core			5	2
Fe	26				6	2
Co	27				7	2
Ni	28				8	2
Cu	29	2	2	6	10	$^2S_{1/2}$
Zn	30				2	1S_0

Blue: No fine structure in the ground state.

Energy ordering for Terms and Levels

- **Energy ordering: Hund's rules**

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

- (1) **S-rule:** For a given configuration, ***the state with the maximum spin multiplicity is lowest in energy.*** The electrons repel each other, and therefore their mutual electrostatic energy is positive. The farther away the electrons get, the lower will be the contribution of the electrostatic energy to the total energy.
- (2) **L-rule:** For a given configuration and spin multiplicity, ***the state with the maximum orbital angular momentum is the lowest in energy.***
- (3) **J-rule:** ***The lowest energy is obtained for lowest value of J in the normal case and for highest J value in the inverted case.***
- The normal case is a shell which is less than half filled. The inverted case is a shell which is more than half full such as the ground state of atomic oxygen.



- If the shell is exactly half-filled (e.g., p^3), the energy order does not obey a simple rule.
- The Hund's rules are only applicable within L - S coupling. They are only rigorous for ground states. However, they are almost always useful for determining the energy ordering of excited states. The rules show increasing deviations with higher nuclear charge.

Selection Rules

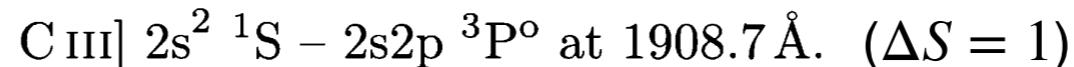
- **Selection Rules**

- (1) one electron jumps
 - (2) Δn any
 - (3) $\Delta l = \pm 1$
 - (4) parity change
 - (5) $\Delta S = 0$
 - (6) $\Delta L = 0, \pm 1$ (except $L = 0 - 0$)
 - (7) $\Delta J = 0, \pm 1$ (except $J = 0 - 0$)
 - (8) $\Delta F = 0, \pm 1$ (except $F = 0 - 0$)
-
- selection rule for configuration
- intercombination** line if only this rule is violated.
- It is only rarely necessary to consider this.

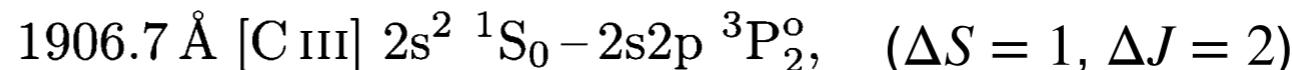
- **Allowed = Electric Dipole** : Transitions which satisfy all the above selection rules are referred to as **allowed transitions**. These transitions are strong and have a typical lifetime of $\sim 10^{-8}$ s. Allowed transitions are denoted without square brackets.

e.g., C IV 1548, 1550 Å

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



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



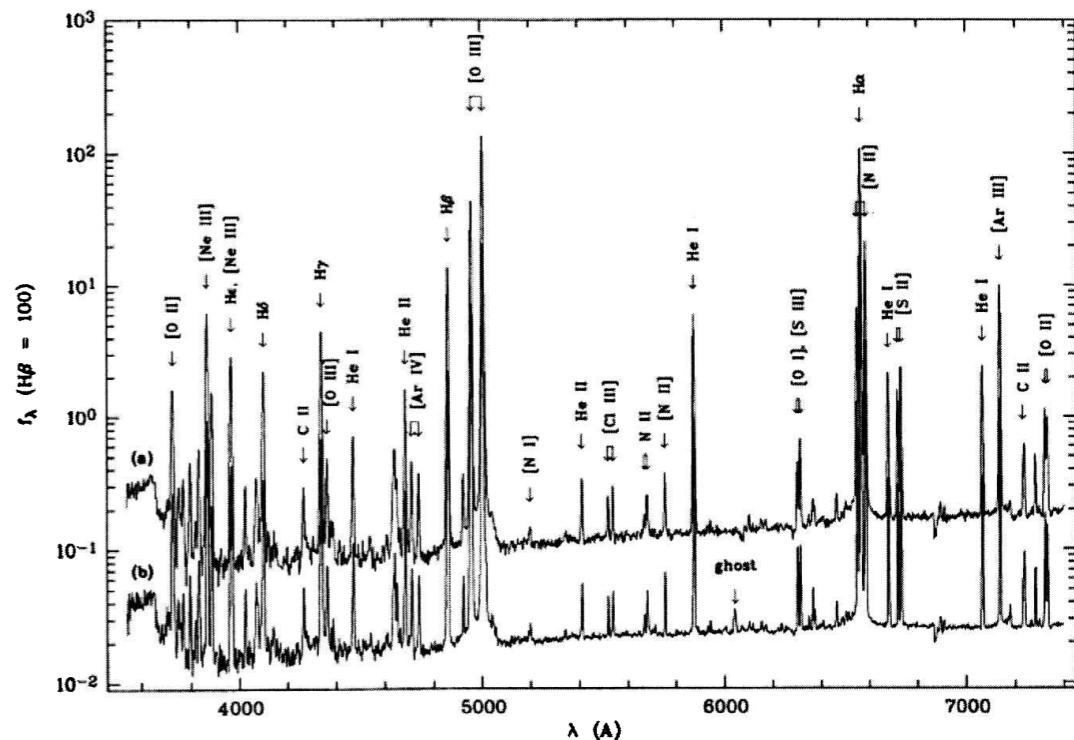
- **Resonance line** denotes the longest wavelength, dipole-allowed transition arising from the ground state of a particular atom or ion.

Forbidden Lines

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

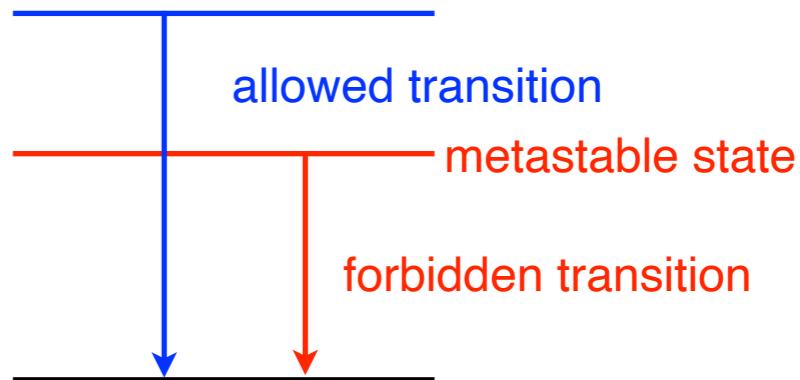
History: Nebulium?

- 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 Bowen (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].



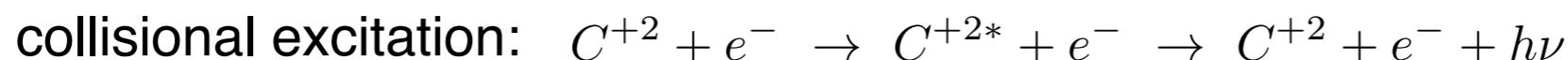
Optical spectra of NGC 6153, Liu et al. (2000, MNRAS)

[O III], [O II], [N II], etc:
We use a pair of square
brackets for a forbidden line.



Notations

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



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

[Hydrogen Atom] : Fine Structure

- The discussion on H-atom levels has assumed that all states 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	$1/2$	$5/2, 7/2$	$^2F^o$	$^2F_{5/2}^o, ^2F_{7/2}^o$

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

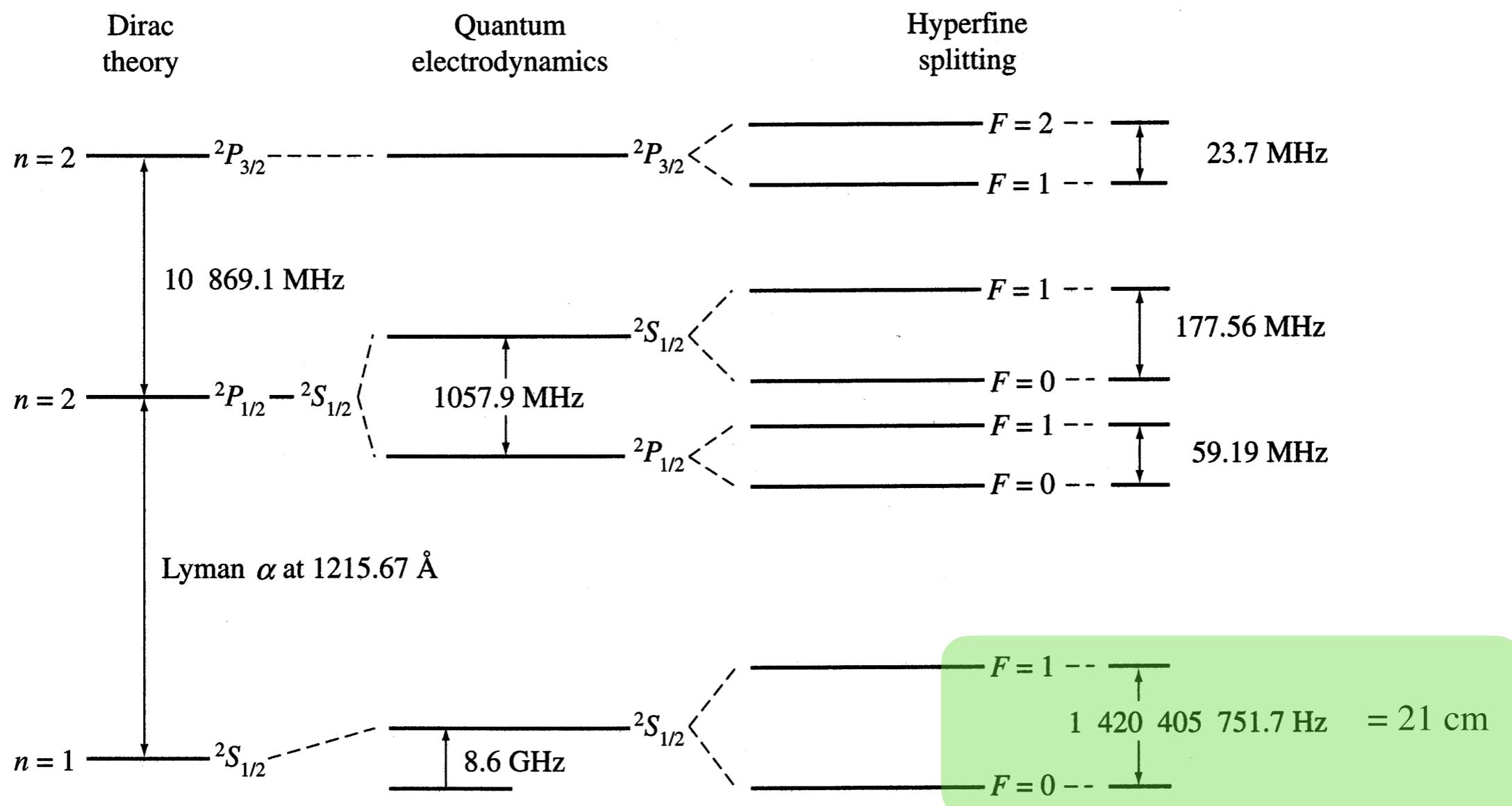
- The above table shows the fine structure levels of the H atom.
- Note that the states with principal quantum number $n = 2$ give rise to three fine-structure levels. In spectroscopic notation, these levels are $^2S_{1/2}$, $^2P_{1/2}^o$ and $^2P_{3/2}^o$.

Hydrogen Atom : Hyperfine Structure

- Hyperfine Structure in the H atom

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

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



Hydrogen Atom : Allowed Transitions

- Selection Rules

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

Δn any selection rule for configuration

$$\Delta l = \pm 1$$

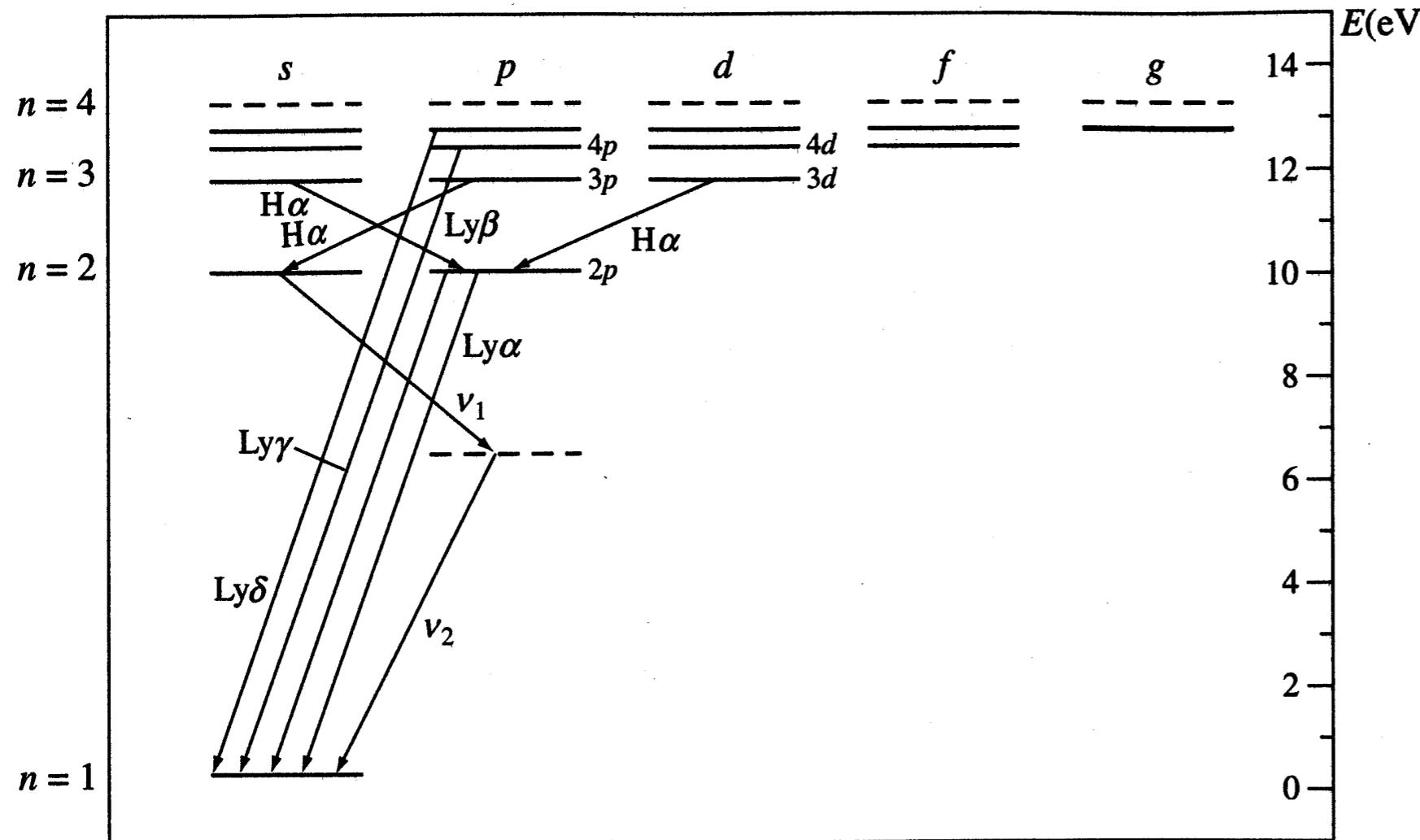
$$\Delta S = 0$$

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

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

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

For H α transitions:



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

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

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

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

- 3d_{3/2} is allowed;

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

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

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

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

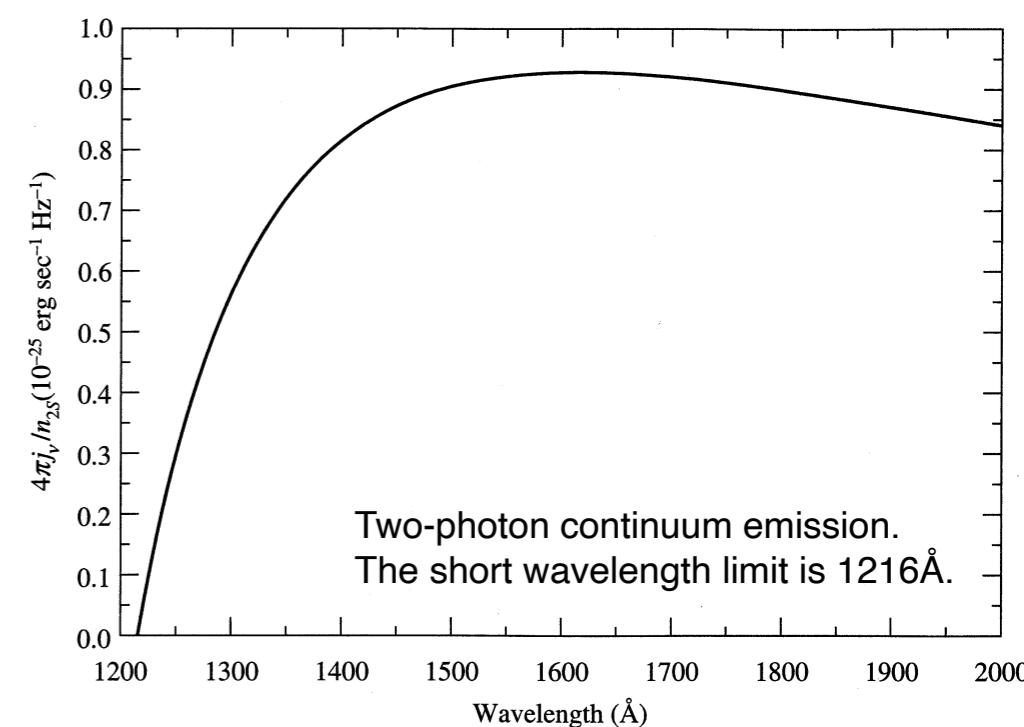
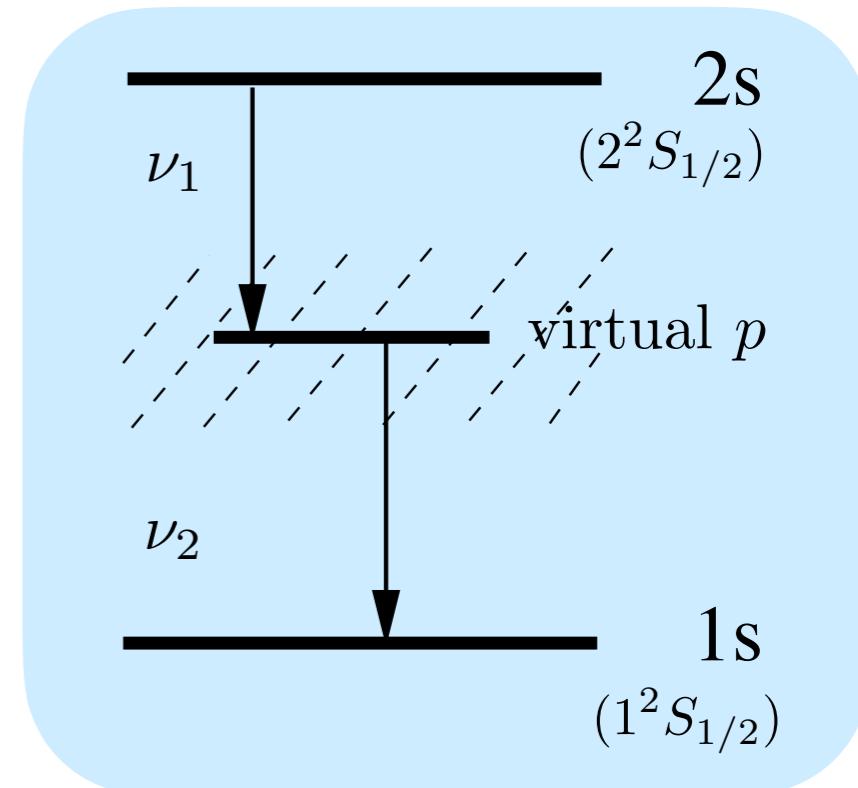
$$\tau_i = \left(\sum_j A_{ij} \right)^{-1} \quad \text{where } A_{ij} \text{ is the Einstein A coefficient}$$

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 short, 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 (e.g., ISM), an electron in the $2^2S_{1/2}$ level can jumps 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.
- Because the radiative lifetime of the 2s level is long, we need to consider the possibility for collisions with electrons and protons to depopulate 2s level before a spontaneous decay occurs. However, the critical density, at which deexcitation by electron and proton collision is equal to the radiative decay rate, is $n_{\text{crit}} \approx 1880 \text{ cm}^{-3}$. In the ISM, the radiative decay is in general faster than the collisional depopulation process.



[Helium Atom]

- (1) The ground state is $1s^2$.

This is a closed shell, with $L = 0$ and $S = 0$, hence it gives rise to a single, even parity term 1S , and level 1S_0 .

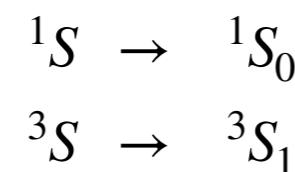
- (2) The first excited configuration is $1s2s$.

This has $l_1 = l_2 = 0$ and hence $L = 0$, but $s_1 = s_2 = \frac{1}{2}$ giving both $S = 0$ (singlet) or $S = 1$ (triplet) states.

S	L	J
0	0	0

$${}^1S \rightarrow {}^1S_0$$

S	L	J
0	0	0
1	0	1



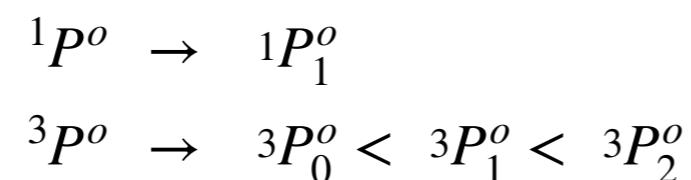
For a given configuration, the state with the maximum spin multiplicity is lowest in energy.

So the 3S term (3S_1 level) is lower in energy than the 1S term (1S_0 level). In practice, the splitting between these terms is 0.80 eV.

- (3) The next excited configuration is $1s2p$, which has odd parity.

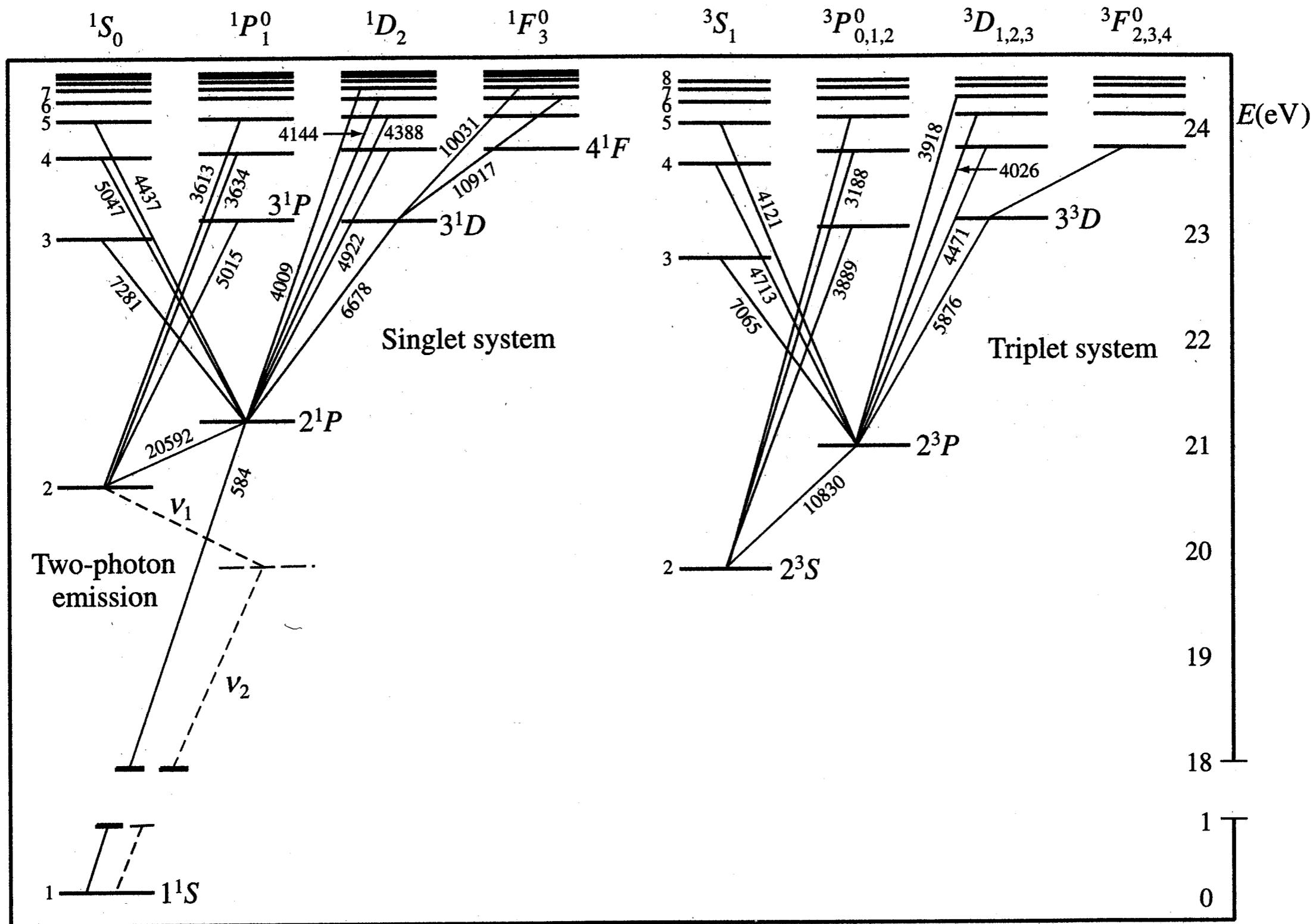
This has $l_1 = 0$ and $l_2 = 1$, giving $L = 1$; again $s_1 = s_2 = \frac{1}{2}$, giving both $S = 0$ and $S = 1$ terms.

S	L	J
0	1	1
1	1	0, 1, 2



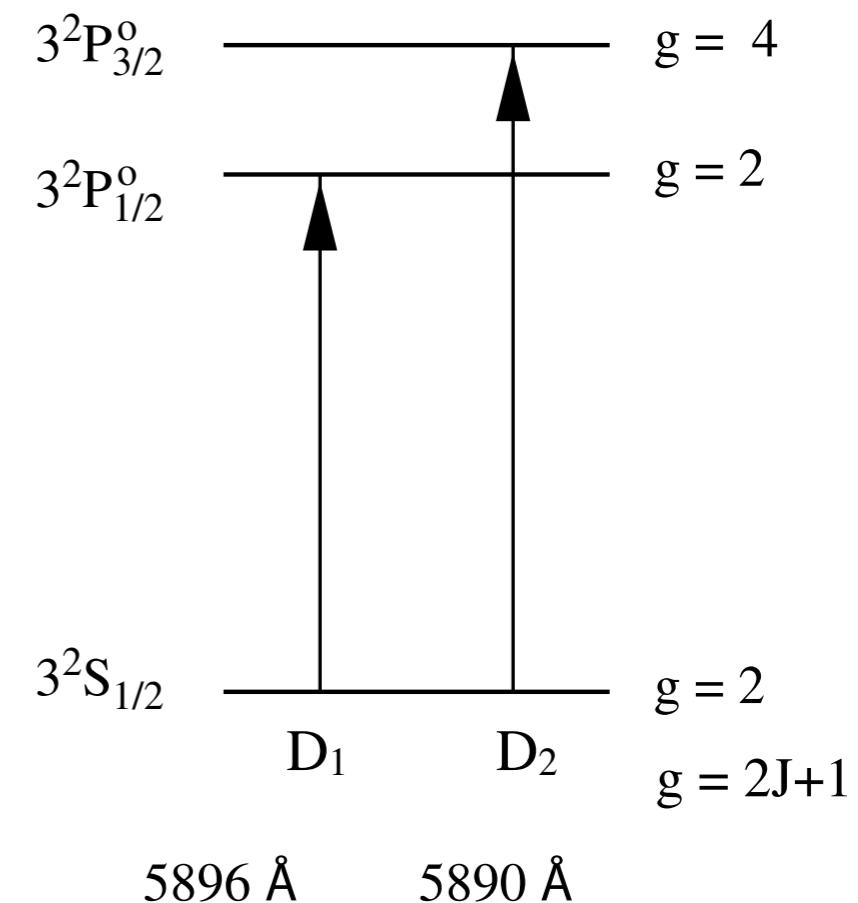
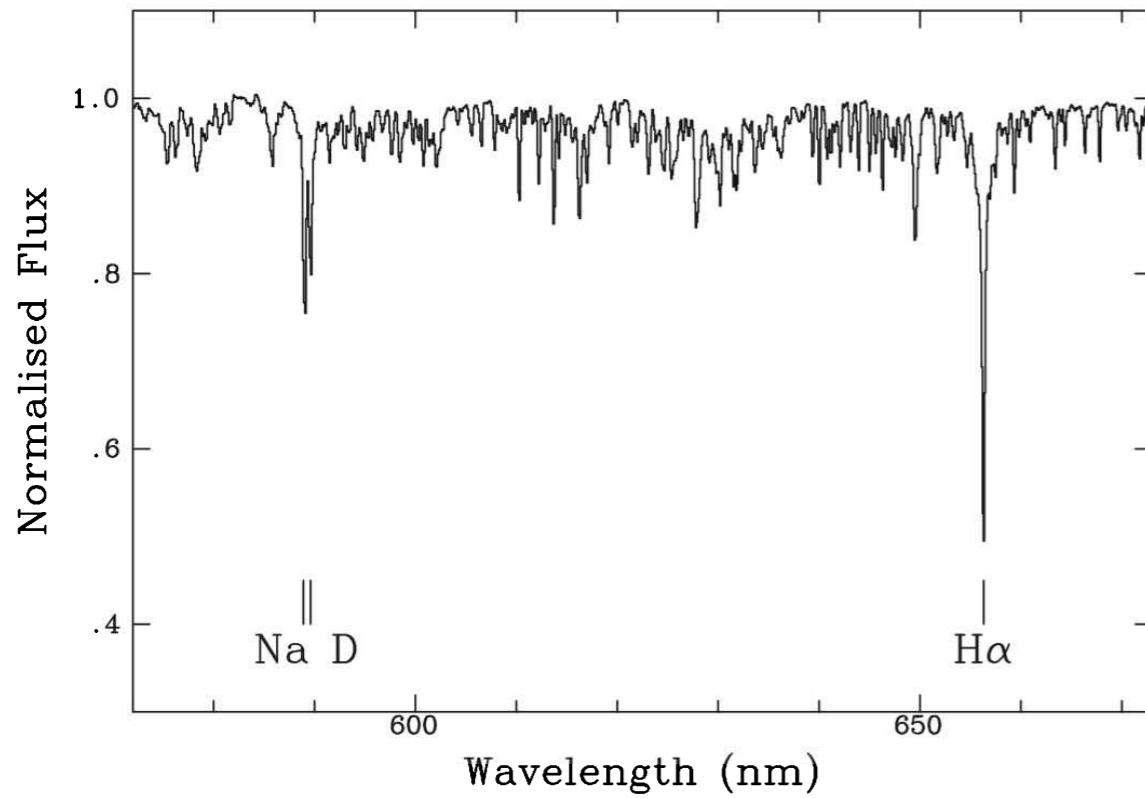
Following the rule above, the ${}^3P^o$ term is lower in energy than the ${}^1P^o$ term, in this case by 0.25 eV.

- Helium (Grotrian diagram)



LS coupling: Alkali Atoms

- Alkali atoms: Lithium, sodium, potassium and rubidium all have ground state electronic structures which consist of one electron in an s orbital outside a closed shell.
- Sodium (Na) : Sodium has $Z = 11$ and the ground state configuration of $1s^2 2s^2 2p^6 3s^1$ and the first excited state configuration of $1s^2 2s^2 2p^6 3p^1$.



A solar spectrum reflected from the Moon just before a lunar eclipse taken at the University of London Observatory (S.J. Boyle).

Na D lines:

D₁ 5896 Å line : $3^2S_{1/2} - 3^2P_{1/2}$

D₂ 5890 Å line : $3^2S_{1/2} - 3^2P_{3/2}$

-
- **Ca II (potassium-like calcium)**

H 3968.47 Å line : $4\ ^2S_{1/2} - 4\ ^2P_{1/2}^o$

K 3933.66 Å line : $4\ ^2S_{1/2} - 4\ ^2P_{3/2}^o$
 - **Mg II (sodium-like magnesium)**

2802.7 Å line : $3\ ^2S_{1/2} - 3\ ^2P_{1/2}^o$

2795.5 Å line : $3\ ^2S_{1/2} - 3\ ^2P_{3/2}^o$
 - **C IV (lithium-like carbon)**

1550.8 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{1/2}^o$

1548.2 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{3/2}^o$
 - **N V (lithium-like nitrogen)**

1242.8 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{1/2}^o$

1238.8 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{3/2}^o$
 - **O VI (lithium-like oxygen)**

1037.6 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{1/2}^o$

1031.9 Å line : $2\ ^2S_{1/2} - 2\ ^2P_{3/2}^o$
- 8498.0 Å line : $4\ ^2P_{3/2}^o - 3\ ^2D_{3/2}$
 8542.1 Å line : $4\ ^2P_{3/2}^o - 3\ ^2D_{5/2}$
 8662.1 Å line : $4\ ^2P_{1/2}^o - 3\ ^2D_{3/2}$
 (Note that $^2P_{1/2}^o - ^2D_{5/2}$ is forbidden because $\Delta J = 2$.)
- 1240.4 Å line : $3\ ^2S_{1/2} - 4\ ^2P_{1/2}^o$
 1239.9 Å line : $3\ ^2S_{1/2} - 4\ ^2P_{3/2}^o$

LS coupling: Excited Configuration of O III

Doubly Ionized Oxygen, O III

Consider O III with the configuration: $1s^2 2s^2 2p3d$.

$1s^2$ and $2s^2$ are closed, so they contribute no angular momentum.

For the 2p electron $l_1 = 1$ and $s_1 = \frac{1}{2}$;

for the 3d electron $l_2 = 2$ and $s_2 = \frac{1}{2}$.

$$\underline{L} = \underline{l}_1 + \underline{l}_2 \Rightarrow L = 1, 2, 3;$$

$$\underline{S} = \underline{s}_1 + \underline{s}_2 \Rightarrow S = 0, 1.$$

Combining these using all possible combinations of L and S , and the rules of vector addition, gives:

	L	S	J	Level
$\underline{J} = \underline{L} + \underline{S} \Rightarrow$	1	0	1	${}^1P_1^o$
	1	1	0, 1, 2	${}^3P_0^o, {}^3P_1^o, {}^3P_2^o$
	2	0	2	${}^1D_2^o$
	2	1	1, 2, 3	${}^3D_1^o, {}^3D_2^o, {}^3D_3^o$
	3	0	3	${}^1F_3^o$
	3	1	2, 3, 4	${}^3F_2^o, {}^3F_3^o, {}^3F_4^o$

In total, 6 terms and 12 levels.

Example: 4p4d

4p4d electron configuration

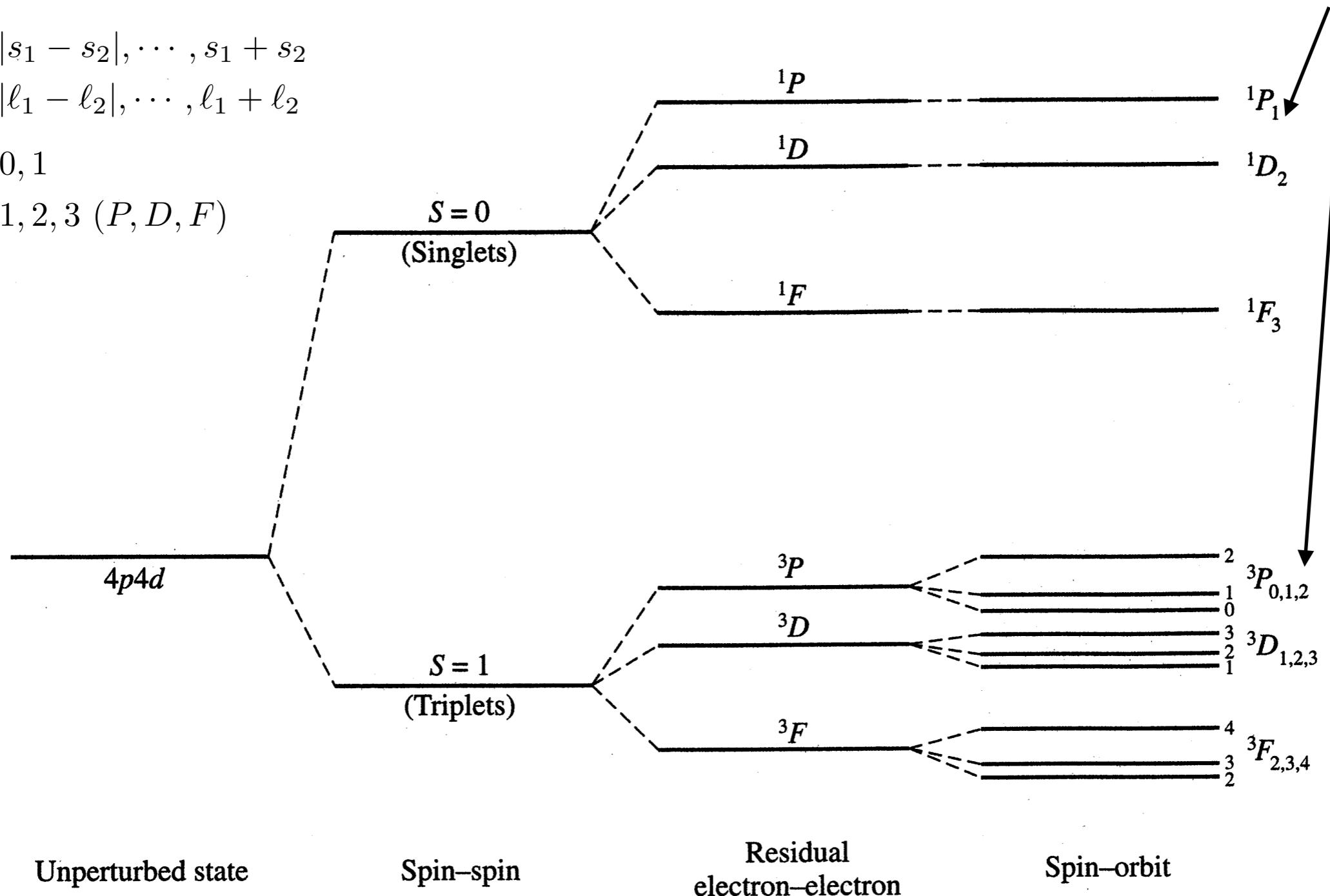
$$J = |L - S|, \dots, L + S$$

$$S = |s_1 - s_2|, \dots, s_1 + s_2$$

$$L = |\ell_1 - \ell_2|, \dots, \ell_1 + \ell_2$$

$$S = 0, 1$$

$$L = 1, 2, 3 \text{ (} P, D, F \text{)}$$



LS Terms: (1) Nonequivalent Electrons, 2p3p

- **Equivalent and Nonequivalent Electrons**

Nonequivalent electrons are those differing in either n or l values, whereas equivalent electrons have the same n and l values.

- **Consider the combination of two p electrons.**

(1) **2p3p** - Two electrons are nonequivalent.

In this nonequivalent case, all possible spectroscopic combinations are available.

$$S = 0, 1, \quad L = 0, 1, 2 \quad \rightarrow \quad ^1S, ^1P, ^1D, ^3S, ^3P, ^3D \\ \rightarrow \quad 6 \text{ spectroscopic terms}$$

$$\rightarrow \quad ^1S_0, ^1P_1, ^1D_2, ^3S_1, ^3P_{0,1,2}, ^3D_{1,2,3} \\ \rightarrow \quad 10 \text{ spectroscopic levels}$$

We can have $(2J+1)$ states for each J value. (The number of m_J is $2J+1$).

Therefore, 36 distinguishable states are available in total.

$$\rightarrow \quad 1 + 3 + 5 + 3 + 9 + 15 = 36$$

There are two possible states $m_s = \pm 1/2$ for spin of each electron, and three states $m_l = -1, 0, 1$ for orbital angular momentum of each electron.

Thus, we expect that there will be $2^2 \times 3^2 = 36$ distinguishable states.

Example: npn'p

npn'p electron configuration

The dashed levels are missing if the two electrons are equivalent ($n = n'$)

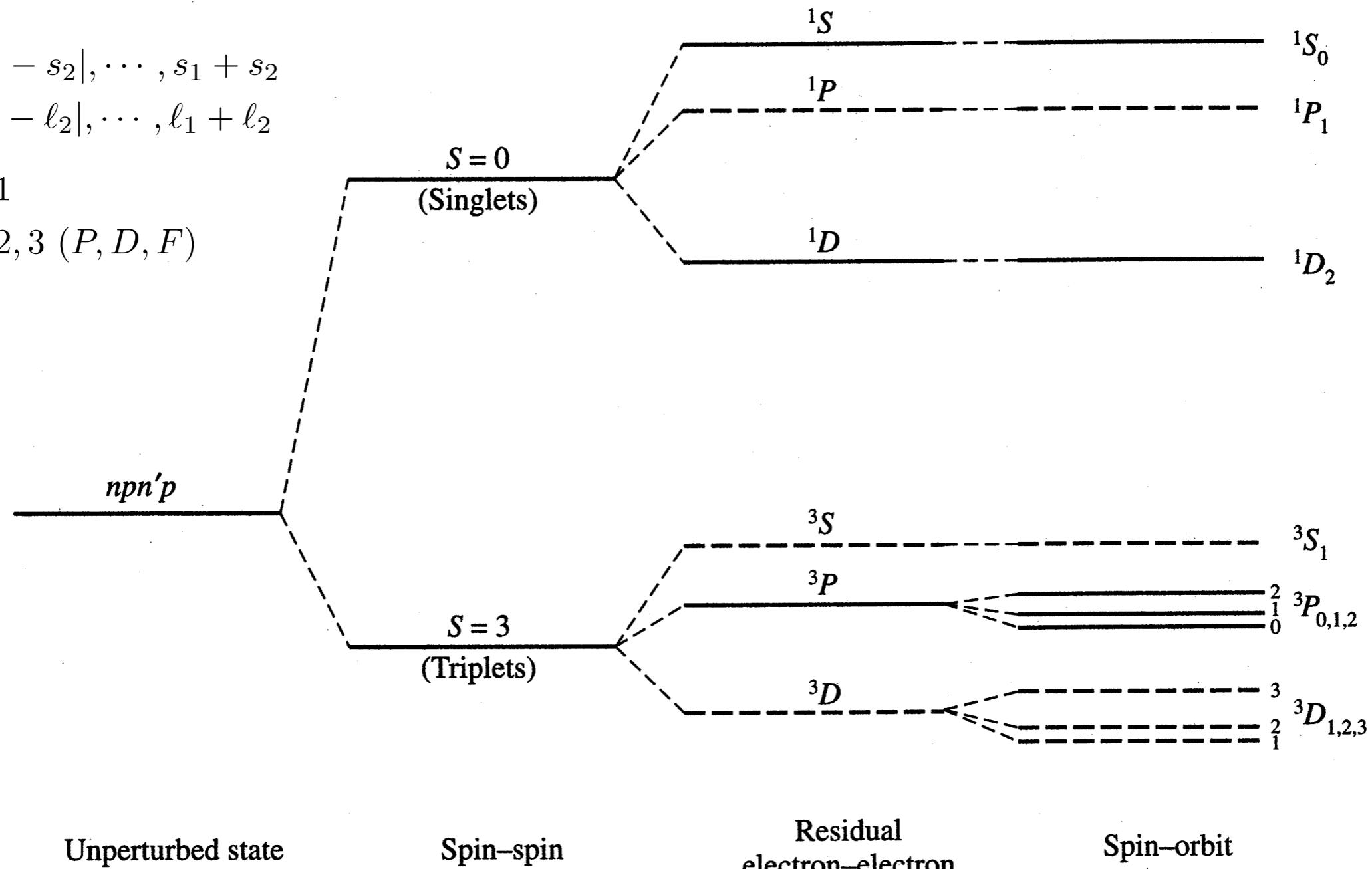
The levels for $n = n'$ will be explained in the next slides.

$$S = |s_1 - s_2|, \dots, s_1 + s_2$$

$$L = |\ell_1 - \ell_2|, \dots, \ell_1 + \ell_2$$

$$S = 0, 1$$

$$L = 1, 2, 3 \text{ (} P, D, F \text{)}$$



Unperturbed state

Spin-spin

Residual
electron-electron

Spin-orbit

(2) Equivalent Electrons, $2p^2$

(2) $2p^2$ - Two electrons are equivalent.

Then, *all the 36 states are not available. Some are ruled out by Pauli exclusion principle, and some are ruled out because they are not distinguishable from others.*

Table 1

Label	m_l	m_s
a	+1	+1/2
b	0	+1/2
c	-1	+1/2
d	+1	-1/2
e	0	-1/2
f	-1	-1/2

- The first step is to make a table to label the states for a single electron (e.g., a, b, c, d, e, f), as shown in Table 1.

Table 2

	States	M_L	M_S
1	ab	1	1
2	ac	0	1
3	ad	2	0
4	ae	1	0
5	af	0	0
6	bc	-1	1
7	bd	1	0
8	be	0	0
9	bf	-1	-1
10	cd	0	0
11	ce	-1	0
12	cf	-2	0
13	de	1	-1
14	df	0	-1
15	ef	-1	-1

- Next step is to make a table for the combination of (M_L, M_S) of two electrons, as shown in Table 2. Here, $M_L = m_{l1} + m_{l2}$, and $M_S = m_{s1} + m_{s2}$.
 - According to Pauli's exclusion principle, the states that have two identical states (aa, bb, cc, dd, ee, and ff) are not allowed.
 - Notice also that "ab" and "ba" states are identical and thus the "ba" state is ignored. Other identical combinations are also ignored.
- Following the above two rules, we construct Table 2 which contains 15 distinguishable states.

Table 3

States	M_L	M_S	Term 1	Term 2	Term 3
ab	1	1		3P	
ac	0	1		3P	
ad	2	0	1D		
ae	1	0	1D		
af	0	0	1D		
bd	1	0		3P	
be	0	0		3P	
cd	0	0			1S

- In addition to the above two rules, we can recognize that every “negative” values have always their “positive” counterparts.
 - Therefore, it is more convenient to remove the states with negative values. This gives us Table 3, which contains only 8 states.
- Now, we pick the states starting with the largest M_L and then the largest M_S .
 - (ad) $M_L = 2$ and $M_S = 0$: The presence of the $M_L = 2, M_S = 0$ indicates that a 1D term is among the possible terms. To this term we must further assign states with $M_L = 1,0$ and $M_S = 0$ (ae, af). What is left?
 - (ab) $M_L = 1$ and $M_S = 1$: This is the next largest values. The combination $M_L = 1, M_S = 1$ indicates that a 3P term is among the possible terms. To this term we must further assign states with $M_L = 1,0$ and $M_S = 1,0$ (ac, bd, be). What is left?
 - (cd) $M_L = 0$ and $M_S = 0$: This is the only remaining combination. This implies that a 1S term is among the possible terms.
 - Finally, we obtain 3 terms 1D , 3P , and 1S .
 - The 3 terms are split into 5 levels : 1D_2 , $^3P_{0,1,2}$, and 1S_0 .

(3) Equivalent Electrons, $2p^3$

(3) $2p^3$ - Three electrons are equivalent.

- According to Pauli's exclusion principle, any states that include two identical states (aaa, aab, aac, add, bbc, bbd, etc) are not allowed.
- We have only seven states that have non-negative values, as shown in Table 4.

Table 4

States	M_L	M_S	Term 1	Term 2	Term 3
abc	0	3/2			4S
abd	2	1/2	2D		
abe	1	1/2	2D		
abf	0	1/2	2D		
acd	1	1/2		2P	
ace	0	1/2		2P	
bcd	0	1/2			4S

Table 1

Label	m_L	m_S
a	+1	+1/2
b	0	+1/2
c	-1	+1/2
d	+1	-1/2
e	0	-1/2
f	-1	-1/2

- Now, we pick the states starting with the largest M_L and then the largest M_S .
 - (abd) $M_L = 2$ and $M_S = 1/2$: This indicates that a 2D term is among the possible terms. To this term we must further assign states with $M_L = 1, 0$ and $M_S = 1/2$ (abe, abf). What is left?
 - (acd) $M_L = 1$ and $M_S = 1/2$: This indicates the presence of a 2P term. To this term we must further assign states with $M_L = 0$ and $M_S = 1/2$ (ace). What is left?
 - (abc) $M_L = 0$ and $M_S = 3/2$: This indicates the presence of a 4S term.
 - **Finally, we obtain three terms (2D , 2P , and 4S) and five levels : $^2D_{3/2, 5/2}$, $^2P_{1/2, 3/2}$, and $^4S_{3/2}$.**

(4) Another method for $2p^2$

When we have only two electrons, we can use the Pauli principle to obtain the terms.

This method is much simpler than the above method. However, this method is not easy to apply to the case of three electrons.

Recall that the Pauli principle states that **the total eigenfunction must be antisymmetric with respect to the exchange of two particles**. Therefore, we can have only two distinct cases:

- (a) symmetric function for the spin + antisymmetric function for the orbital angular momentum $\Rightarrow {}^3P$
- (b) antisymmetric function for the spin + symmetric function for the orbital angular momentum $\Rightarrow {}^1S, {}^1D$

Note that among the six terms ${}^1S, {}^1P, {}^1D, {}^3S, {}^3P, {}^3D$, the following terms are all excluded.

1P is antisymmetric for both spin and orbital angular momenta

3S is symmetric for both spin and orbital angular momenta

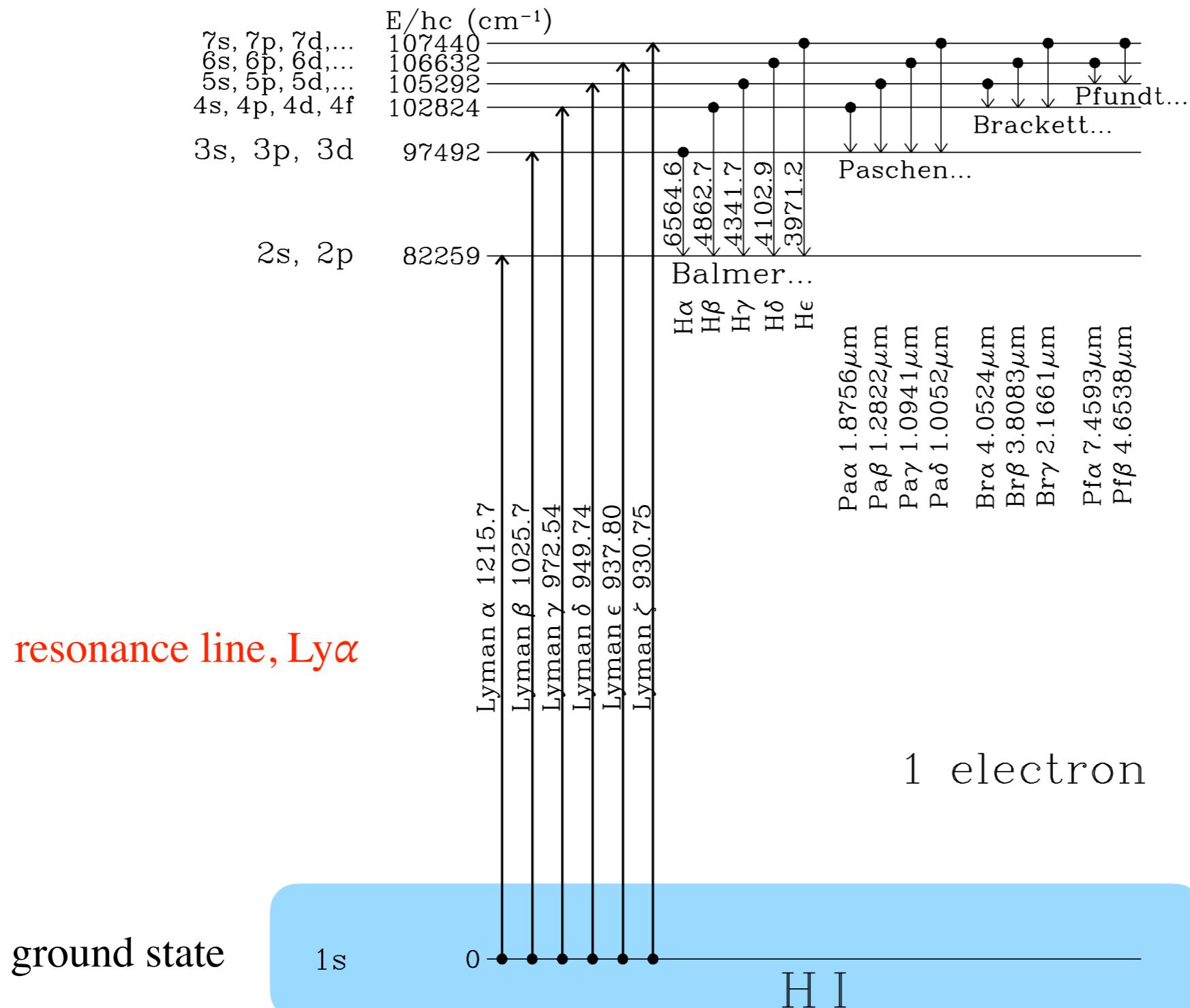
3D is also symmetric for both spin and orbital angular momenta

Because

- | | |
|---|--|
| $S = 0 \rightarrow s_1 = 1/2, s_2 = -1/2$ | : Product of two spin functions are antisymmetric w.r.t. the exchange |
| $S = 1 \rightarrow s_1 = 1/2, s_2 = 1/2$ | : Product of two spin functions are symmetric. |
| $L = 1 \rightarrow l_1 = 1, l_2 = 0$ | : The first wavefunction is antisymmetric and the second one is symmetric.
Therefore, their product is antisymmetric w.r.t. the exchange. |
| $L = 2 \rightarrow l_1 = 1, l_2 = 1$ | : Both are antisymmetric. Therefore, their product is symmetric. |

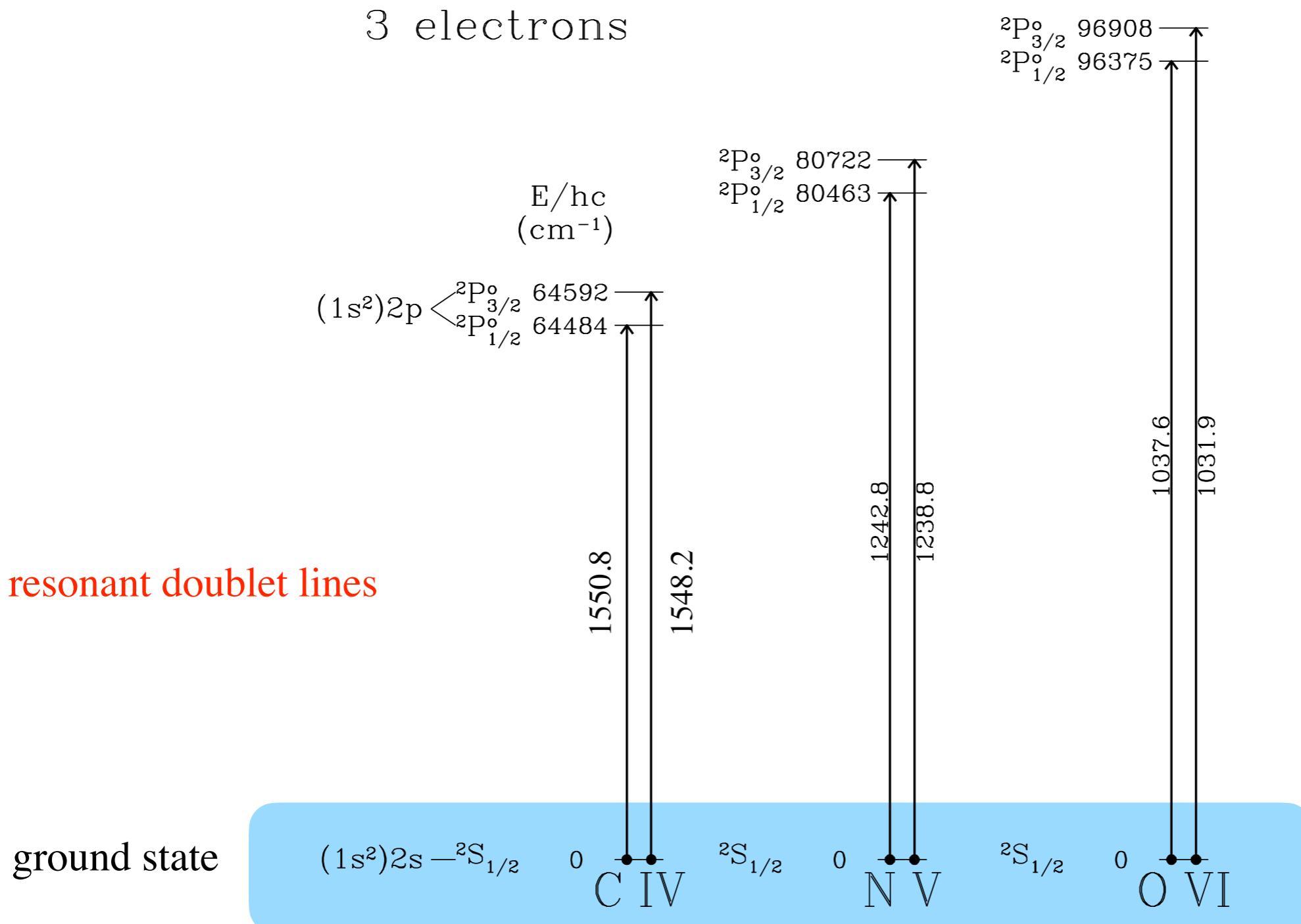
Energy Level Diagrams

- 1 electron



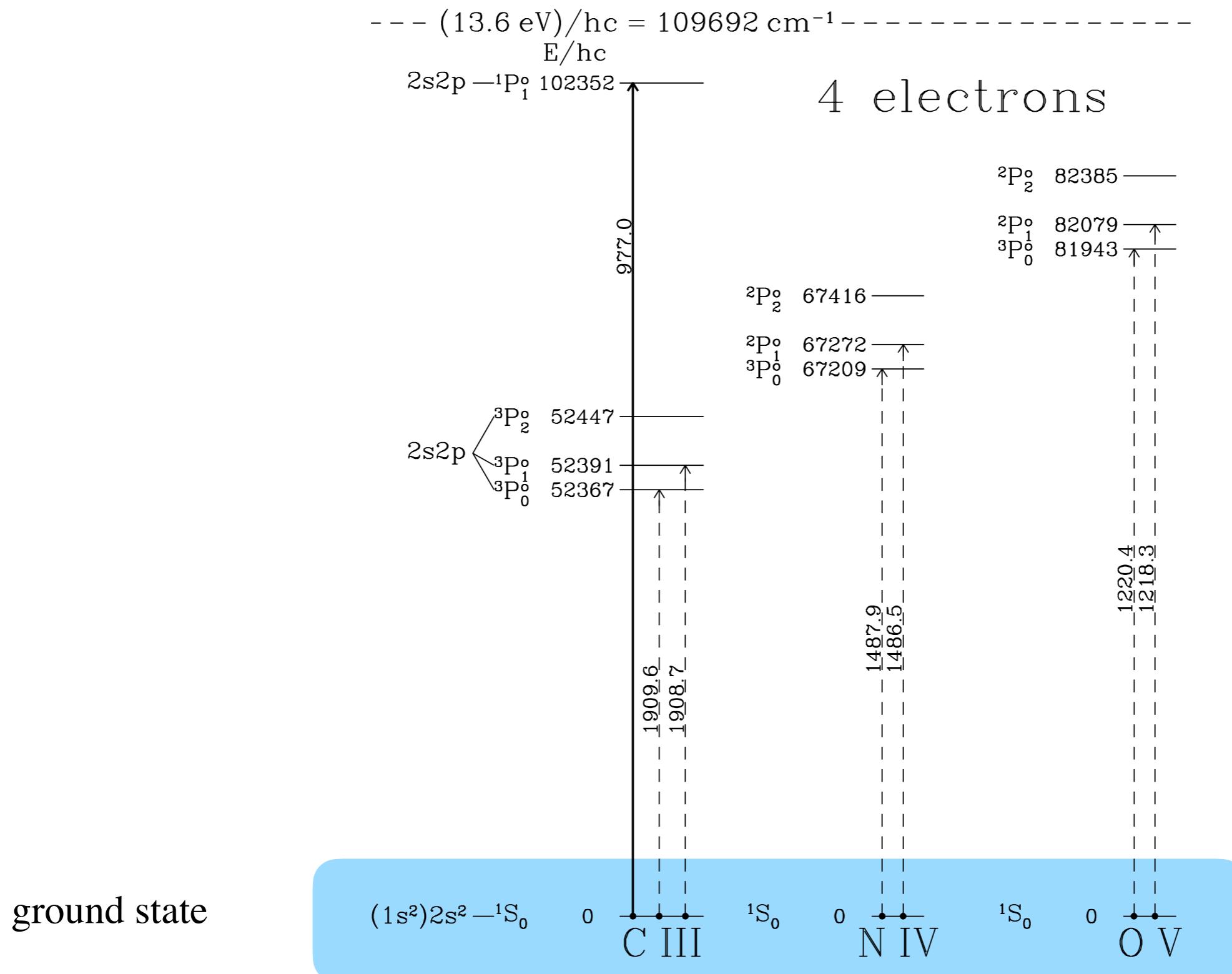
- 3 electrons (Lithium-like ions)

$$\dots (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \dots$$



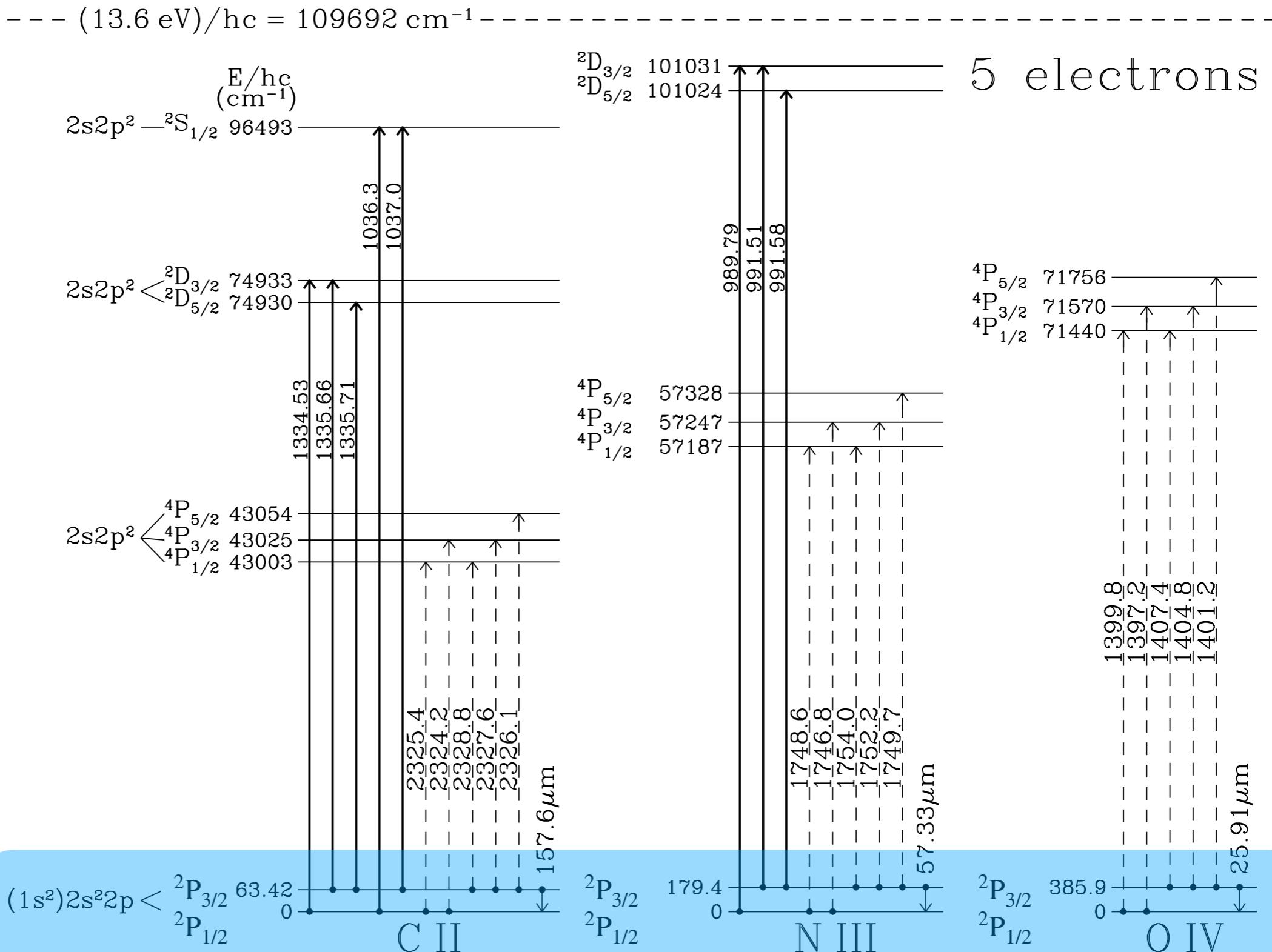
- 4 electrons

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



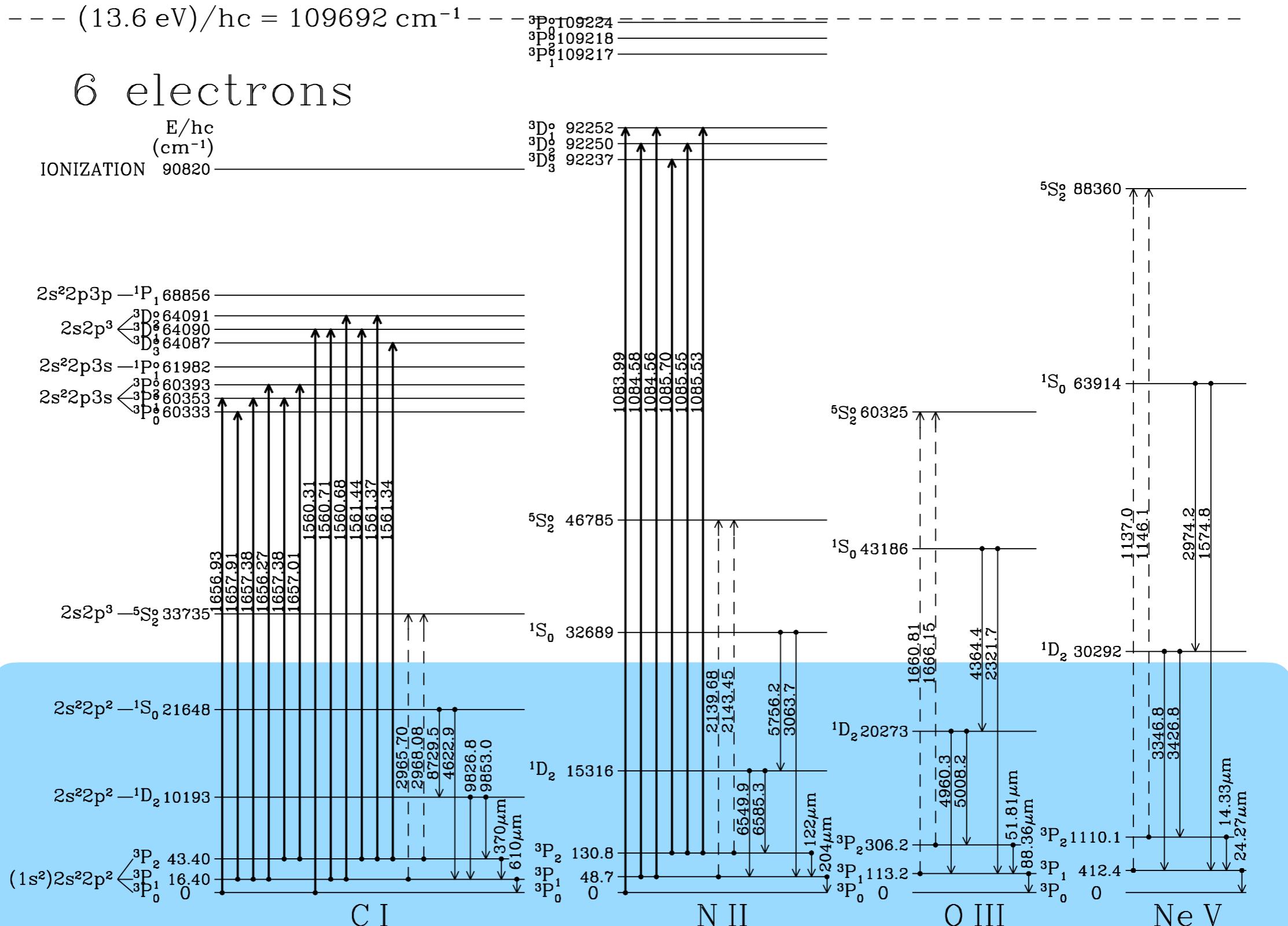
- 5 electrons

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



- 6 electrons

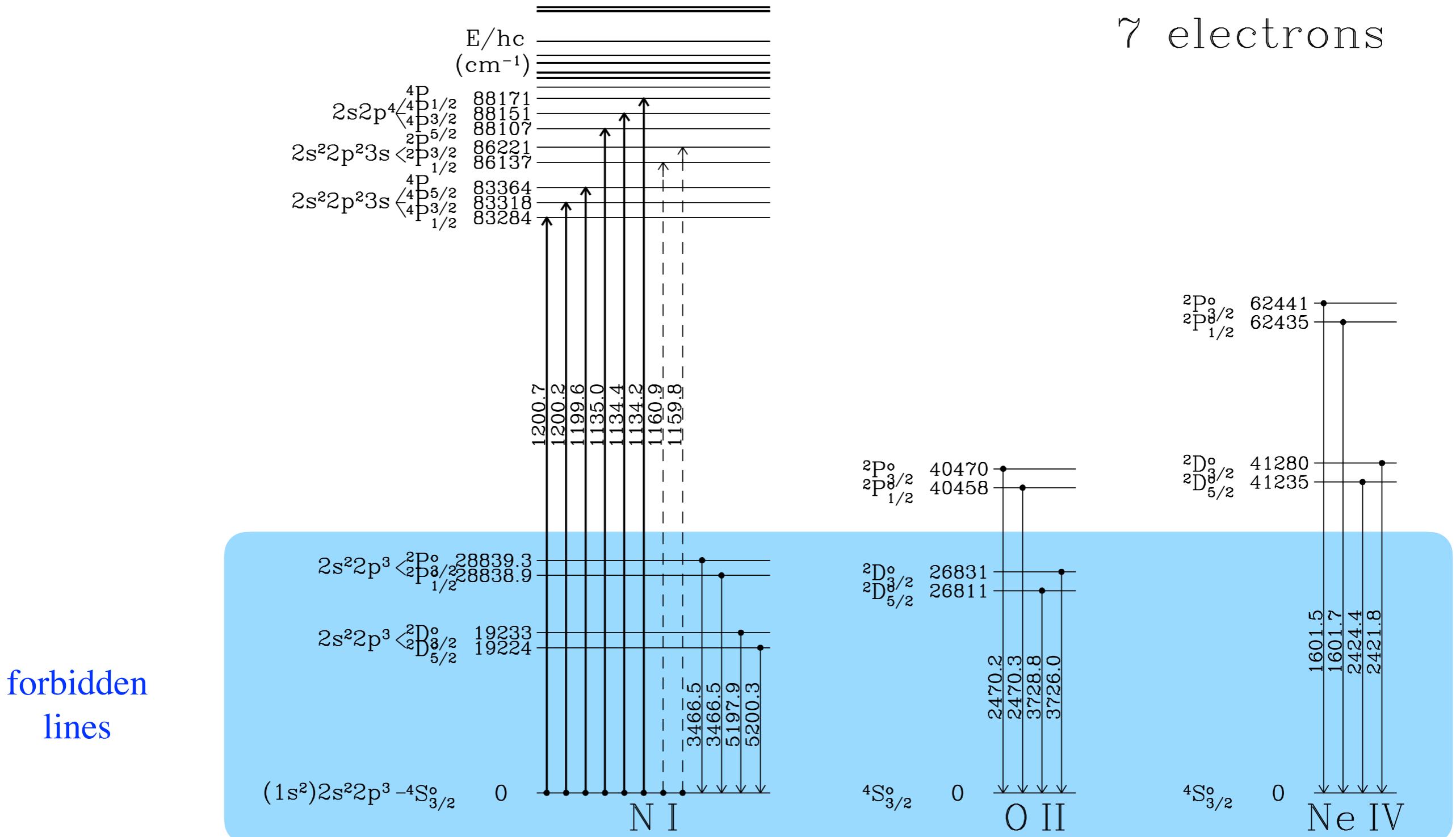
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



- 7 electrons

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

$$\text{---} (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{---} \text{---} \text{---}$$

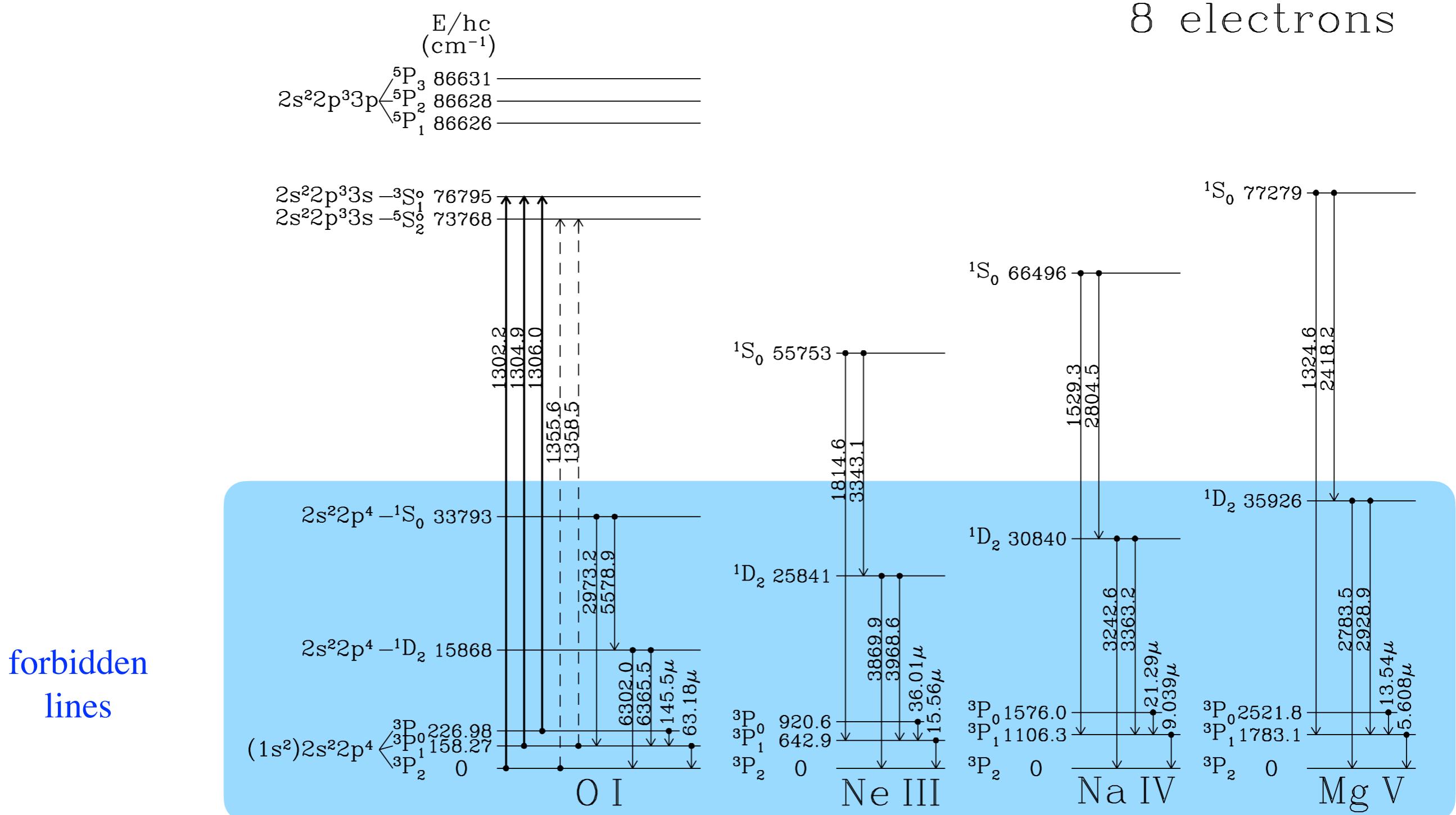


forbidden
lines

- 8 electrons

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

$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{ ---}$$



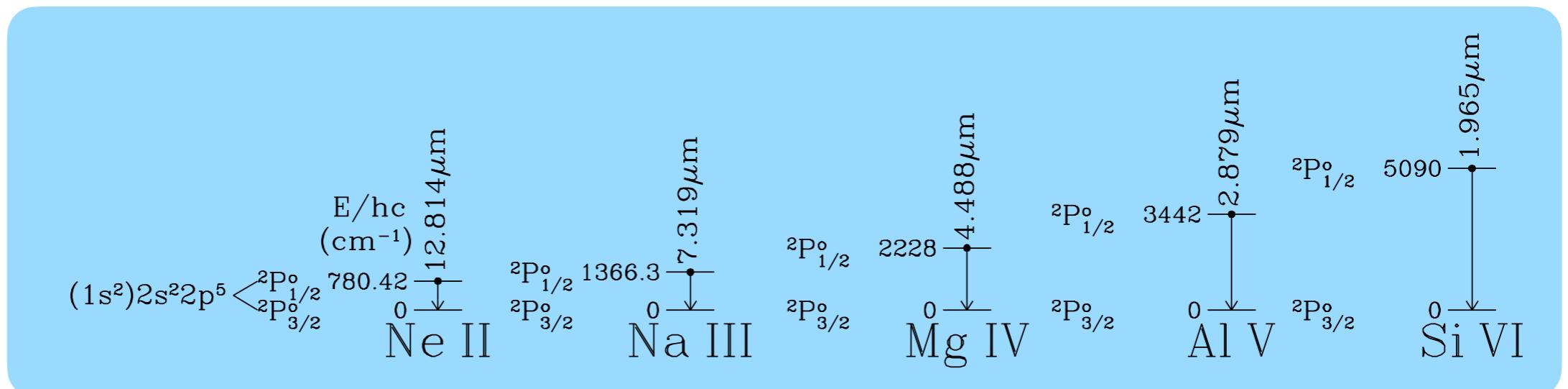
- 9 electrons

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

$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{-----}$$

9 electrons

forbidden
lines

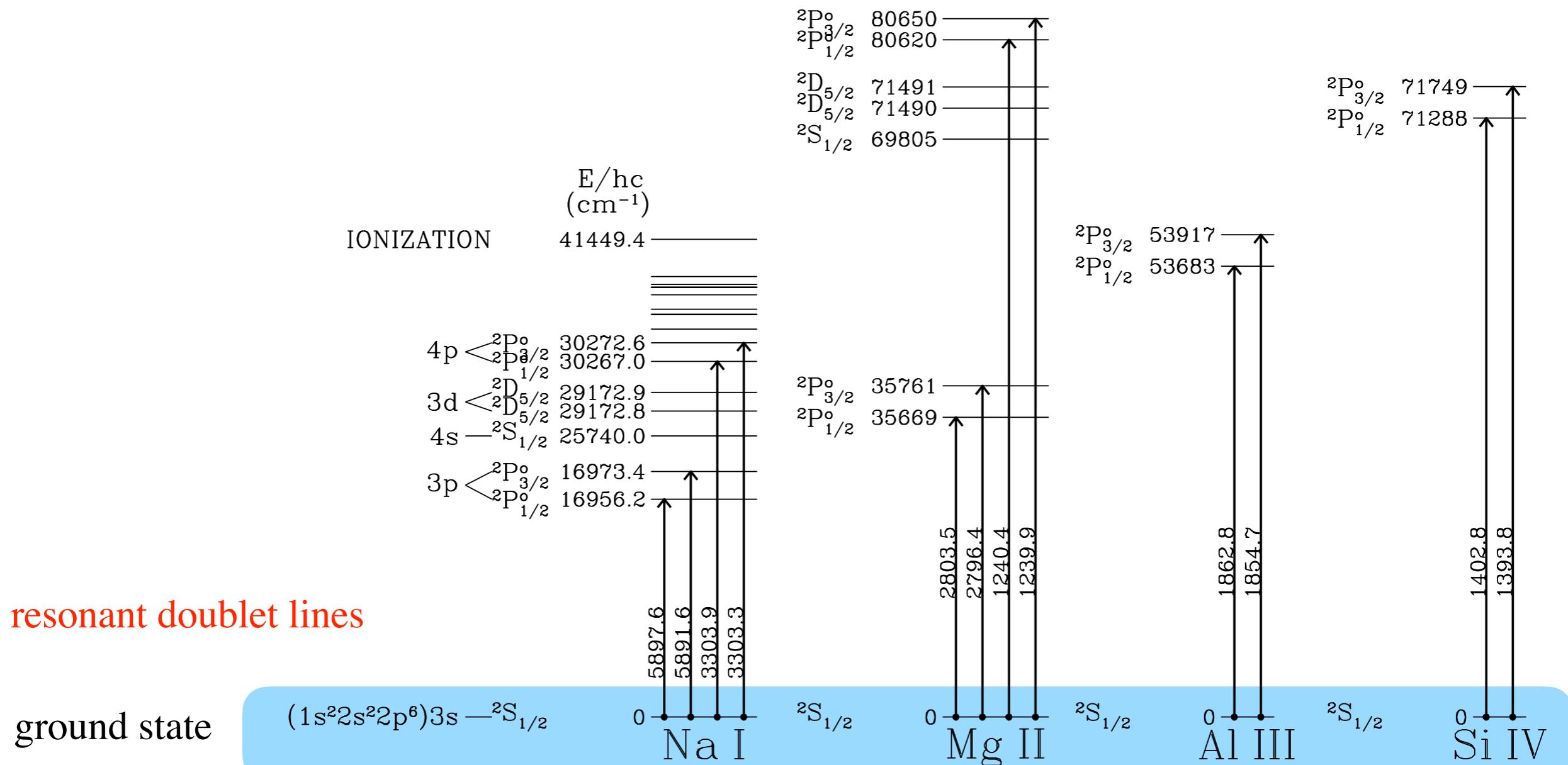


- 11 electrons

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

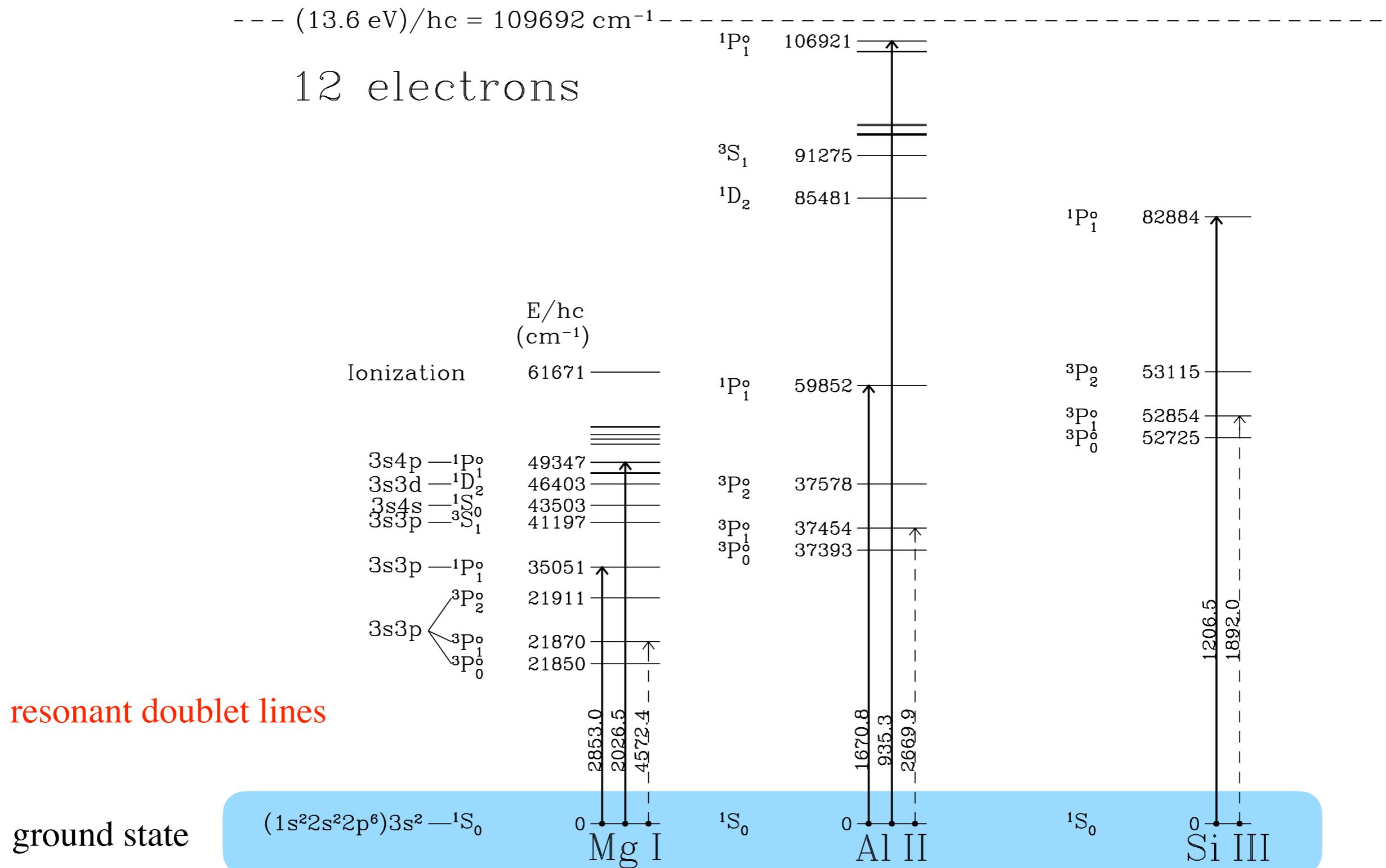
$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{-----}$$

11 electrons



- 12 electrons

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

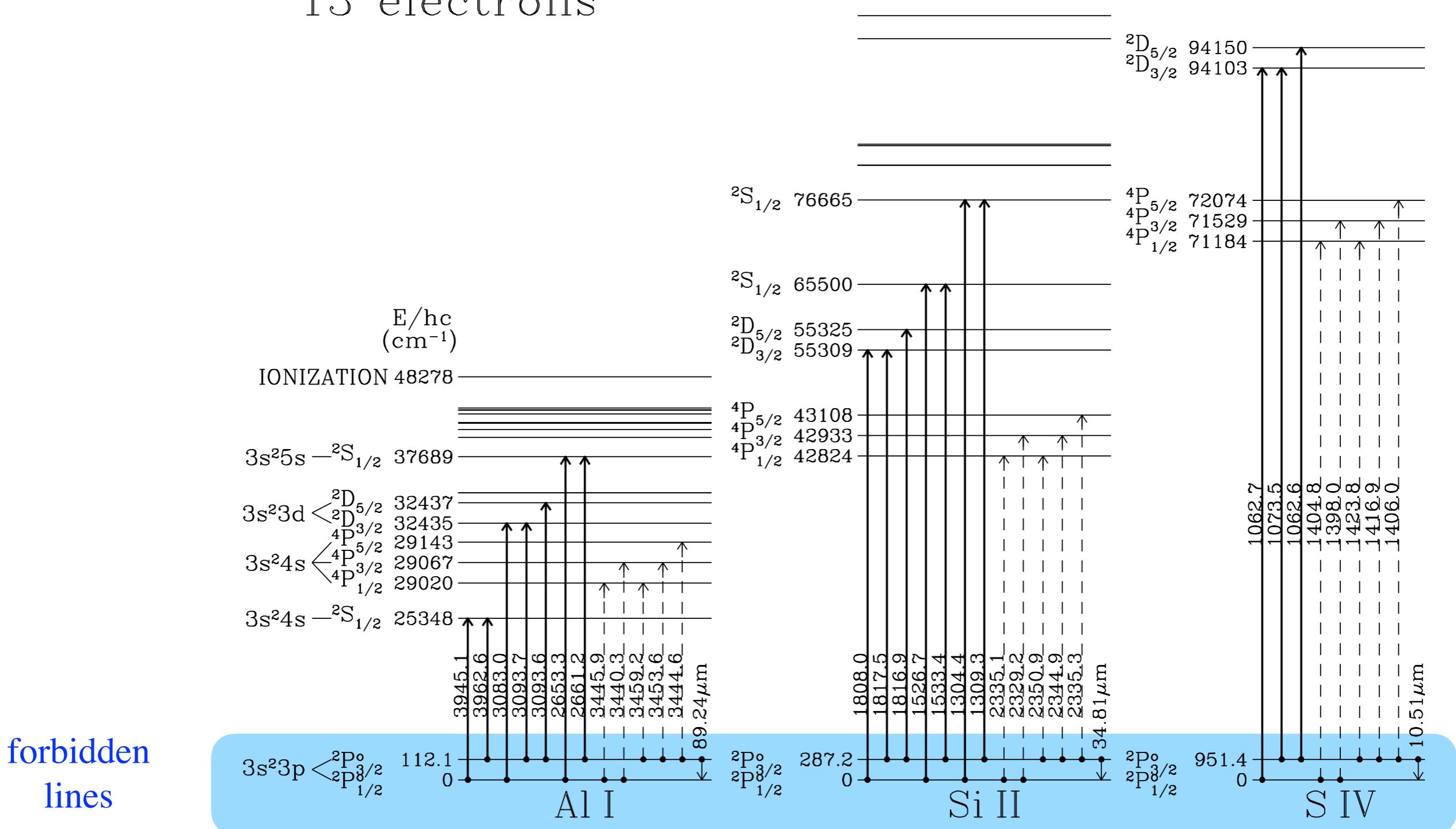


- 13 electrons

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

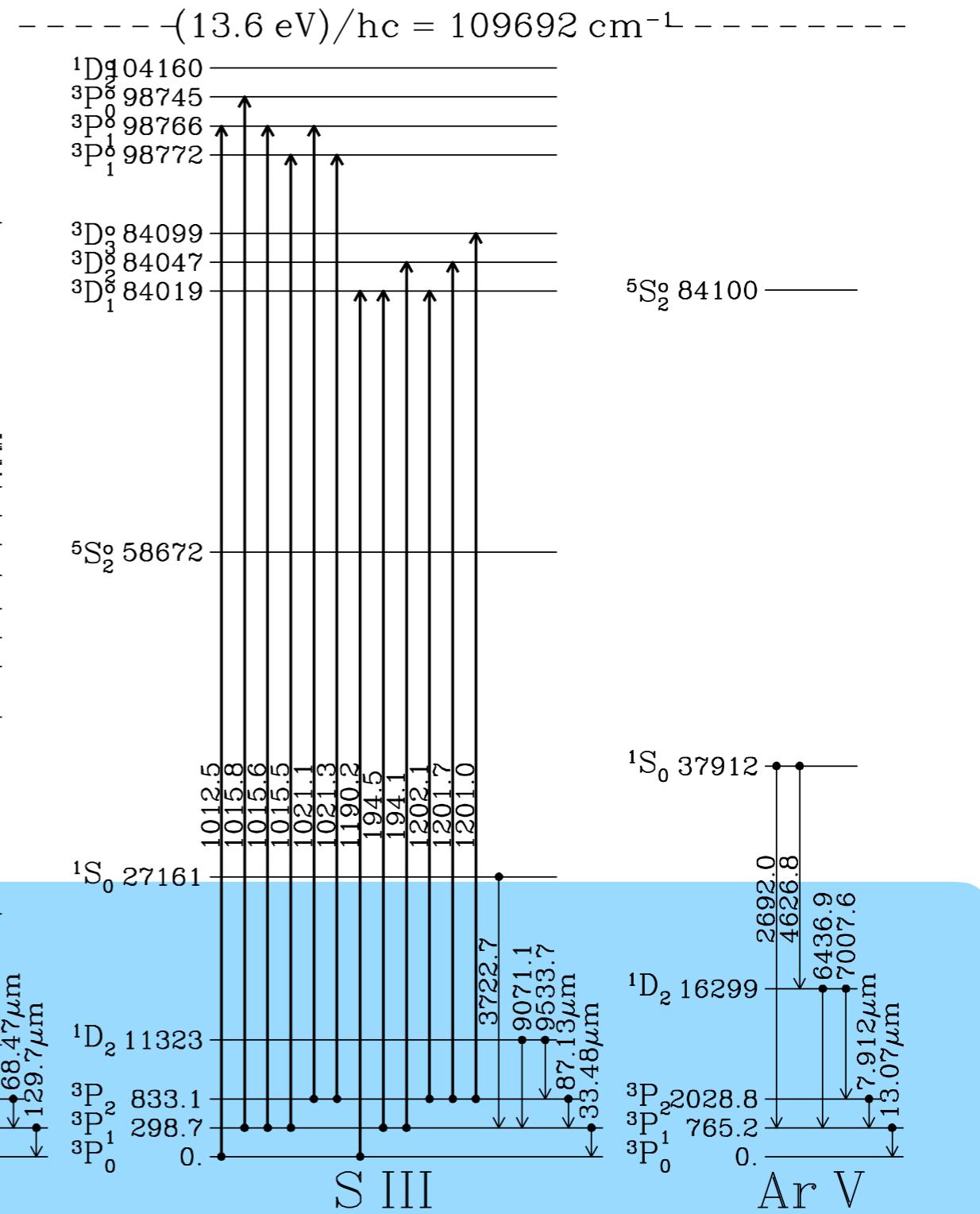
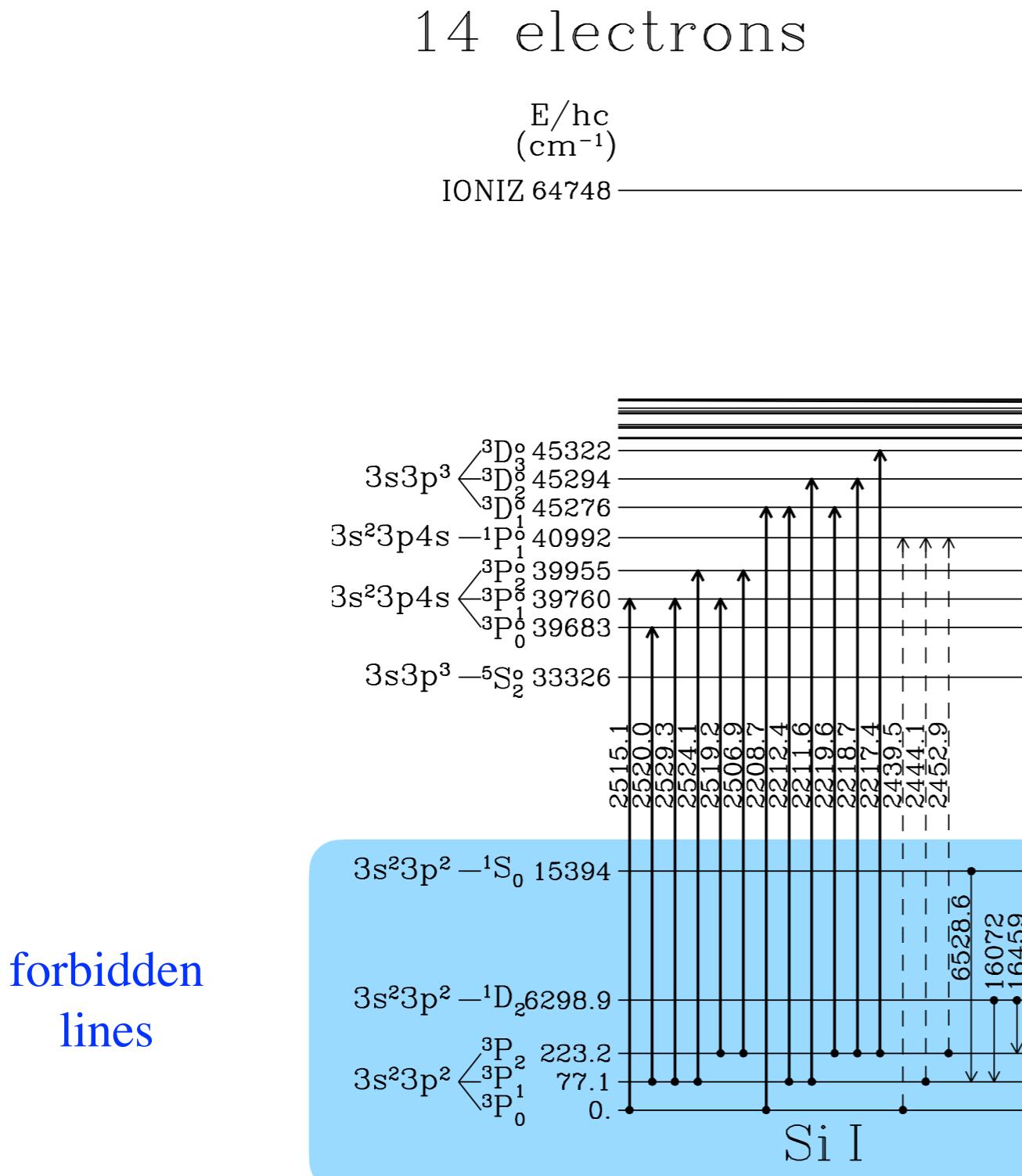
$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1}$$

13 electrons



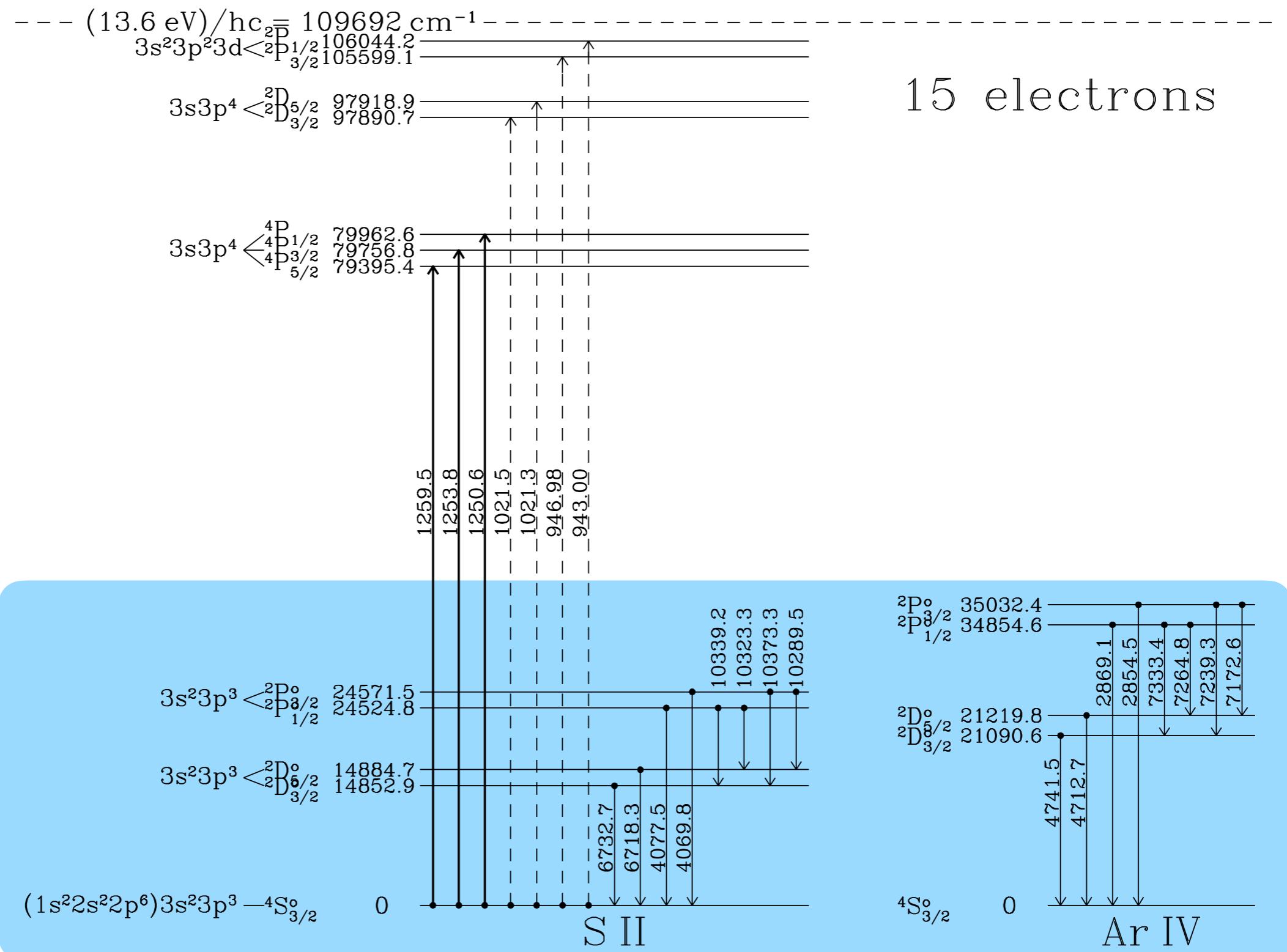
- 14 electrons

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



- 15 electrons

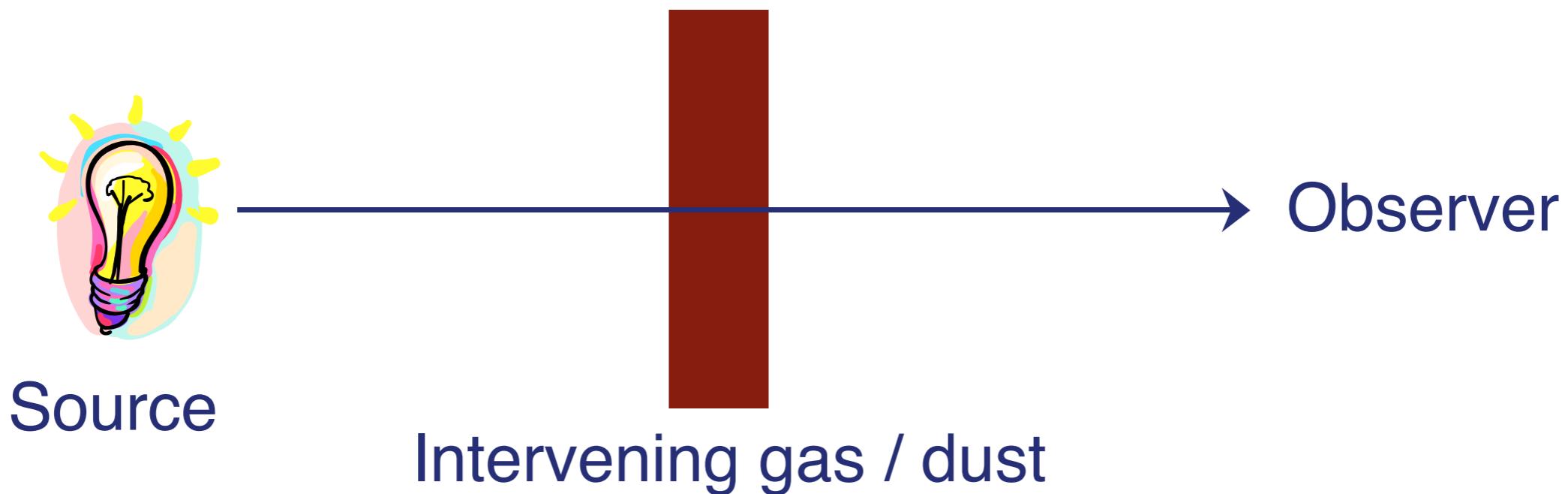
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



Radiative Transfer

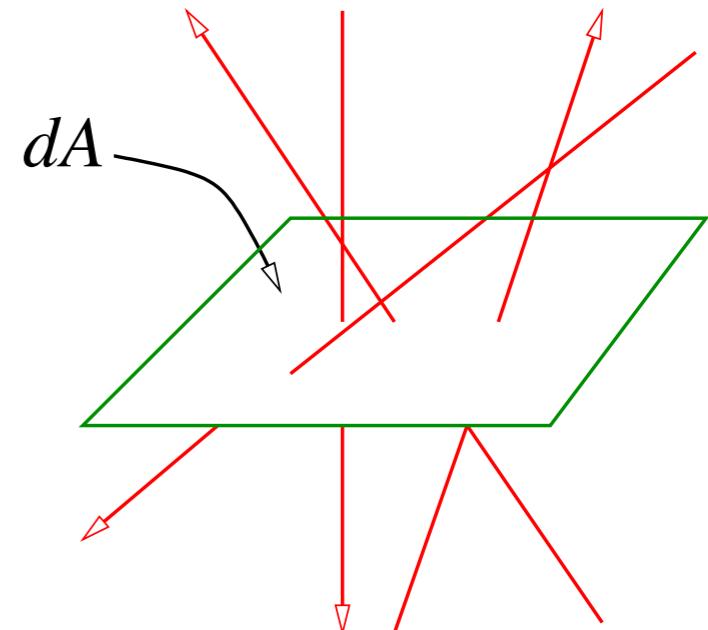
Radiative Transfer

- How is radiation affected as it propagates through intervening gas and dust media to the observer?



Simplification & Complexity

- Simplification:
 - Astronomical objects are normally much larger than the wavelength of radiation they emit.
 - Diffraction can be neglected.
 - Light rays travel to us along straight lines.
- Complexity:
 - At one point, photons can be traveling in several different directions.
 - For instance, at the center of a star, photons are moving equally in all directions. (However, radiation from a star seen by a distant observer is moving almost exactly radially.)
 - Full specification of radiation needs to say how much radiation is moving in each direction at every point. Therefore, we are dealing with the five- or six-dimensional problem. ($[x, y, z] + [\theta, \phi] + [t]$)

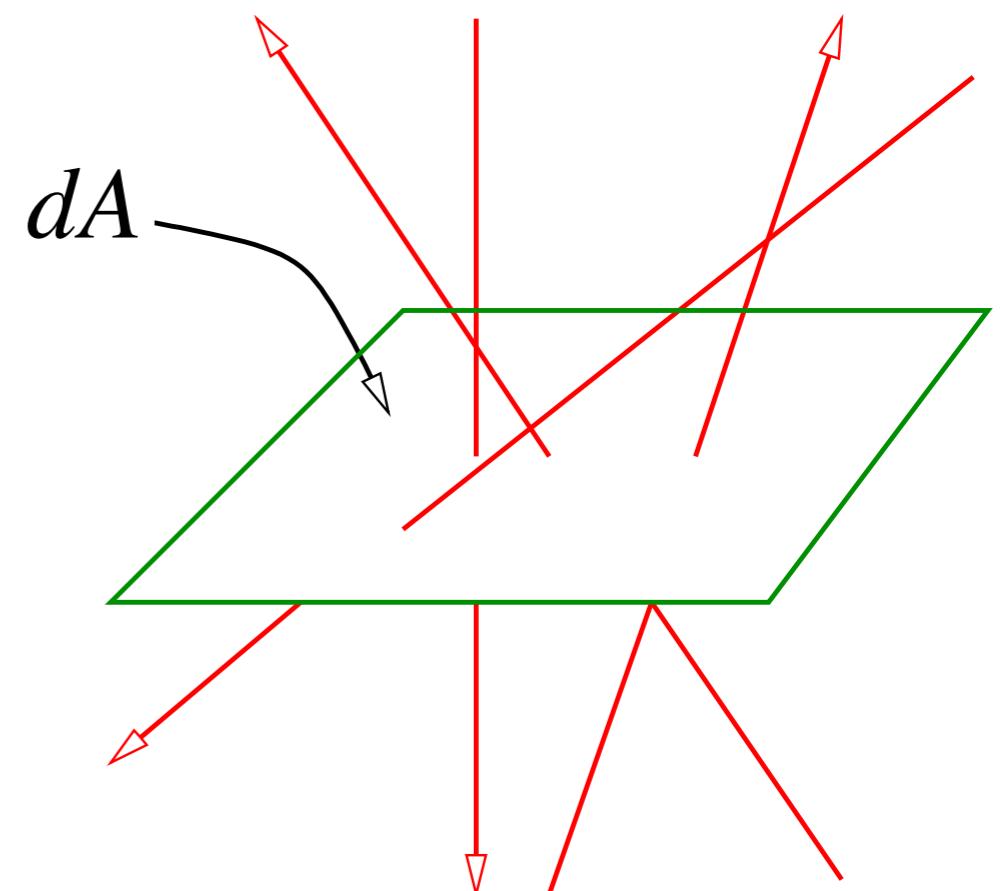


Energy Flux

- Definition
 - Consider a small area dA , exposed to radiation for a time dt .
 - Energy flux F is defined as ***the net energy dE passing through the element of area in all directions in the time interval*** so that

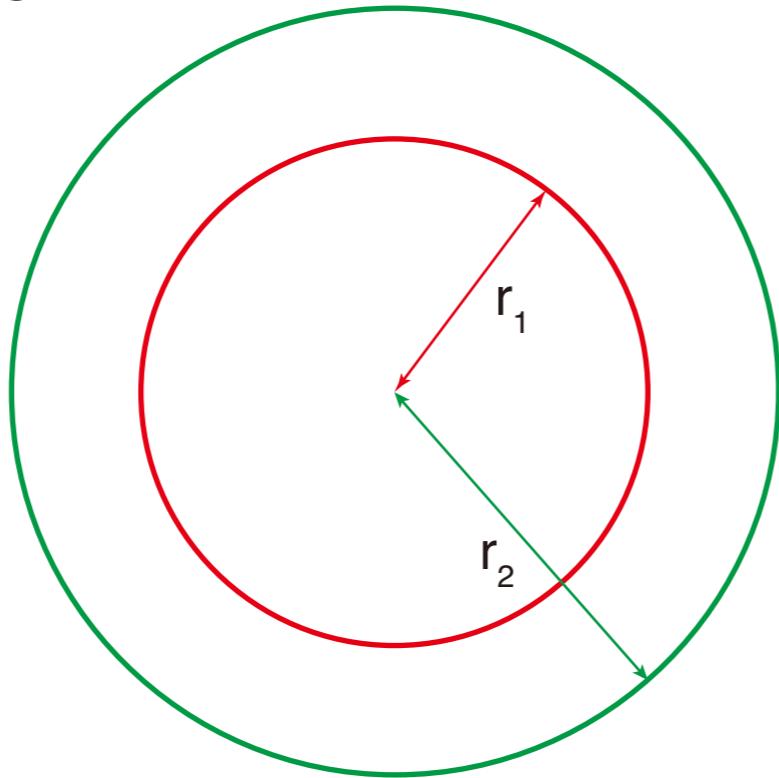
$$dE = F \times dA \times dt$$

- Note that F ***depends on the orientation of the area element dA .***
- Unit: erg cm⁻² s⁻¹



Inverse Square Law

- Flux from an isotropic radiation source, i.e., a source emitting equal amounts of energy in all directions.



- Because of energy conservation, flux through two shells around the source must be the same.

$$4\pi r_1^2 F(r_1) = 4\pi r_2^2 F(r_2)$$

- Therefore, we obtain the inverse square law.

$$F = \frac{\text{const.}}{r^2}$$

Energy Flux Density

- Real detectors are sensitive to a limited range of wavelengths. We need to consider how the incident radiation is distributed over frequency.

Total energy flux: $F = \int F_\nu d\nu$ Integral of F_ν over all frequencies

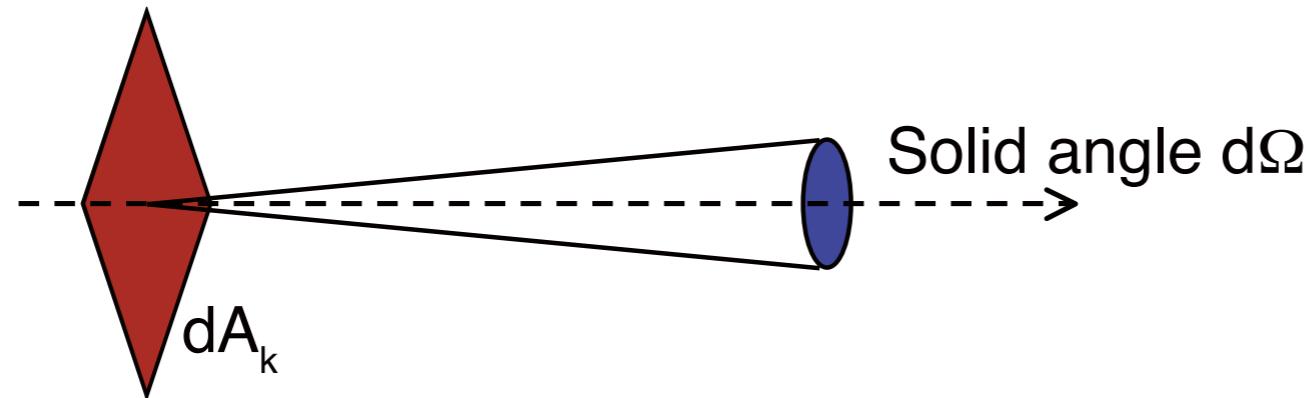
↓

Units: erg s⁻¹ cm⁻² Hz⁻¹

- F_ν is often called the “flux density.”
- Radio astronomers use a special unit to define the flux density:
1 Jansky (Jy) = 10⁻²³ erg s⁻¹ cm⁻² Hz⁻¹

Specific Intensity or Surface Brightness

- Recall that ***flux is a measure of the energy carried by all rays passing through a given area***
- Intensity is the energy carried along by individual rays.***



- Let dE_ν be the amount of radiant energy which crosses the area dA in a direction \mathbf{k} within solid angle $d\Omega$ about in a time interval dt with photon frequency between ν and $\nu + d\nu$.
- The monochromatic specific intensity I_ν is then defined by the equation.

$$dE_\nu = I_\nu(\mathbf{k}, \mathbf{x}, t) dA_{\mathbf{k}} d\Omega d\nu dt$$

- Unit: $\text{erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1} \text{ Hz}^{-1}$
- From the view point of an observer, the specific intensity is called ***surface brightness***.

Relation between the flux and the specific intensity

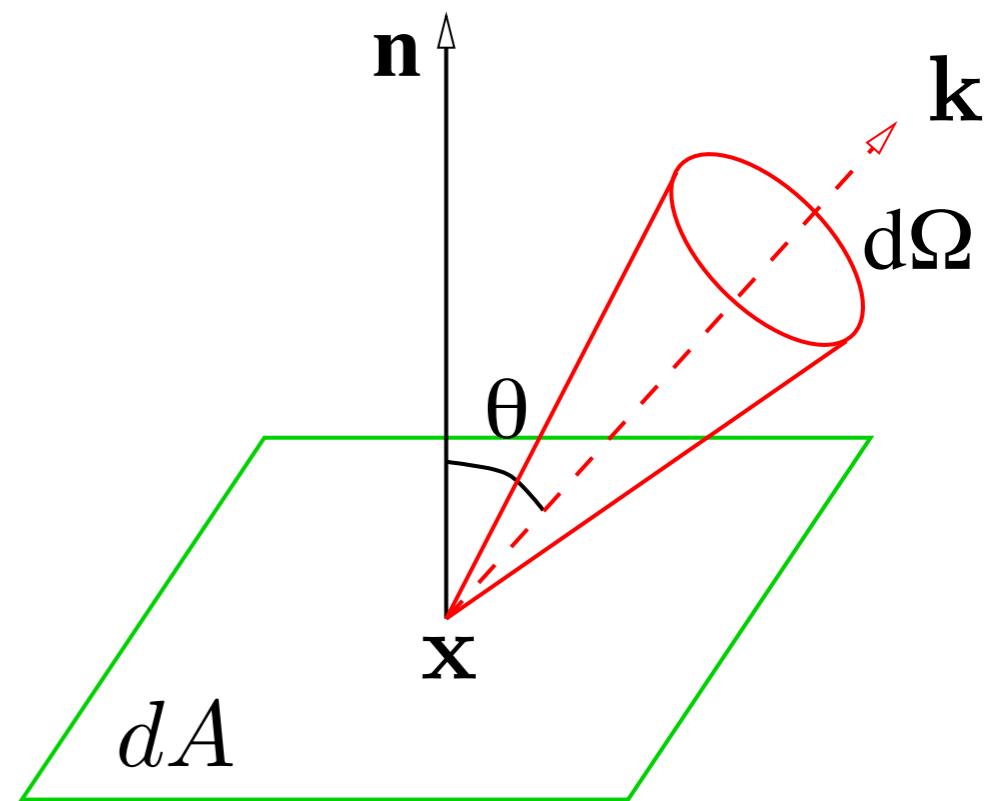
- Let's consider a small area dA , with light rays passing through it at all angles to the normal vector \mathbf{n} of the surface.
- For rays centered about \mathbf{k} , the area normal to \mathbf{k} is

$$dA_{\mathbf{k}} = dA \cos \theta$$

- By the definition,

$$F_{\nu} dAd\nu dt = \int I_{\nu}(\mathbf{k}, \mathbf{x}, t) dA_{\mathbf{k}} d\Omega d\nu dt$$

- Hence, net flux in the direction of \mathbf{n} is given by integrating over all solid angles:



$$F_{\nu} = \int I_{\nu} \cos \theta d\Omega = \int_0^{2\pi} \int_0^{\pi} I_{\nu} \cos \theta \sin \theta d\theta d\phi$$

[Note] **flux** = “sum of all ray vectors” which is then projected onto a normal vector
intensity = magnitude of a single ray vector

Note

- Intensity can be defined as per wavelength interval.

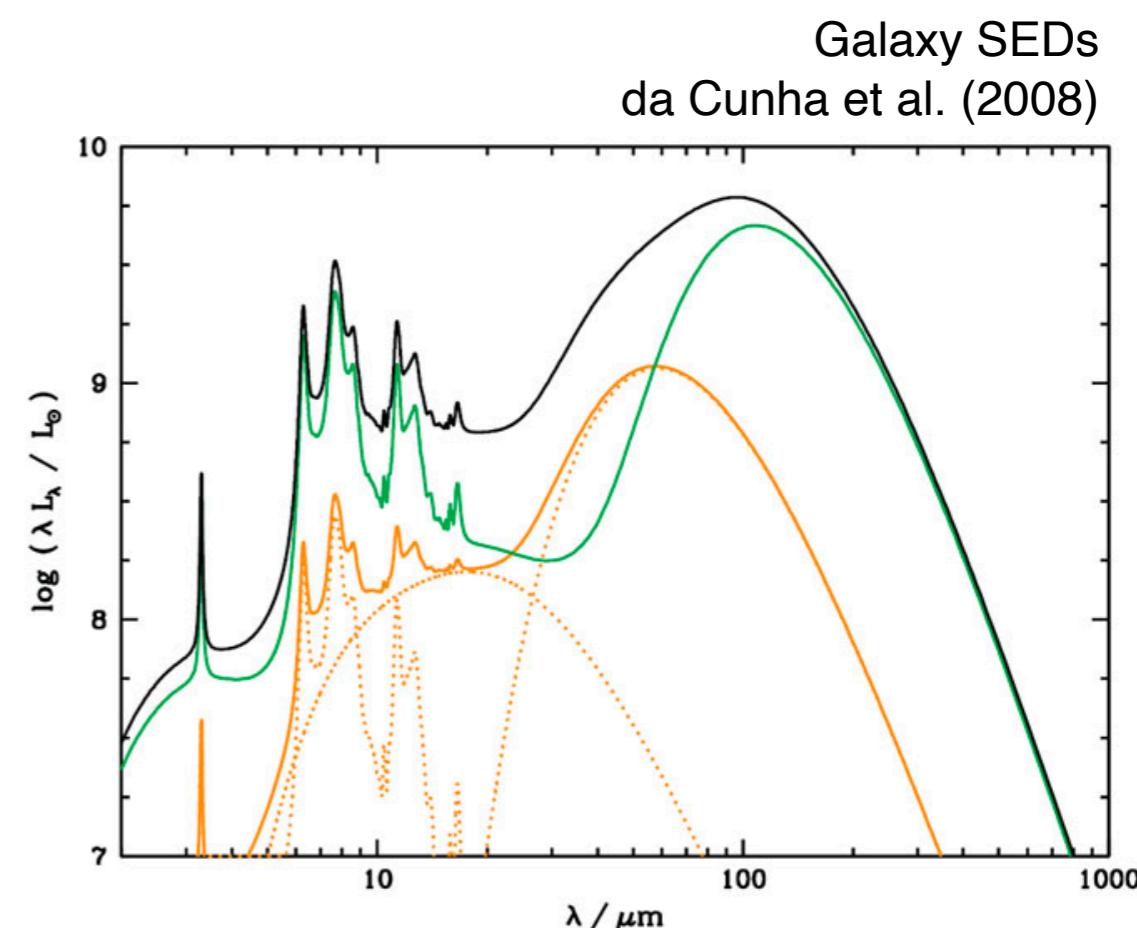
$$I_\nu |d\nu| = I_\lambda |d\lambda| \quad \leftarrow \left| \frac{d\nu}{d\lambda} \right| = \frac{c}{\lambda^2} = \frac{\nu}{\lambda} \quad \leftarrow \quad \nu = \frac{c}{\lambda}$$

$$\nu I_\nu = \lambda I_\lambda$$

- Integrated intensity is defined as the intensity over all frequencies.

$$I = \int_0^\infty I_\nu d\nu = \int_0^\infty I_\lambda d\lambda$$

- In astrophysics, we plot the **spectral energy distribution (SED)** as νI_ν versus ν or λI_λ versus λ .



How does specific intensity changes along a ray in free space

- Consider a bundle of rays and any two points along the rays. Construct areas dA_1 and dA_2 normal to the rays at these points.
 - Consider the energy carried by the rays passing through both areas. Because energy is conserved,

$$dE_1 = I_1 dA_1 d\Omega_1 d\nu dt = dE_2 = I_2 dA_2 d\Omega_2 d\nu dt$$

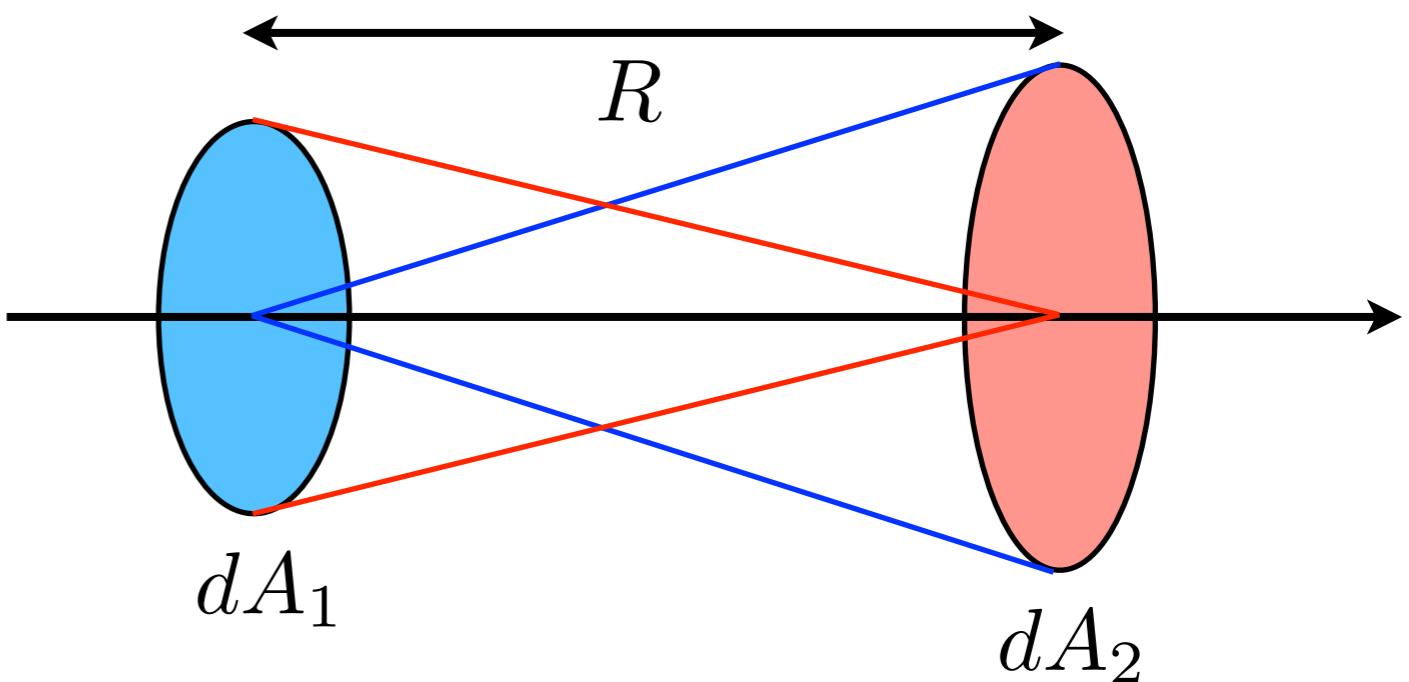
- Here, $d\Omega_1$ is the solid angle subtended by dA_2 at the location 1 and so forth.

$$d\Omega_1 = \frac{dA_2}{R^2}$$

$$d\Omega_2 = \frac{dA_1}{R^2}$$

\rightarrow

$$I_1 = I_2$$



-
- Conclusion (the constancy of intensity):
 - the specific intensity remains the same as radiation propagates through free space.

$$I_1 = I_2$$

- If we measure the distance along a ray by variable s , we can express the result equivalently in differential form:

$$\frac{dI}{ds} = 0$$

- We receive the same specific intensity at the telescope as is emitted at the source.
 - Imagine looking at a uniformly lit wall and walking toward it. As you get closer, a field-of-view with fixed angular size will see a progressively smaller region of the wall, but this is exactly balanced by the inverse square law describing the spreading of the light rays from the wall.

Specific Energy Density

- Consider a bundle of rays passing through a volume element dV in a direction Ω .
 - Then, the energy density per unit solid angle is defined by

$$dE = u_\nu(\Omega) dV d\Omega d\nu$$

- Since radiation travels at velocity c , the volume element is

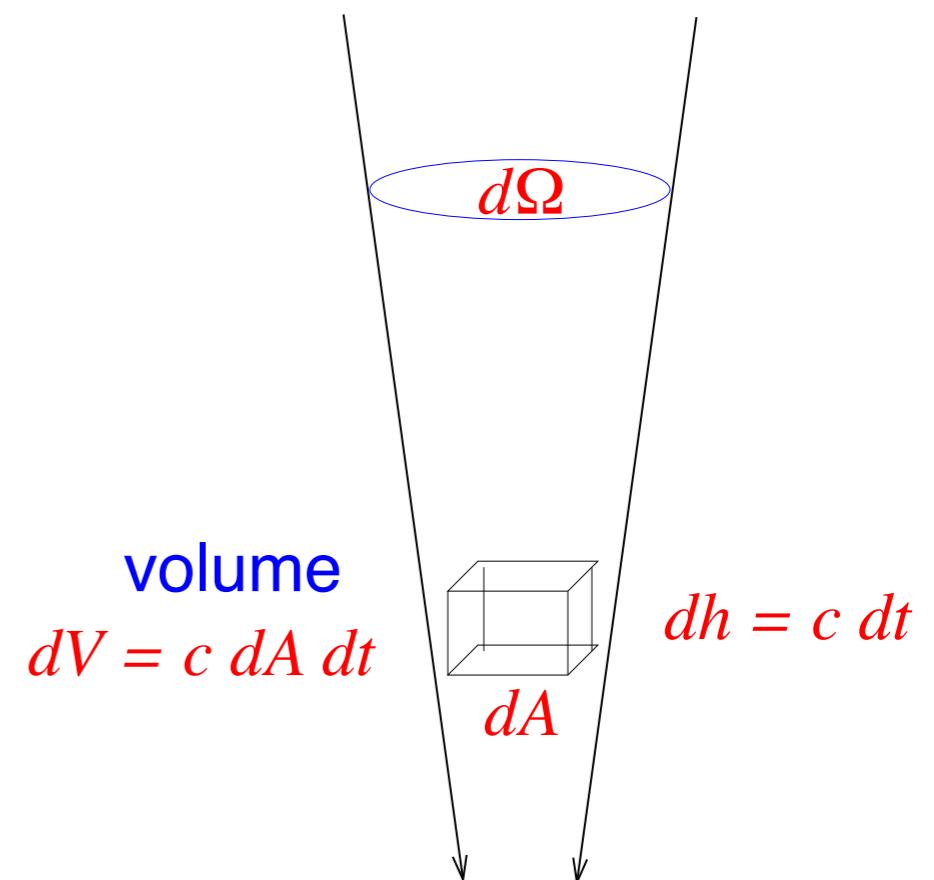
$$dV = dA(cdt)$$

- According to the definition of the intensity,

$$dE = I_\nu dA dt d\Omega d\nu$$

- Then, we have

$$u_\nu(\Omega) = I_\nu(\Omega)/c$$



Energy Density and Mean Intensity

- Integrating over all solid angle, we obtain

$$u_\nu = \int u_\nu(\Omega) d\Omega = \frac{1}{c} \int I_\nu d\Omega$$

- Mean intensity** is defined by

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

- Then, the energy density is

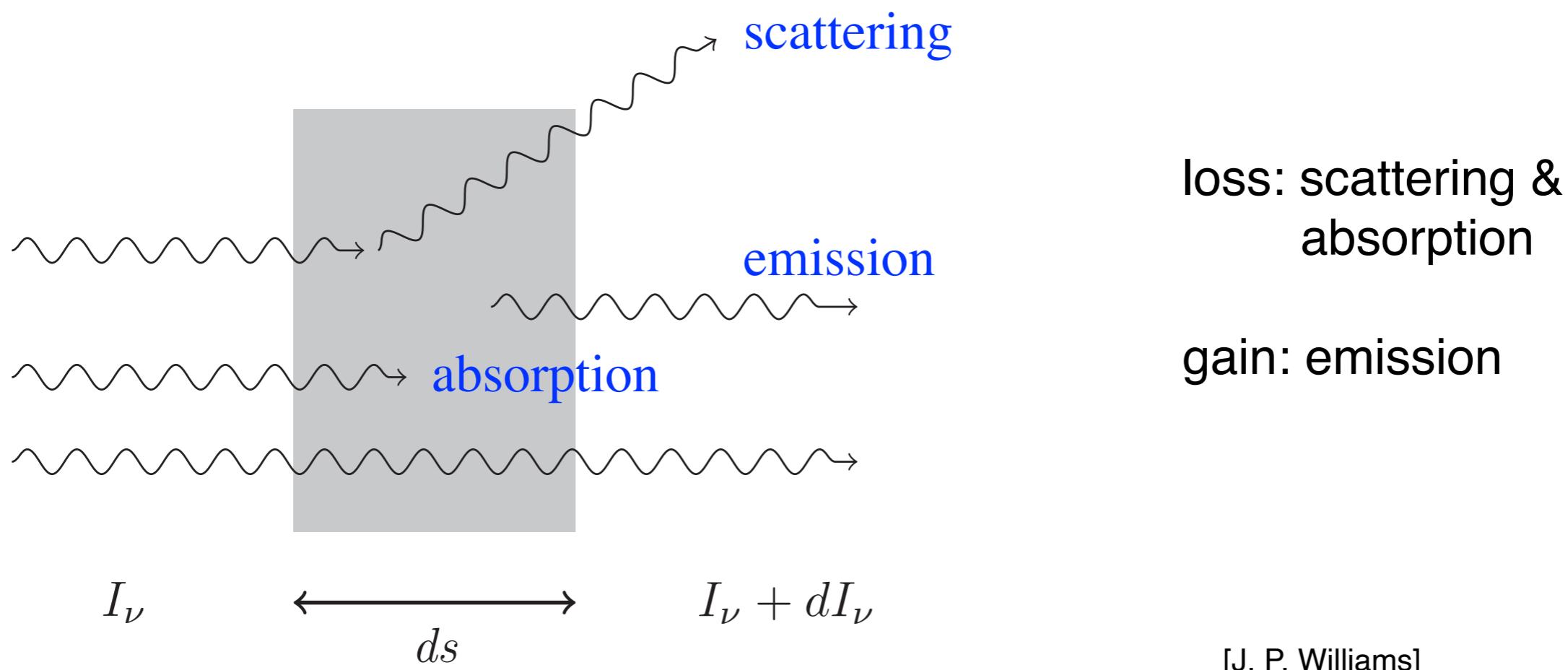
$$u_\nu = \frac{4\pi}{c} J_\nu$$

- Total energy density is obtained by integrating over all frequencies.

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

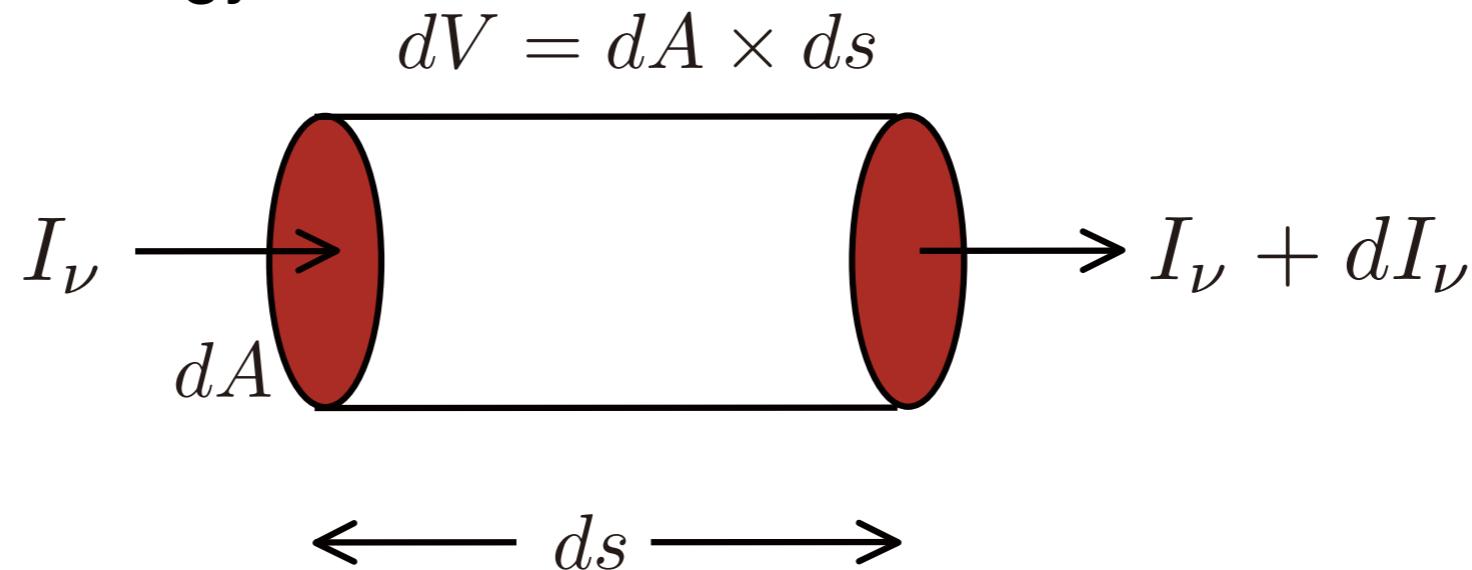
Radiative Transfer Equation in reality

- In reality, as a ray passes through matter, energy may be added, subtracted, or scattered from it by emission, absorption, or scattering.
- The intensity will not in general remain constant.
- These interactions are described by the ***radiative transfer equation***.



Emission

- If the radiation travels through a medium which is itself emitting radiation, that will add to the energy:



- Spontaneous “**emission coefficient**” or “**emissivity**” j_ν is the amount of energy emitted per unit time, per unit solid angle, per unit frequency, and per unit volume:

$$dE = j_\nu dV d\Omega dt d\nu \quad (j_\nu : \text{erg cm}^{-3} \text{ s}^{-1} \text{ sr}^{-1} \text{ Hz}^{-1})$$

- In going a distance ds , a beam of cross section dA travels through a volume $dV = dA ds$. Thus the intensity added to the beam is by ds is

$$dI_\nu = j_\nu ds \qquad \longleftrightarrow \qquad dE = (dI_\nu) dA d\Omega dt d\nu$$

-
- Therefore, the equation of radiative transfer for pure emission becomes:

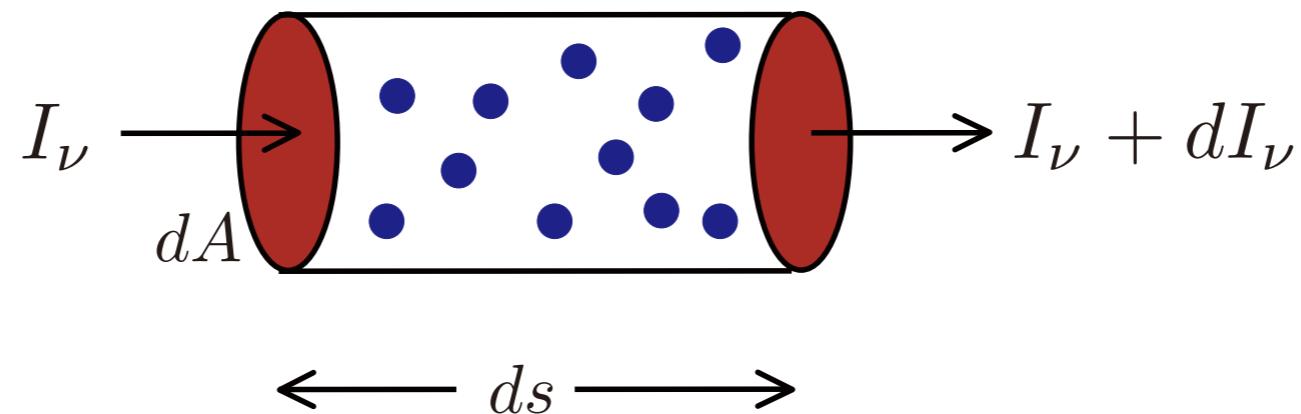
$$\frac{dI_\nu}{ds} = j_\nu$$

- If we know what j_ν is, we can integrate this equation to find the change in specific intensity as radiation propagates through the medium:

$$I_\nu(s) = I_\nu(0) + \int_0^s j_\nu(s')ds'$$

Absorption

- If the radiation travels through a medium which absorbs radiation, the energy in the beam will be reduced:



- Let n denote the number density of absorbers (particles per unit volume).
- Assume that each absorber has a cross-sectional area of σ_ν (in units of cm^2).
- If a beam travels through ds , total area of absorbers is

$$\text{number of absorbers} \times \text{cross-section} = n \times dA \times ds \times \sigma_\nu$$

Fraction of radiation absorbed = fraction of area blocked:

$$\frac{dI_\nu}{I_\nu} = - \frac{ndAds\sigma_\nu}{dA} = -n\sigma_\nu ds \quad \longrightarrow \quad \frac{dI_\nu}{ds} = -\kappa_\nu I_\nu$$

$$dI_\nu = -n\sigma_\nu I_\nu ds \equiv -\kappa_\nu I_\nu ds$$

- **Absorption coefficient** is defined as $\kappa_\nu \equiv n\sigma_\nu$ (units: cm^{-1}), meaning the ***total cross-sectional area per unit volume***.
- If we include the effect of stimulated emission in the absorption coefficient, it may be referred to as the **attenuation coefficient**. (as in Draine's book)

-
- Rearranging the previous equation, we obtain the equation of radiative transfer for pure absorption:

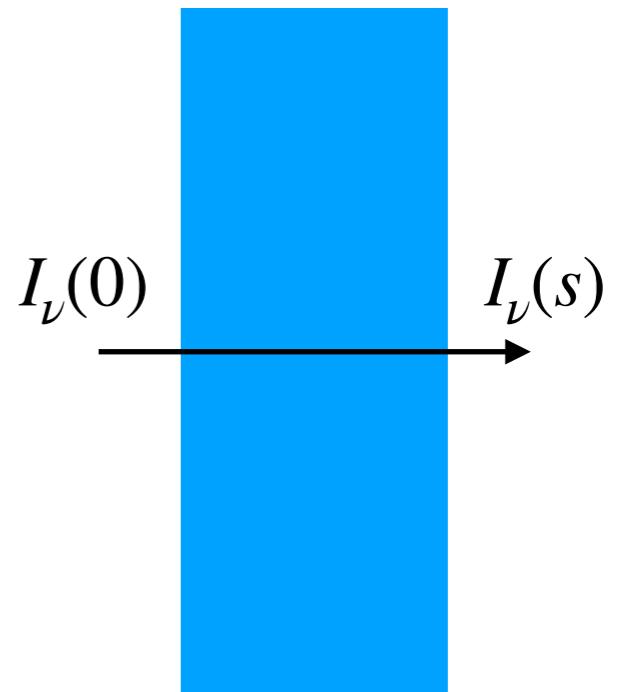
$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu$$

- The amount of reduced energy depends on how much radiation we already have.
- Integrate to find how radiation changes along path:

$$\int_0^s \frac{dI_\nu}{I_\nu} = - \int_0^s \kappa_\nu(s') ds'$$

$$[\ln I_\nu]_0^s = - \int_0^s \kappa_\nu(s') ds'$$

$$I_\nu(s) = I_\nu(0) \exp \left[- \int_0^s \kappa_\nu(s') ds' \right]$$



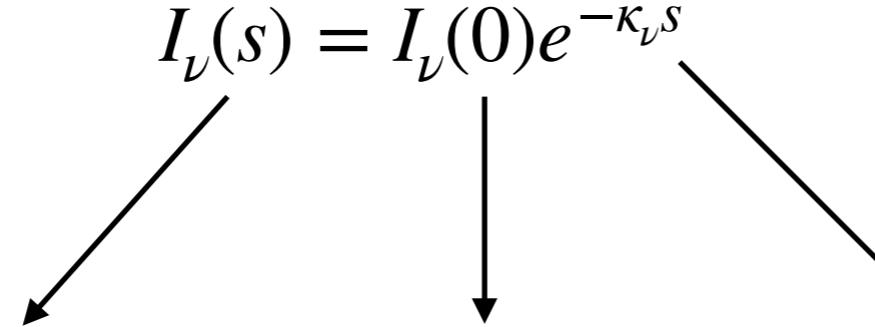
-
- If the absorption coefficient is a constant (example: a uniform density gas of ionized hydrogen), then we obtain

$$I_\nu(s) = I_\nu(0)e^{-\kappa_\nu s}$$

specific intensity
after distance s

initial intensity
at $s = 0$.

radiation exponentially
absorbed with distance



- ***Optical depth:***
 - Imagine radiation traveling into a cloud of absorbing gas, exponential defines a scale over which radiation is attenuated.
 - When $\int_0^s \kappa_\nu(s')ds' = 1$, the intensity will be reduced to $1/e$ of its original value.

-
- We define the optical depth τ_ν as:

$$\tau_\nu(s) = \int_0^s \kappa_\nu(s')ds' \quad \text{or} \quad d\tau_\nu = \kappa_\nu ds \quad \longrightarrow \quad I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu}$$

- A medium is said to be ***optically thick*** at a frequency ν if the optical depth for a typical path through the medium satisfies:

$$\tau_\nu(s) > 1$$

- The medium is ***optically thin*** if, instead:

$$\tau_\nu(s) < 1$$

- An optically thin medium is one which a typical photon of frequency ν can pass through without being (significantly) absorbed.

Mean Free Path

- From the exponential absorption law, the **probability of a photon absorbed** between optical depths τ_ν and $\tau_\nu + d\tau_\nu$ is

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} \quad \xrightarrow{\hspace{1cm}}$$

probability =
$$\frac{|dI_\nu|}{I_\nu(0)} = \left| \frac{dI_\nu}{\tau_\nu} \right| d\tau_\nu = e^{-\tau_\nu} d\tau_\nu \quad \rightarrow \quad P(\tau_\nu) = e^{-\tau_\nu}$$

- The mean optical depth traveled is thus equal to unity:

$$\langle \tau_\nu \rangle = \int_0^\infty \tau_\nu P(\tau_\nu) d\tau_\nu = \int_0^\infty \tau_\nu e^{-\tau_\nu} d\tau_\nu = 1$$

= **probability density function** for
the absorption at an optical depth τ_ν

- The mean free path is defined as the average distance a photon can travel through an absorbing material until it is absorbed.** In a homogeneous medium, the mean free path is determined by

$$\langle \tau_\nu \rangle = \kappa_\nu \ell_\nu = 1 \quad \rightarrow \quad \ell_\nu = \frac{1}{\kappa_\nu} = \frac{1}{n\sigma_\nu}$$

- A local mean path at a point in an inhomogeneous material can be also defined.
- The **probability of a photon being absorbed within an optical depth τ_ν** is

$$\int_0^{\tau_\nu} P(\tau'_\nu) d\tau'_\nu = 1 - e^{-\tau_\nu}$$

Radiative Transfer Equation

- ***Radiative transfer equation*** with both absorption and emission is

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + j_\nu$$

absorption emission

- We can rewrite the radiative transfer equation using the optical depth as a measure of ‘distance’ rather than s :

$$\frac{dI_\nu}{\kappa_\nu ds} = -I_\nu + \frac{j_\nu}{\kappa_\nu}$$

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu$$

- where $S_\nu \equiv j_\nu/\kappa_\nu$ **is called the *source function***. This is an alternative and sometimes more convenient way to write the equation.

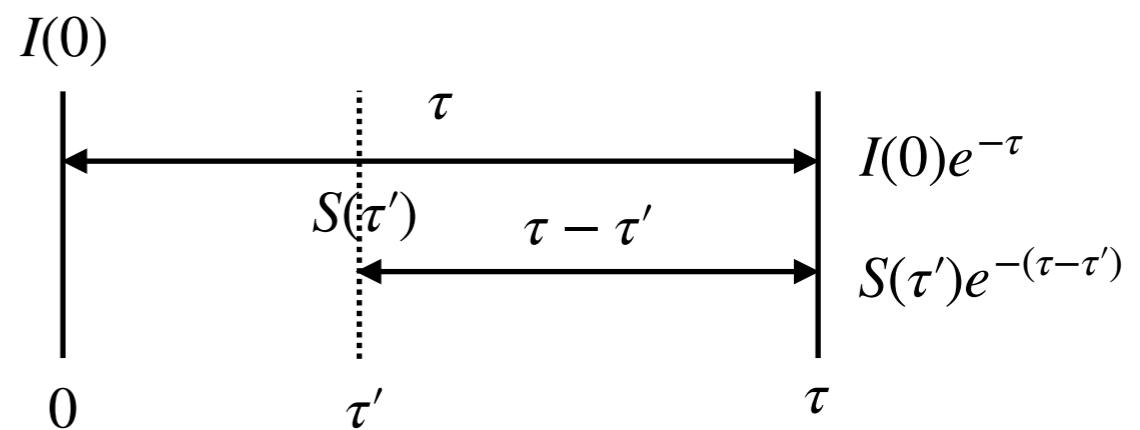
Formal Solution of the RT equation

$$\frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu$$

$$e^{\tau_\nu} \frac{dI_\nu}{d\tau_\nu} + e^{\tau_\nu} I_\nu = e^{\tau_\nu} S_\nu$$

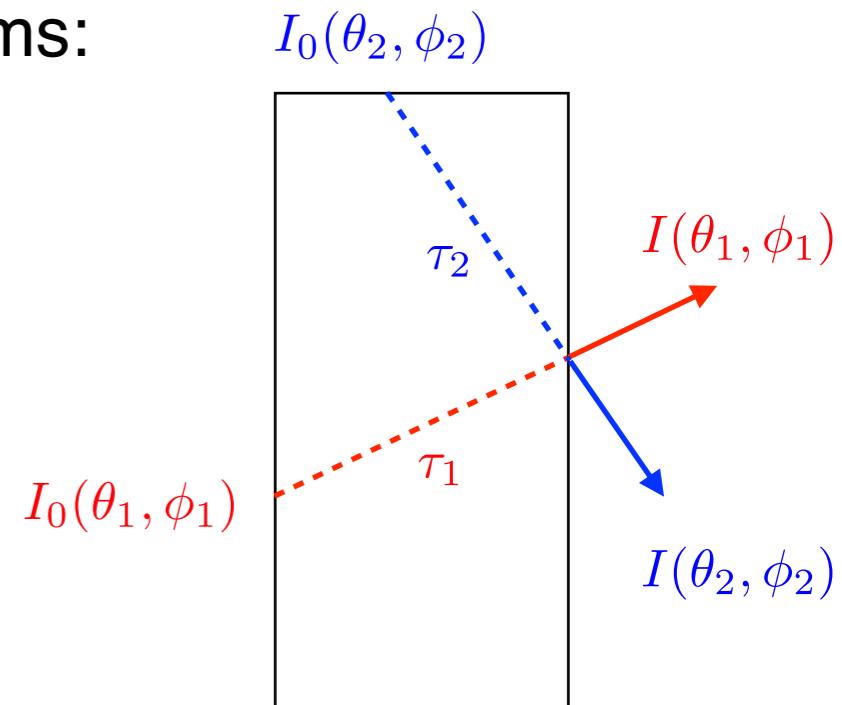
$$\frac{d}{d\tau_\nu} (e^{\tau_\nu} I_\nu) = e^\tau S_\nu$$

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu) d\tau'_\nu$$



- The solution is easily interpreted as the sum of two terms:
 - the initial intensity diminished by absorption
 - the integrated source diminished by absorption.
- For a constant source function, the solution becomes

$$\begin{aligned} I_\nu(\tau_\nu) &= I_\nu(0)e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu}) \\ &= S_\nu + e^{-\tau_\nu} (I_\nu(0) - S_\nu) \end{aligned}$$



Relaxation

- “Relaxation”

$$\frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu$$

$I_\nu > S_\nu \rightarrow \frac{dI_\nu}{d\tau_\nu} < 0$, then I_ν tends to decrease along the ray

$I_\nu < S_\nu \rightarrow \frac{dI_\nu}{d\tau_\nu} > 0$, then I_ν tends to increase along the ray

- ***The source function is the quantity that the specific intensity tries to approach***, and does approach if given sufficient optical depth.

As $\tau_\nu \rightarrow \infty$, $I_\nu \rightarrow S_\nu$

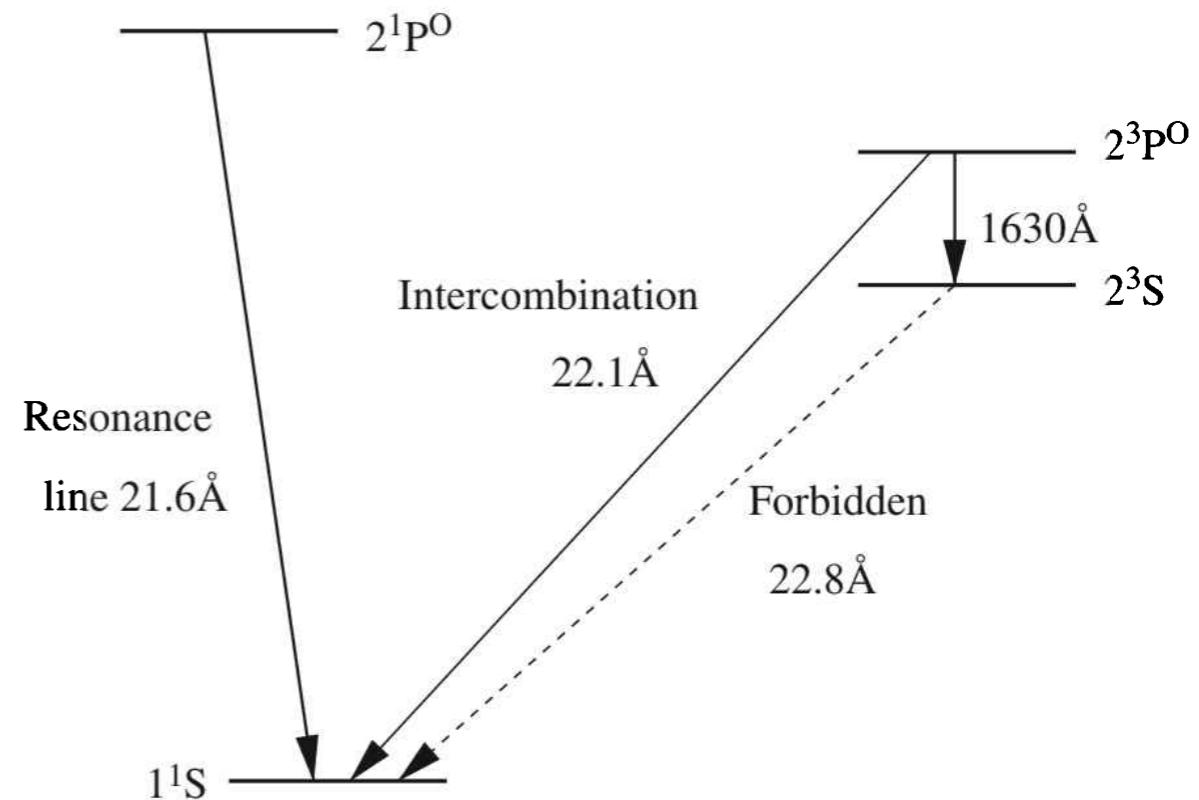
Homework (due date: 04/10)

[Q3] Atomic Spectroscopy

1. What is the ground-state configuration, term and level of the beryllium atom, Be? One of the outer electrons in Be is promoted to the 3rd orbital. What terms and levels can this configuration have?
2. Symbols for particular levels of three different atoms are written as 1D_1 , $^0D_{3/2}$ and $^3P_{3/2}$. Explain in each case why the symbol must be wrong.
3. Give the spectroscopic terms arising from the following configurations, using L-S coupling. Include parity and J values. Give your arguments in detail for deriving these results.
 - (a) $2s^2$
 - (b) $2p3s$
 - (c) $3p4p$

4. The lithium atom, Li, has three electrons. Consider the following configurations of Li: (a) $1s^22p$, (b) $1s2s3s$, (c) $1s2p3p$. By considering the configuration only, state which of the three sets of transitions between the configuration (a), (b) and (c) are allowed and forbidden transitions?

5. The right figure shows the term diagram for helium-like oxygen, O VII, showing transitions from the $1s2l$ states. Explain why 22.1\AA line is an intercombination line and why 22.8\AA is a forbidden line.



[Q4] Radiative Transfer

Suppose a sphere of gas with a radius R emits a forbidden line, and its emissivity is constant over the sphere, i.e., $j(x, y, z) = j_0$ (erg cm $^{-3}$ s $^{-1}$ sr $^{-1}$). An observer is located at a distance d from the sphere's center. The observer measures the intensity of the emission toward a direction with an angle θ , as shown in Figure (a). Without the loss of generality, we can assume that the direction vector of the line of sight is in the xy plane. The line of sight intersects the outer boundary of the sphere at two points, a and b .

- (1). If we make the assumption that there is an absence of dust, and the emission line is forbidden, then, there will be no absorption. In this case, show that the intensity at the angle θ is given by:

$$I(\theta) = j_0 \int_a^b ds = j_0 s_\theta, \text{ where } s_\theta \text{ is the distance between the points } a \text{ and } b.$$

- (2). Show that the distance is $s_\theta = 2\sqrt{R^2 - d^2 \sin^2 \theta}$ and therefore the intensity at angle θ is

$$I(\theta) = 2j_0 \sqrt{R^2 - d^2 \sin^2 \theta}.$$

- (3). Now, assume the case where $d \rightarrow \infty$ and $\theta \rightarrow 0$ (see Figure (b)). Then, the intensity at θ can be approximated as the intensity of a parallel ray that passes through the sphere at an impact parameter defined by $p = d \tan \theta$. In this limit, show that $p \approx d \sin \theta$ and

$$I(p) = 2j_0 \sqrt{R^2 - p^2}.$$

Assume that the emissivity is a function of the radial distance from the sphere's center r , i.e., $j(r)$.

- (4). In the limit of $d \rightarrow \infty$ (Figure (b)), show that $I(p) = \int_a^b j(r) ds = 2 \int_p^R j(r) \frac{r dr}{\sqrt{r^2 - p^2}}$.

Note that this integral is called the Abel transform of $j(r)$.

- (5). Now, use the equation of (4) and derive the same result $\left(I(p) = 2j_0 \sqrt{R^2 - p^2} \right)$ as in (3) if $j(r) = j_0 = \text{constant}$.

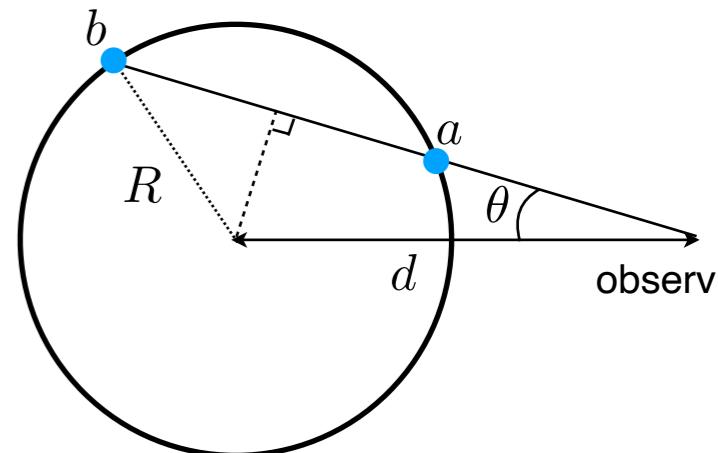


Figure (a)

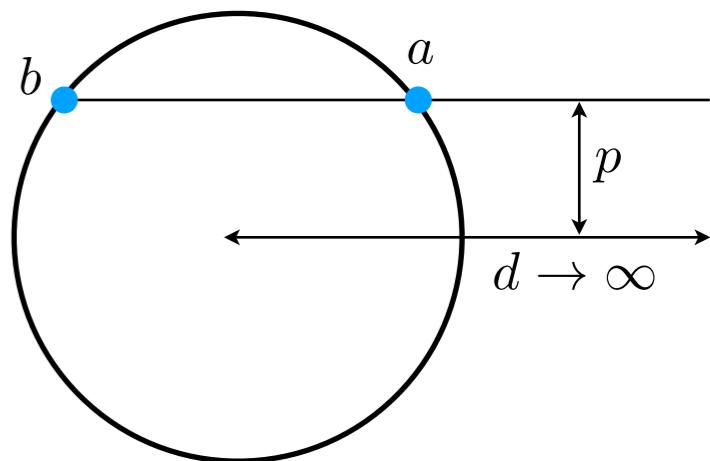


Figure (b)