

Astrophysics

Lecture 13

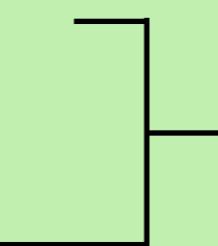
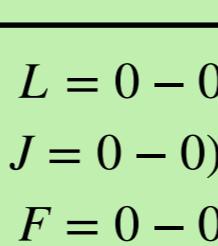
November 27 (Mon.), 2023

updated 11/20 14:42

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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 |
| | 
<i>intercombination</i> line if only this rule is violated. |
| | It is only rarely necessary to consider this. |

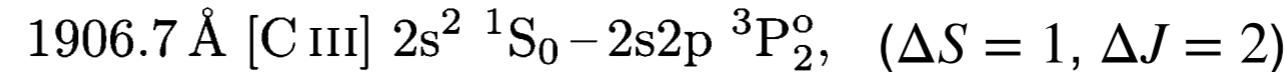
- **Allowed = Electric Dipole** : Transitions which satisfy all the above selection rules are referred to as **allowed transitions**. These transitions are strong and have a typical lifetime of $\sim 10^{-8}$ s. Allowed transitions are denoted without square brackets.

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.



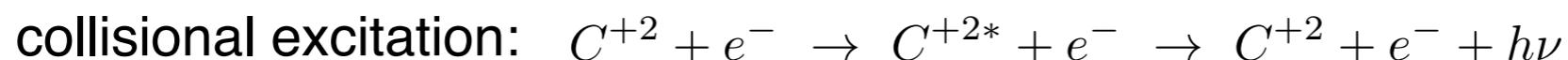
- **Resonance line** denotes the longest wavelength, dipole-allowed transition arising from the ground state of a particular atom or ion.

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.*

[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.



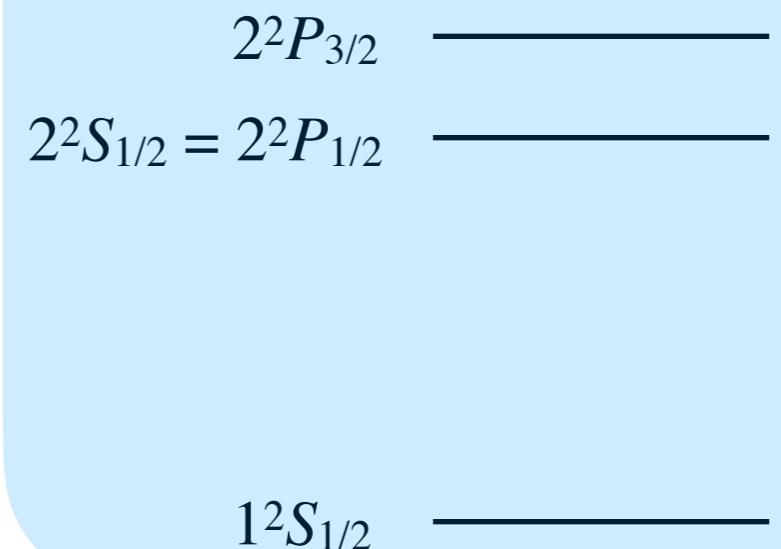
- There is no ambiguity in absorption line studies - only C⁺² can produce a C III absorption line. This had caused many people to think that C III refers to the matter rather than the spectrum.
- But this notation is ambiguous in the case of emission lines.

[Hydrogen Atom - Fine Structure]

- Fine structure of the hydrogen atom

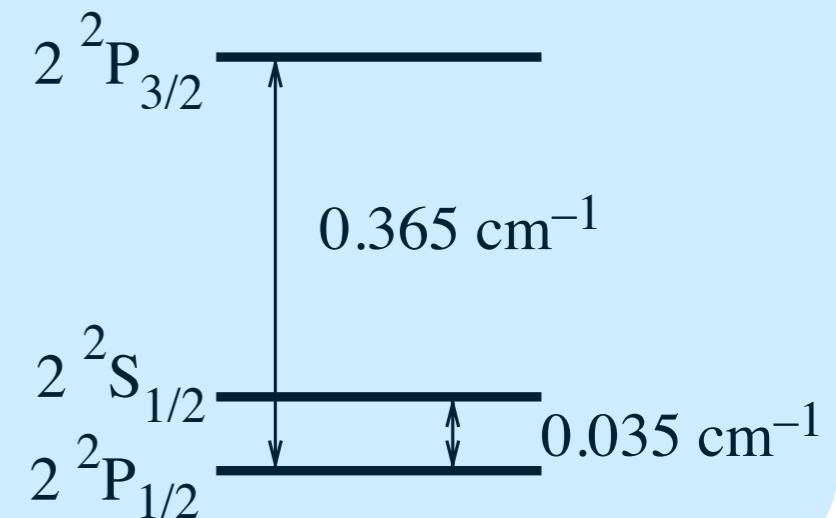
configuration	L	S	J	term	level
ns	0	$1/2$	$1/2$	2S	$^2S_{1/2}$
np	1	$1/2$	$1/2, 3/2$	$^2P^o$	$^2P_{1/2}^o, ^2P_{3/2}^o$
nd	2	$1/2$	$3/2, 5/2$	2D	$^2D_{3/2}, ^2D_{5/2}$
nf	3	$1/2$	$5/2, 7/2$	$^2F^o$	$^2F_{5/2}^o, ^2D_{7/2}^o$

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 $^2P_{1/2}$ orbitals 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

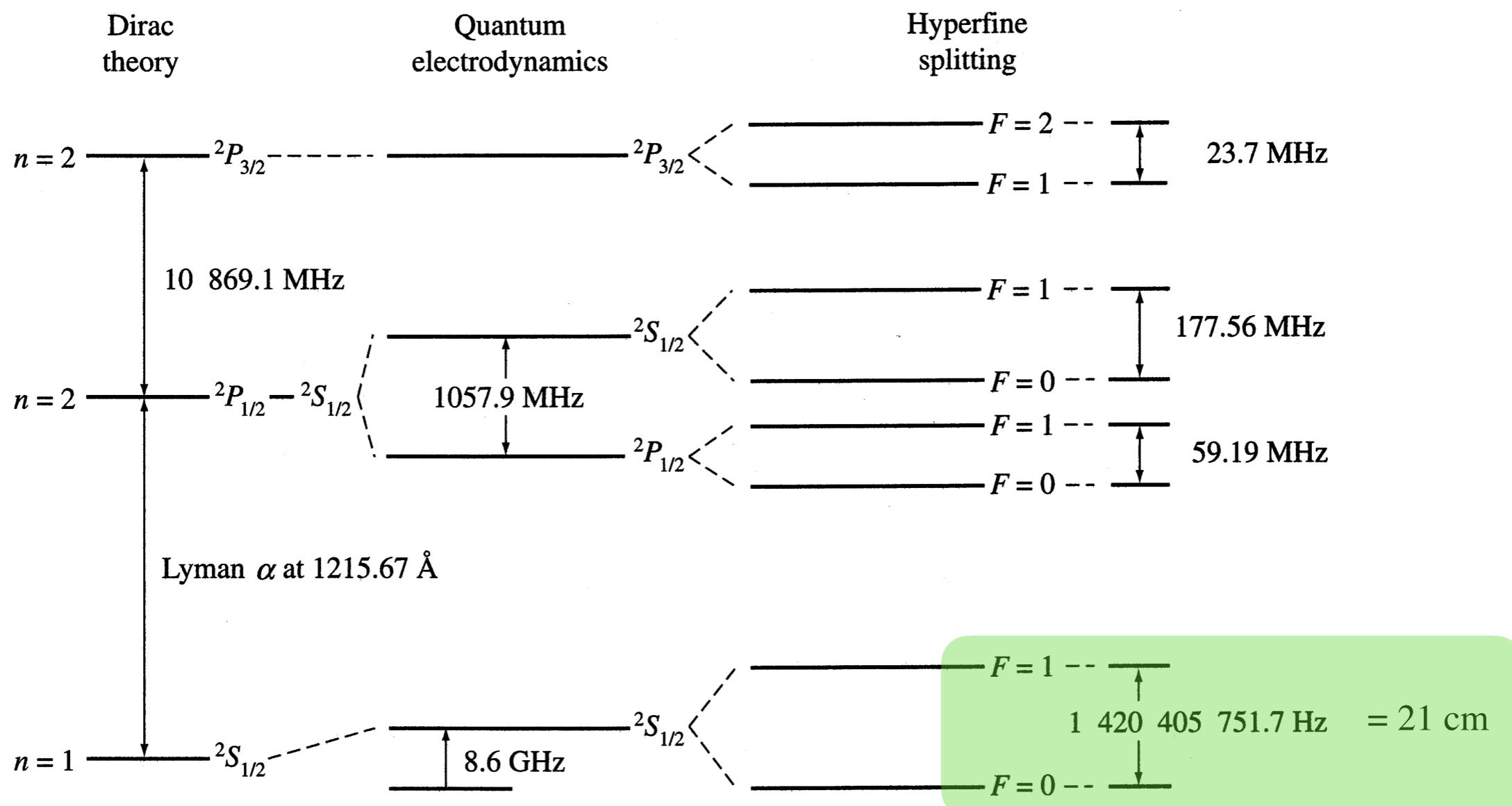


Hydrogen Atom : Hyperfine Structure

- 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

$\Delta l = \pm 1$

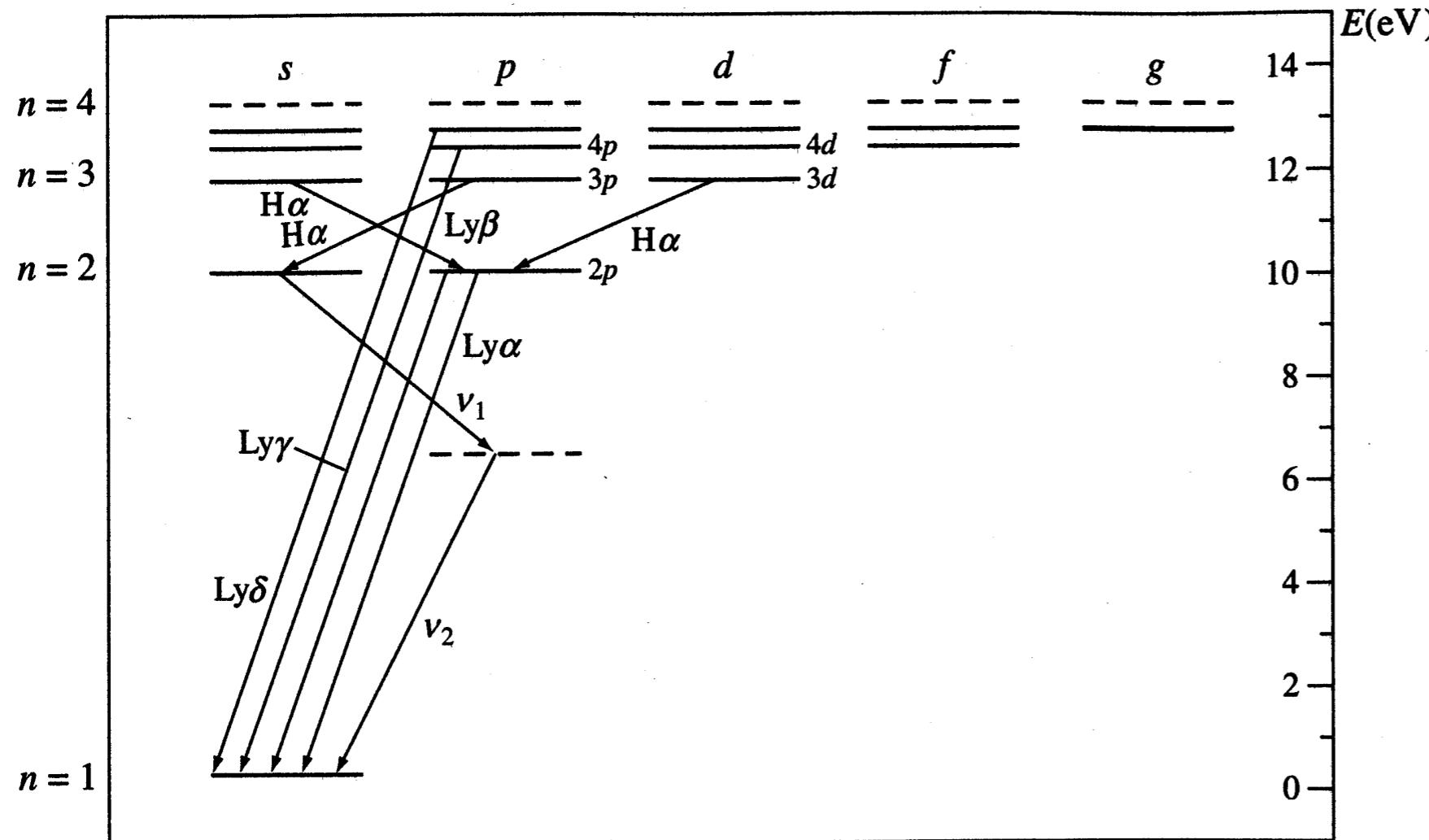
$\Delta S = 0$  For H atom, this is always satisfied as $S = 1/2$ for all states.

$\Delta L = 0, \pm 1$ (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 $H\alpha$ transitions:



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

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

$- 3p_{3/2}$ is allowed;

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

$- 3s_{1/2}$ is allowed;

$- 3d_{3/2}$ is allowed;

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

$- 3d_{3/2}$ is allowed;

$- 3d_{5/2}$ is allowed .

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

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

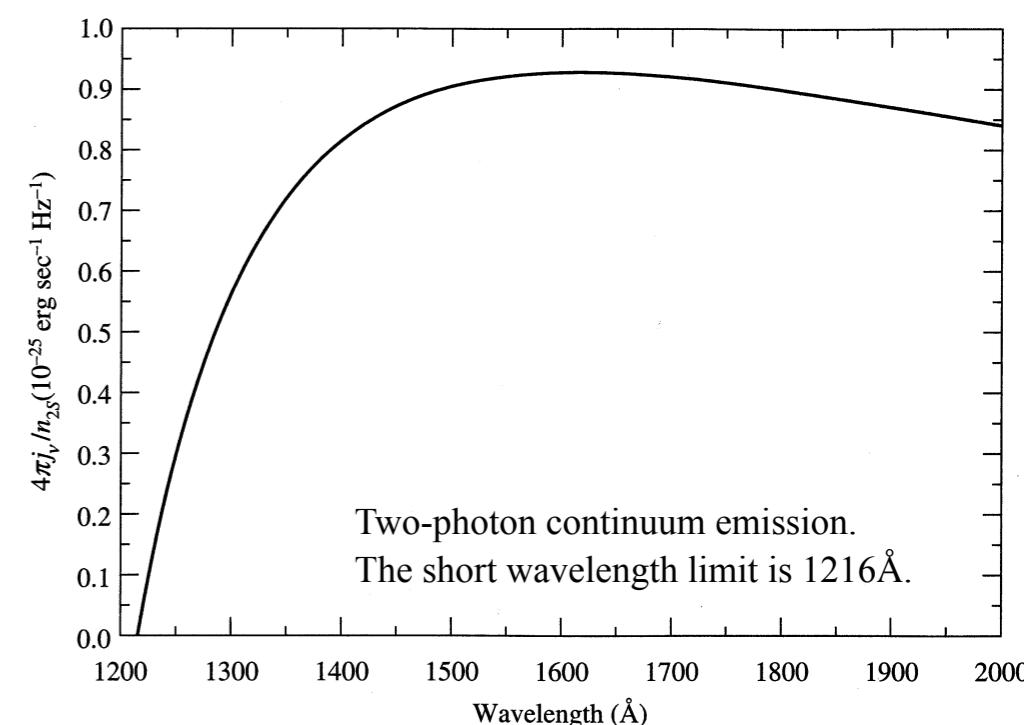
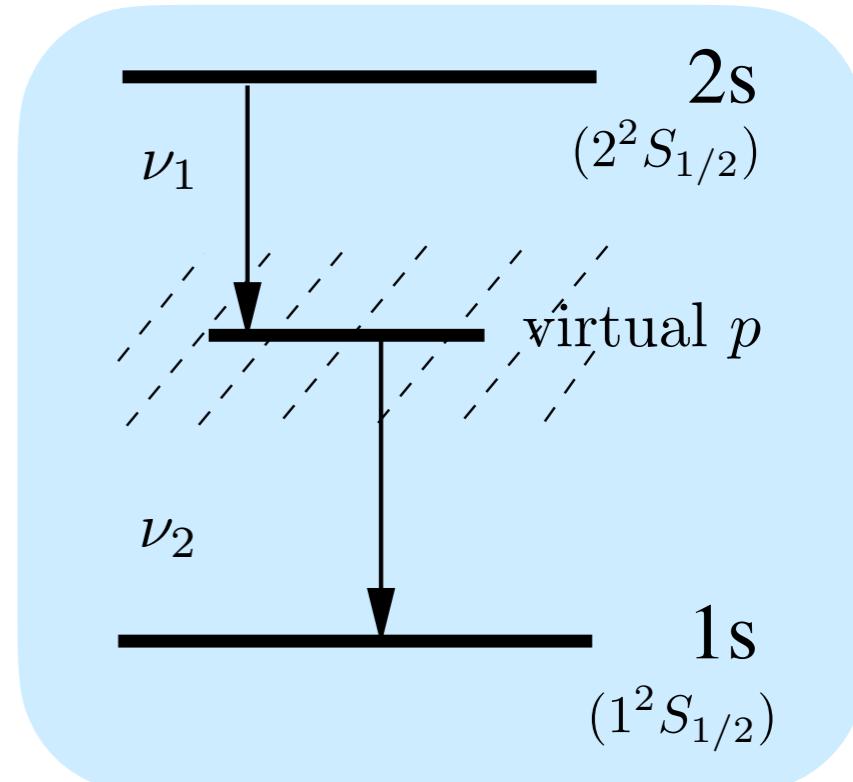
$$\tau_i = \left(\sum_j A_{ij} \right)^{-1} \quad \text{where } A_{ij} \text{ is the Einstein A coefficient}$$

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 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.
- 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 .

S	L	J
0	0	0

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

- (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
1	0	1

$$\begin{aligned} {}^1S &\rightarrow {}^1S_0 \\ {}^3S &\rightarrow {}^3S_1 \end{aligned}$$

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.

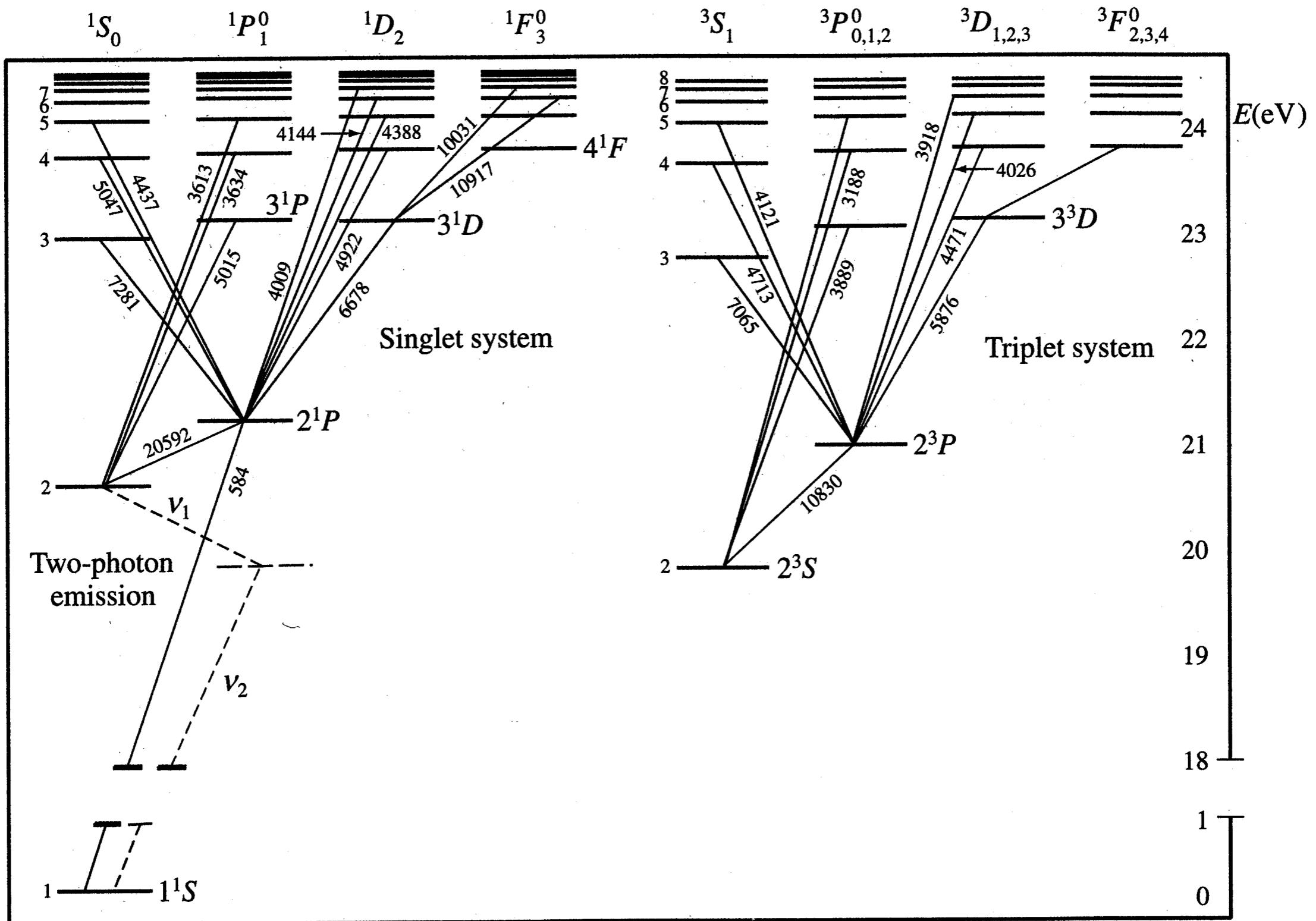
This has $l_1 = 0$ and $l_2 = 1$, giving $L = 1$; again $s_1 = s_2 = \frac{1}{2}$, giving both $S = 0$ and $S = 1$ terms.

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

$$\begin{aligned} {}^1P^o &\rightarrow {}^1P_1^o \\ {}^3P^o &\rightarrow {}^3P_0^o < {}^3P_1^o < {}^3P_2^o \end{aligned}$$

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 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.

$$S = 0, 1, \quad L = 0, 1, 2 \quad \rightarrow \quad ^1S, ^1P, ^1D, ^3S, ^3P, ^3D$$

→ 6 spectroscopic terms

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

→ 10 spectroscopic levels

We can have $(2J+1)$ states for each J value.

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.

(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. |

Example: Helium

- (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 .

S	L	J
0	0	0

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

- (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
1	0	1

$$\begin{aligned} {}^1S &\rightarrow {}^1S_0 \\ {}^3S &\rightarrow {}^3S_1 \end{aligned}$$

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

$$\begin{aligned} {}^1P^o &\rightarrow {}^1P_1^o \\ {}^3P^o &\rightarrow {}^3P_0^o < {}^3P_1^o < {}^3P_2^o \end{aligned}$$

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

Example : 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

(Example) 4p4d electron configuration

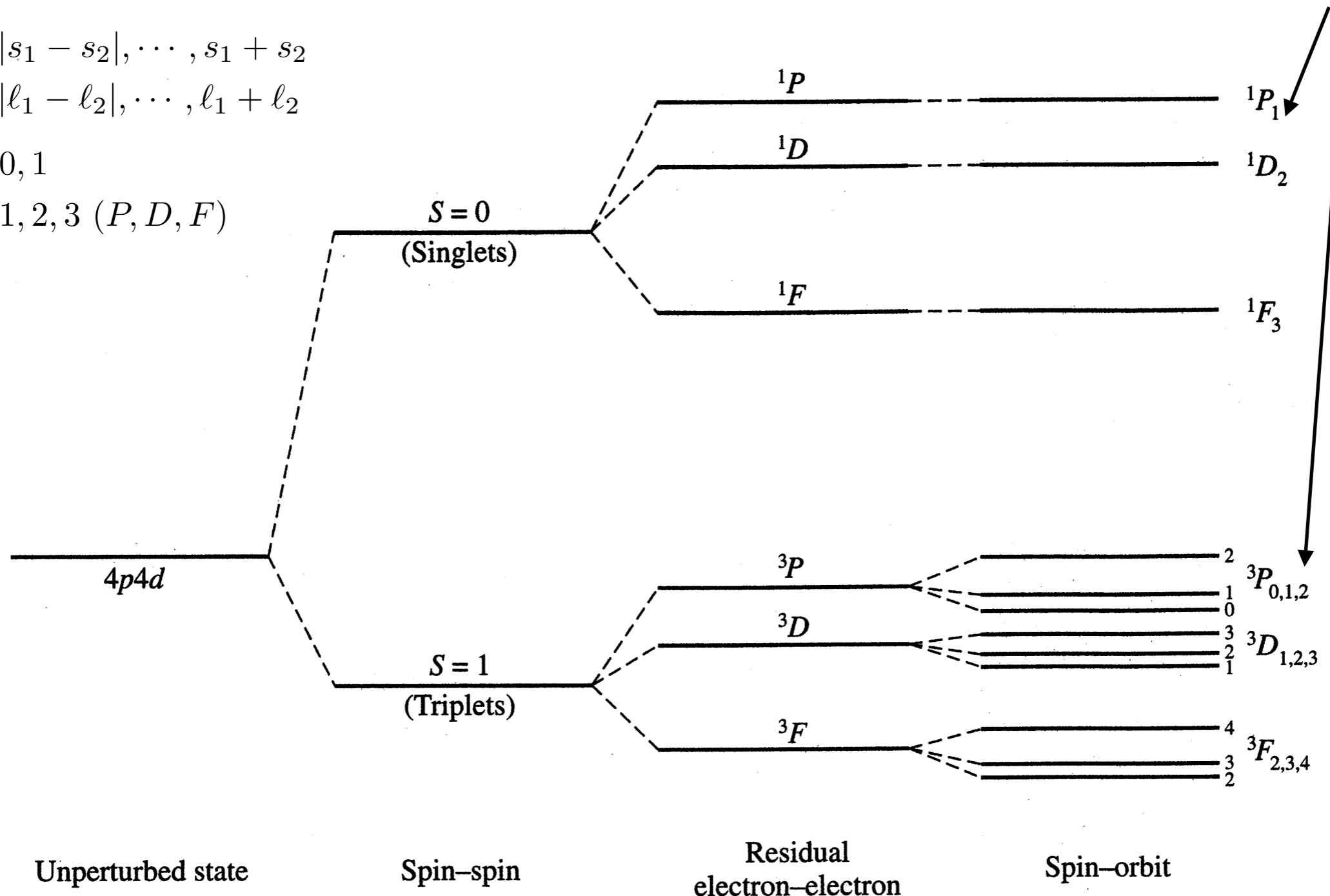
$$J = |L - S|, \dots, L + S$$

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

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

$$S = 0, 1$$

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



Example npn'p

(Example) $nnp'n'p$ electron configuration

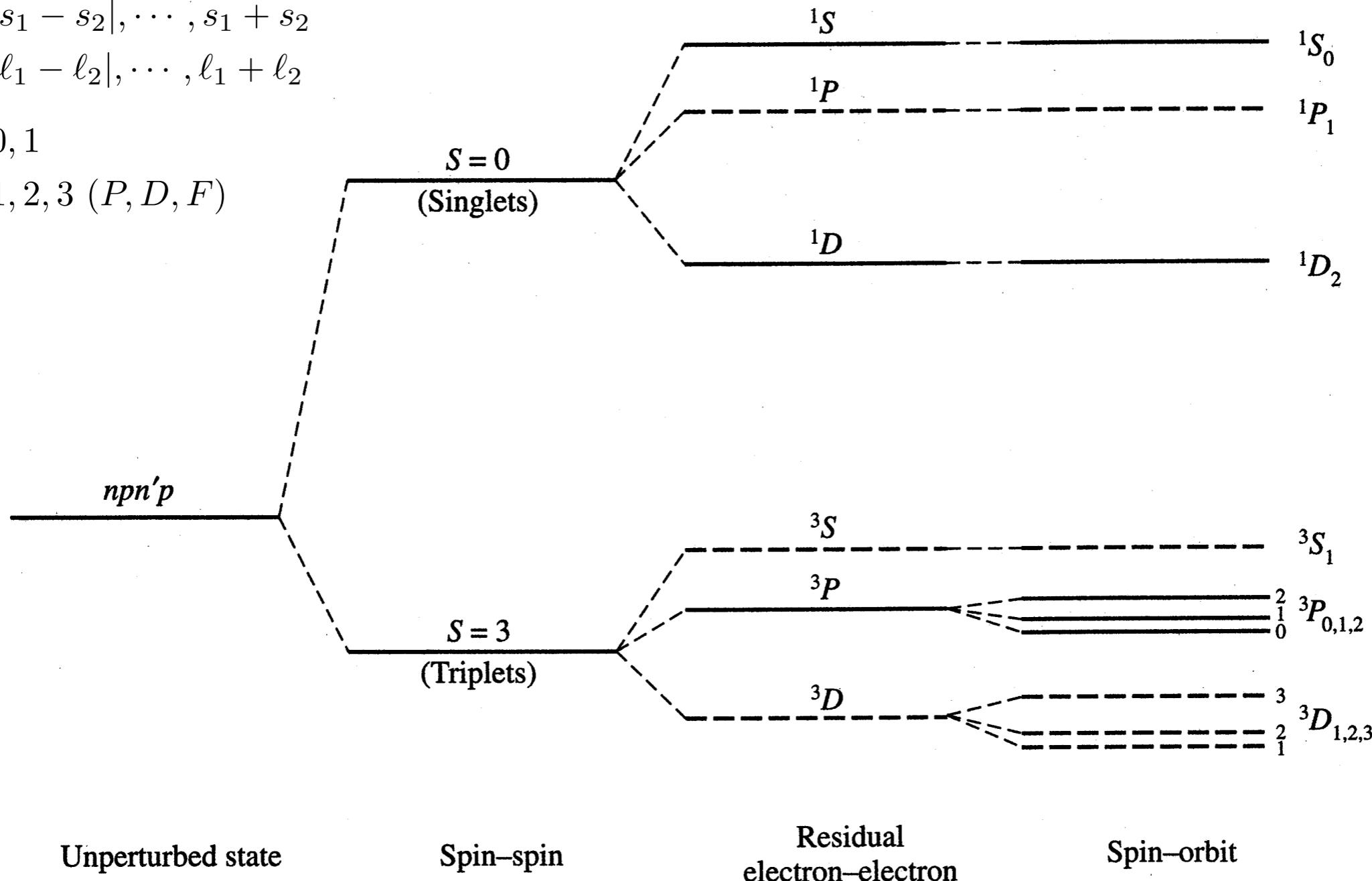
The dashed levels are missing if the two electrons are equivalent ($n = n'$)

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

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

$$S = 0, 1$$

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



[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.

[Draine, Physics of the ISM and IGM]

Table 4.1 Terms for ns and np Subshells

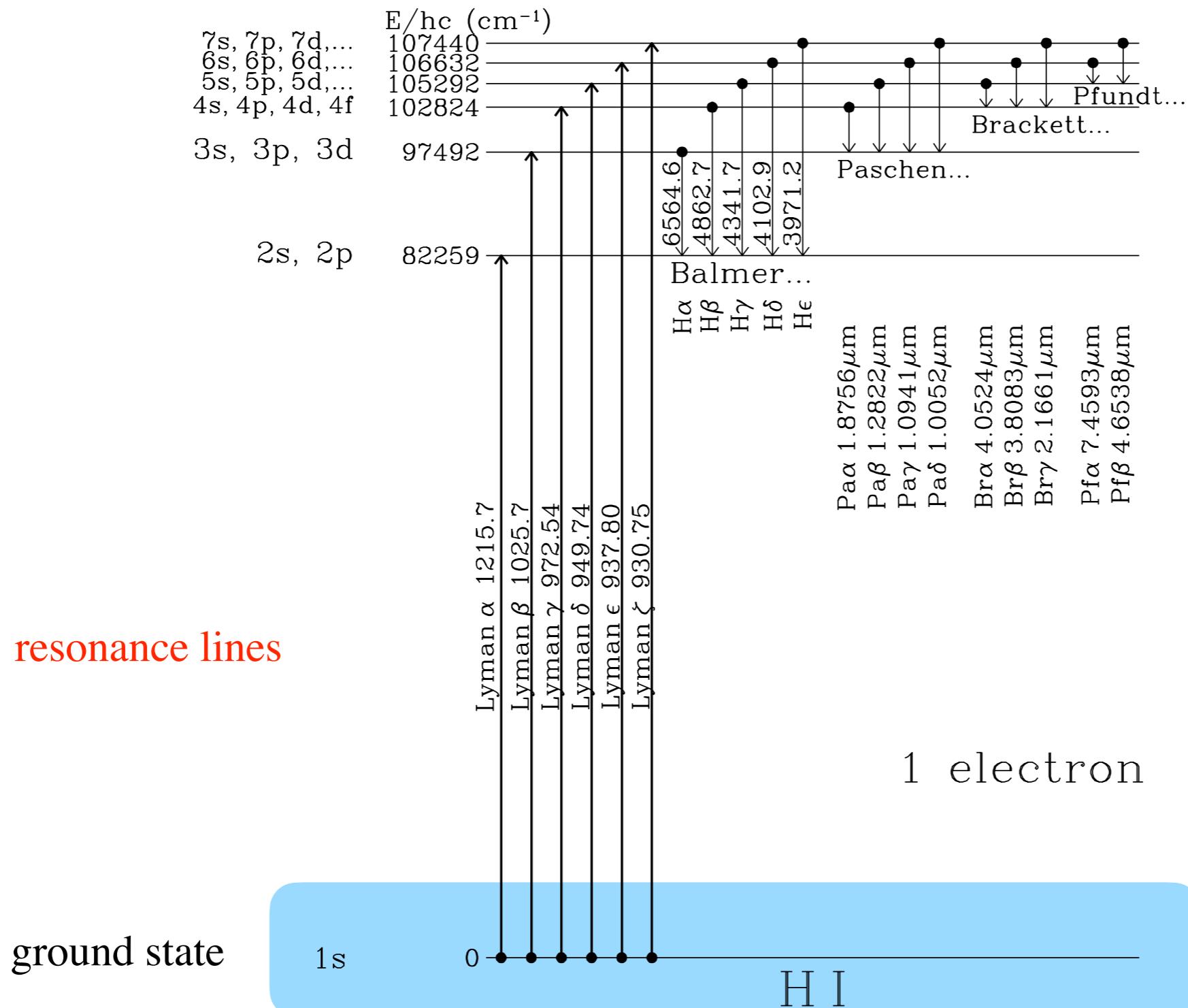
Ground configuration	Terms (in order of increasing energy)	Examples
$\dots ns^1$	$^2S_{1/2}$	HI, He II, C IV, N V, O VI
$\dots ns^2$	1S_0	He I, C III, N IV, O V
$\dots np^1$	$^2P_{1/2,3/2}^o$	C II, N III, O IV
$\dots np^2$	$^3P_{0,1,2}, ^1D_2, ^1S_0$	CI, N II, O III, Ne V, S III
$\dots np^3$	$^4S_{3/2}^o,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

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	1	$^2S_{1/2}$
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.

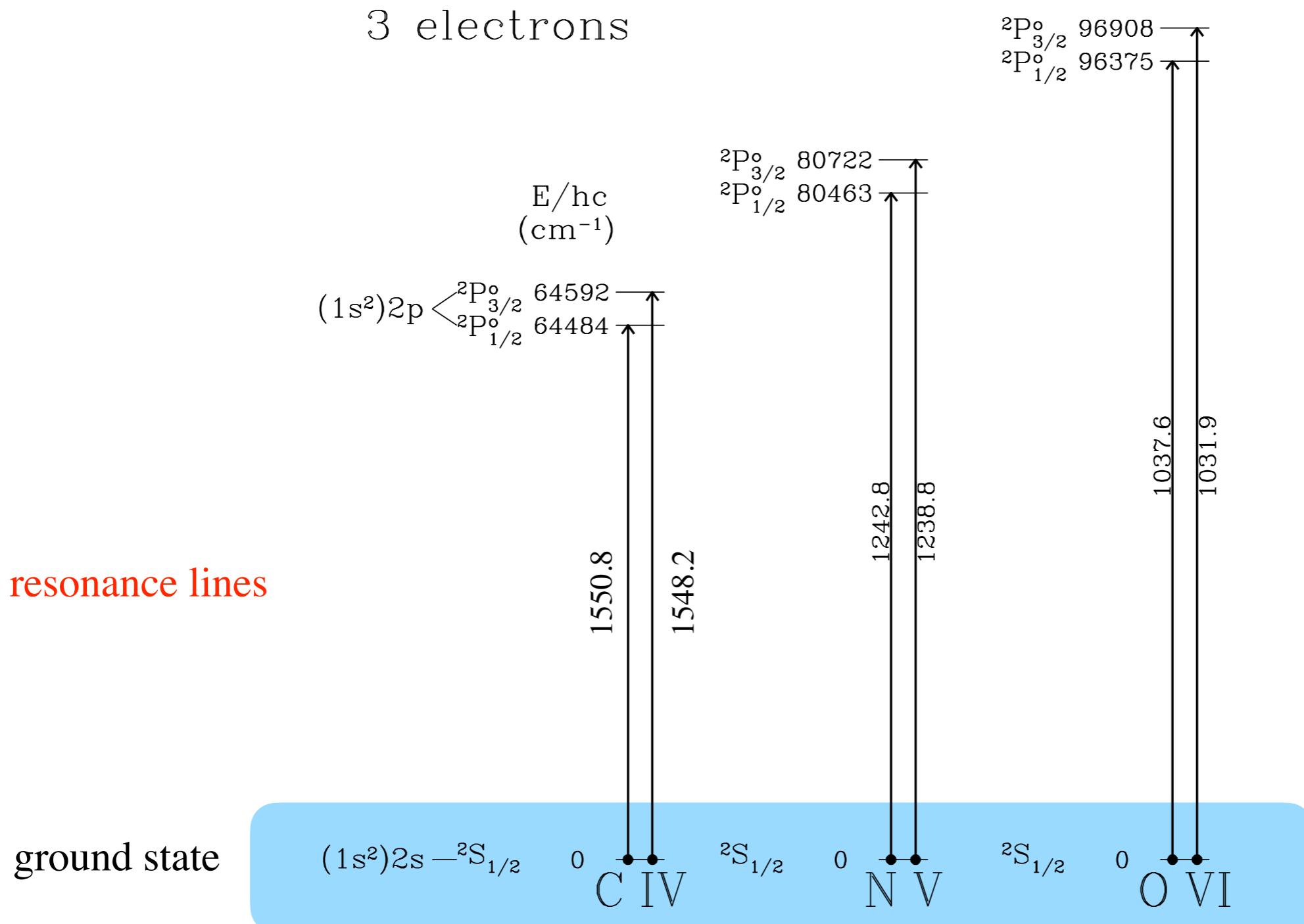
[Energy Level Diagrams]

- 1 electron



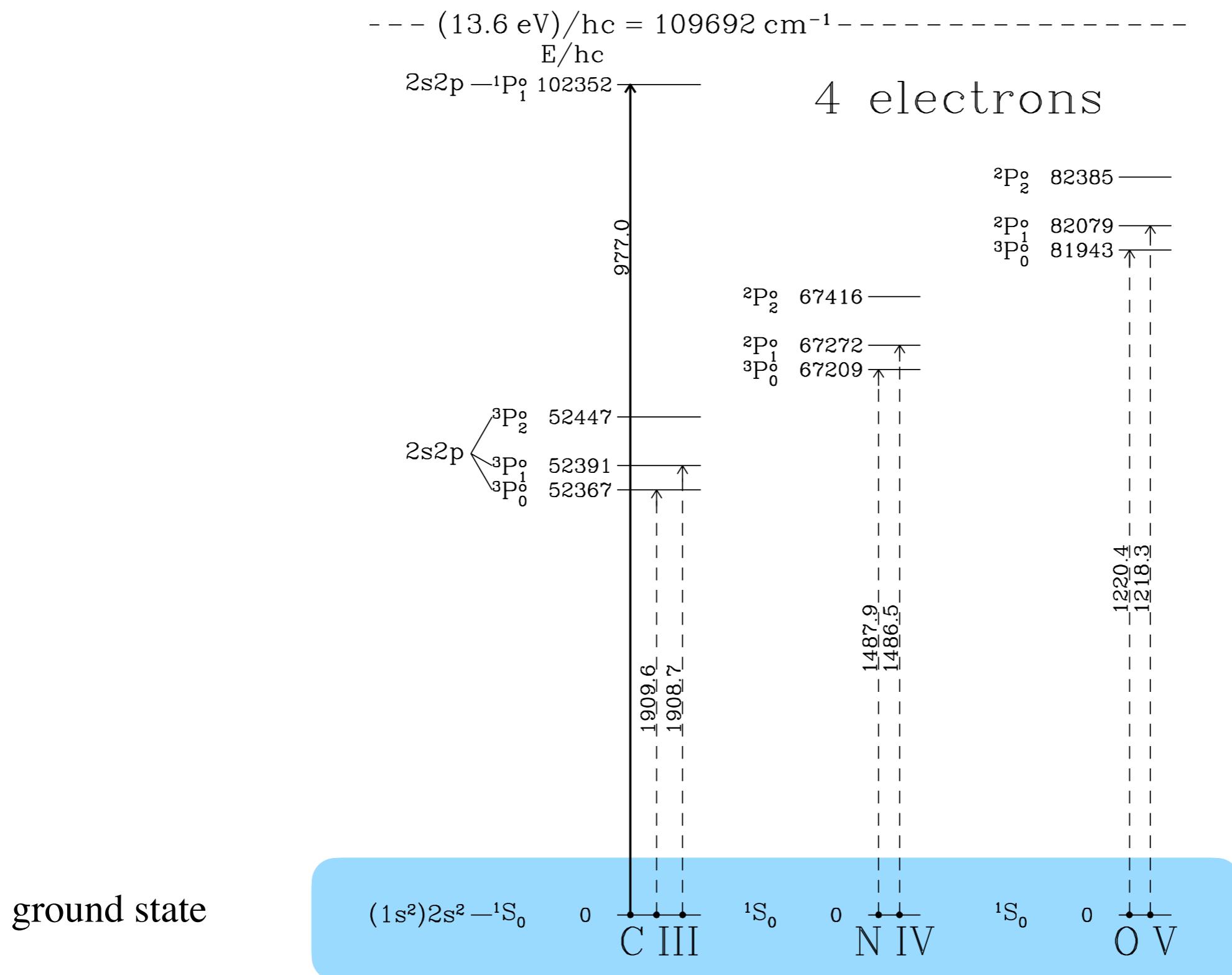
- 3 electrons (Lithium-like ions)

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



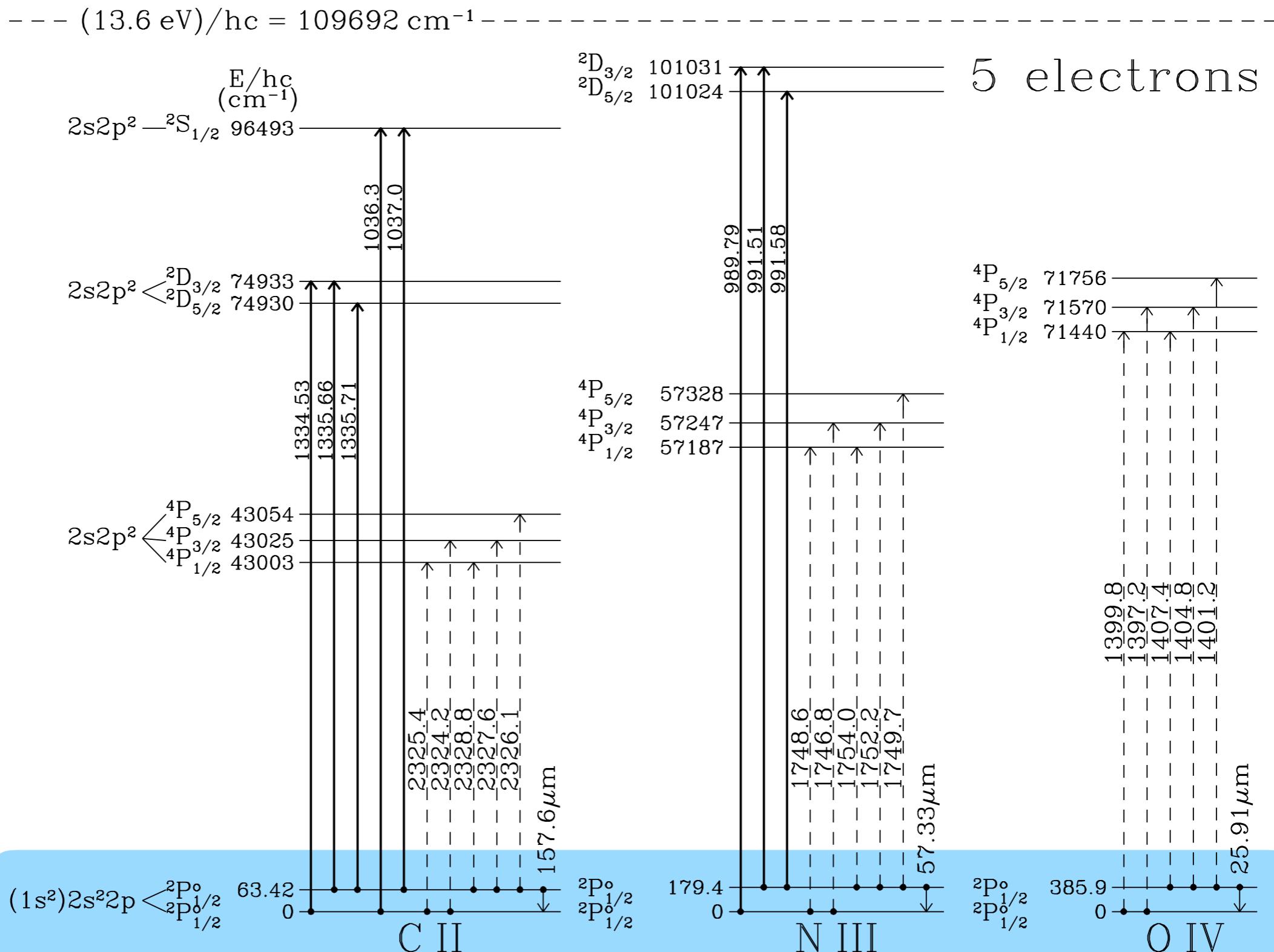
- 4 electrons

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



- 5 electrons

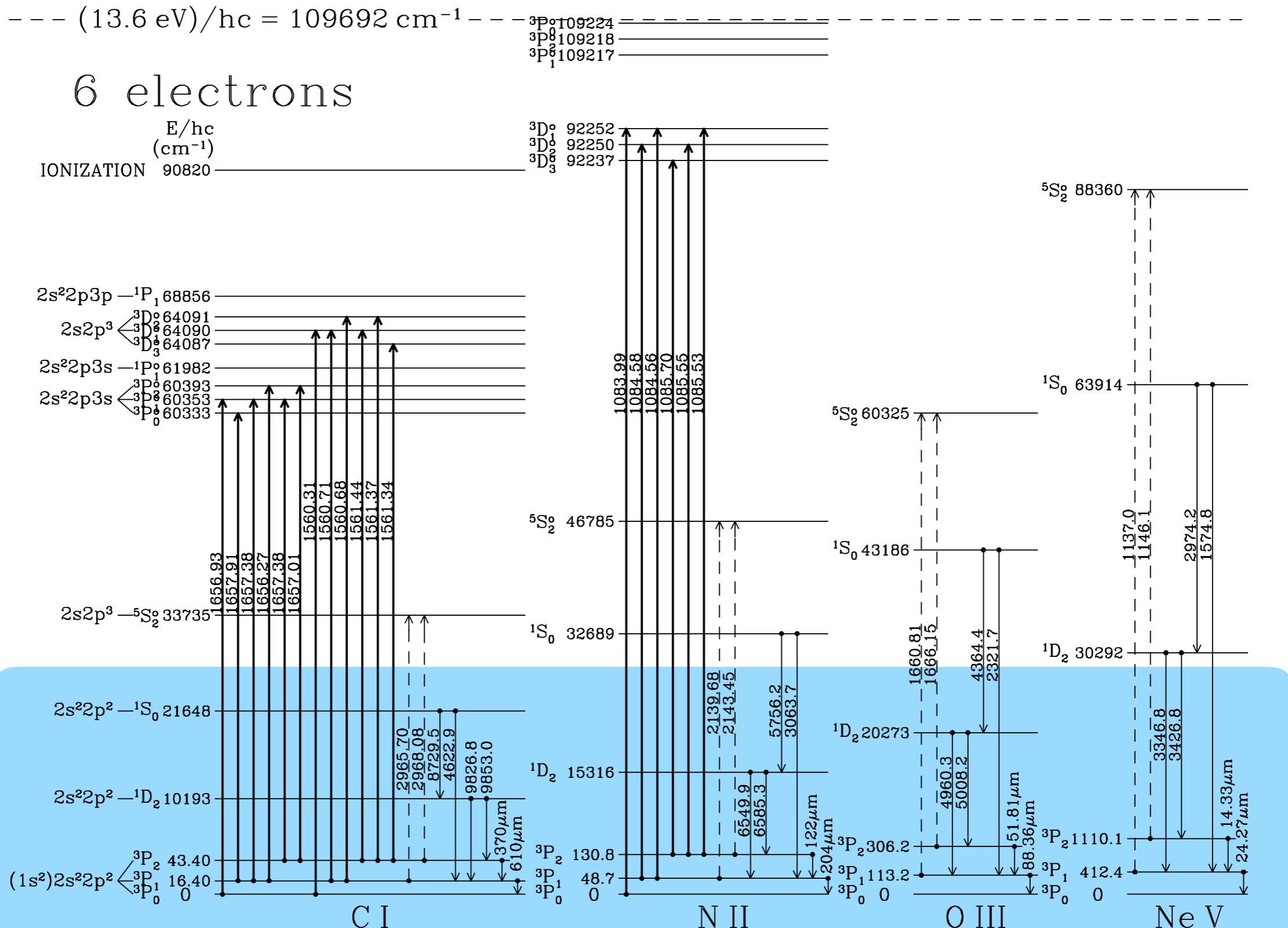
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



forbidden
lines

- 6 electrons

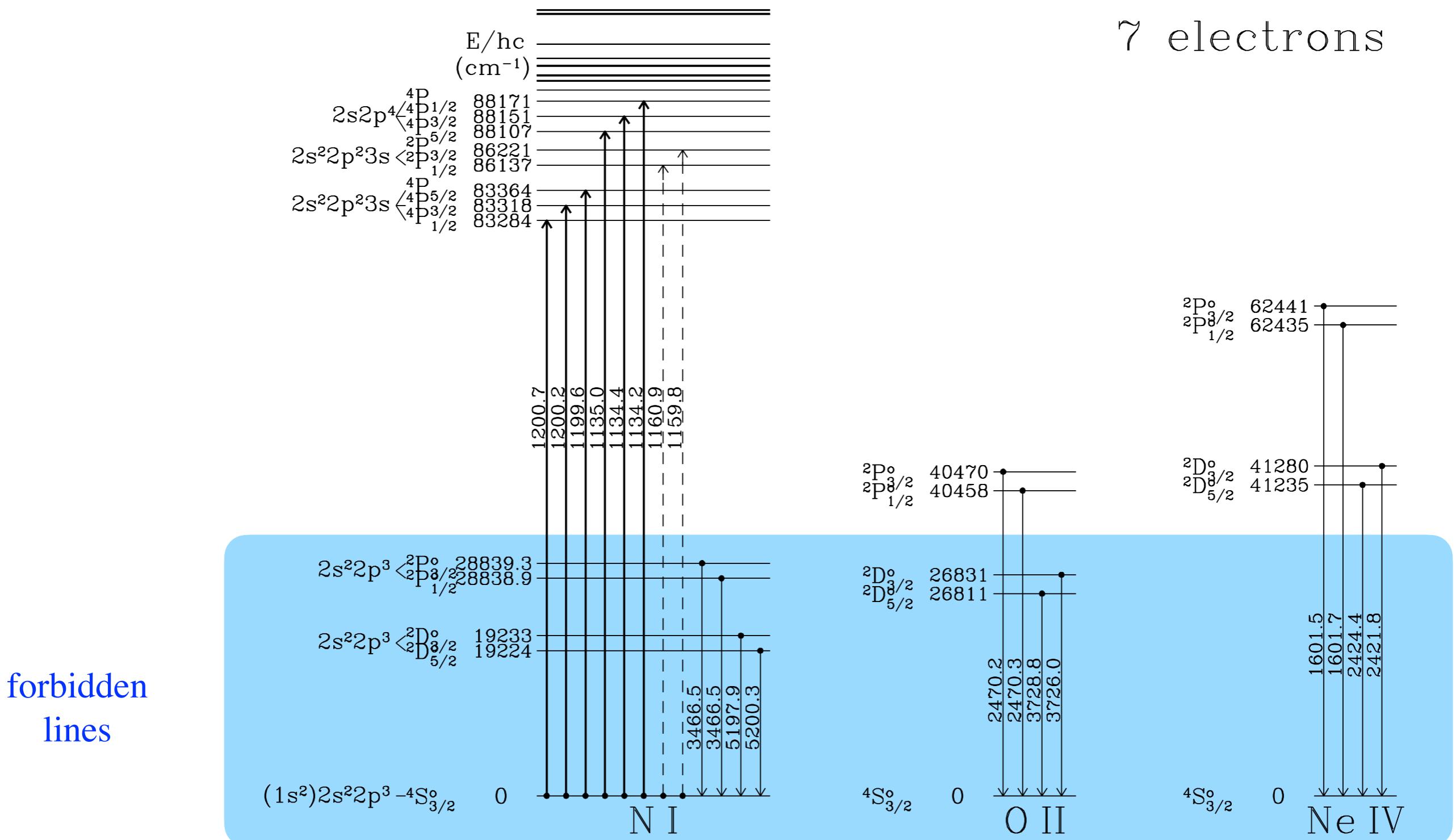
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



- 7 electrons

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

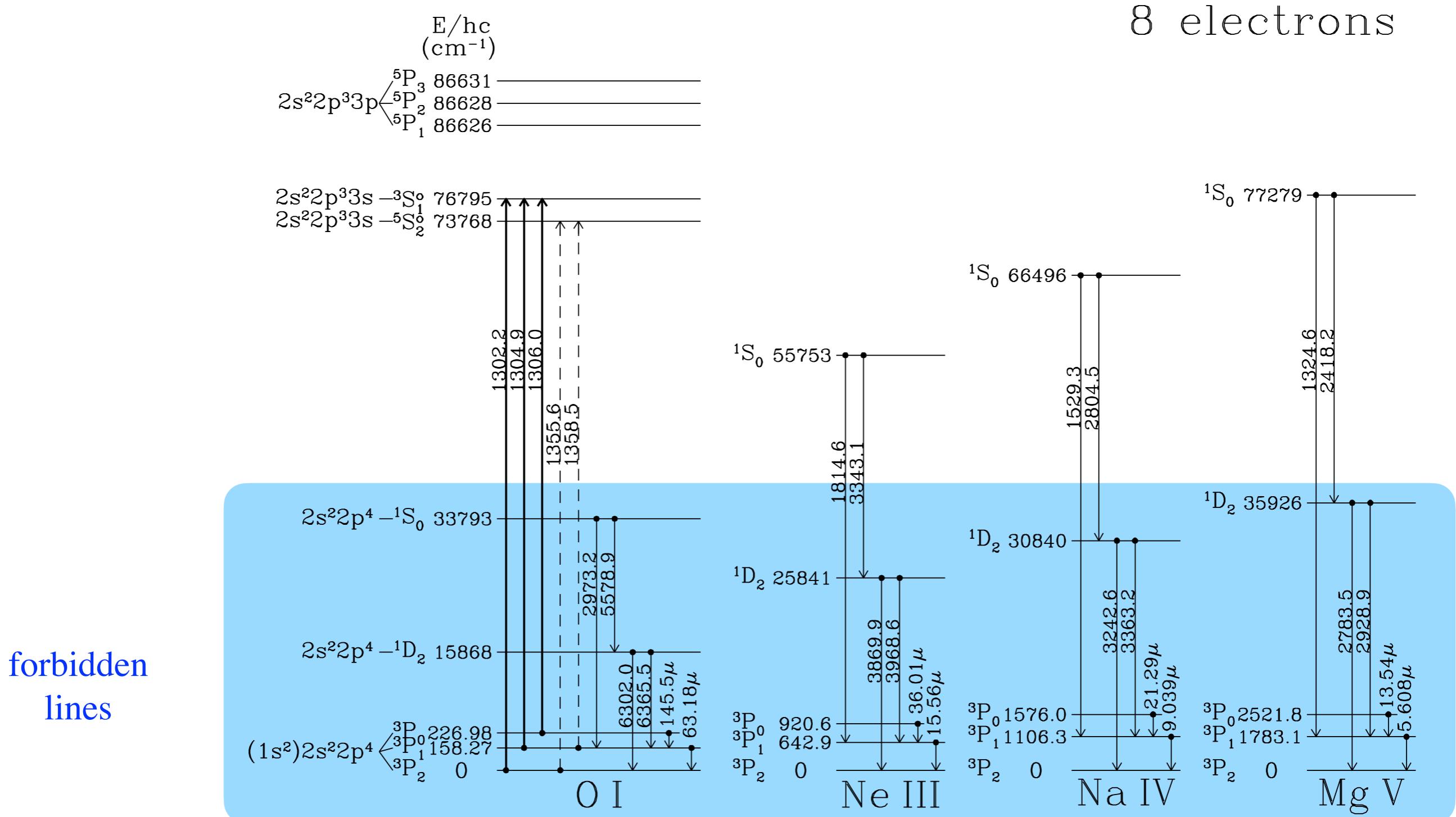
$$\text{---} (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{---} \text{---} \text{---}$$



- 8 electrons

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

--- (13.6 eV)/hc = 109692 cm⁻¹ -----



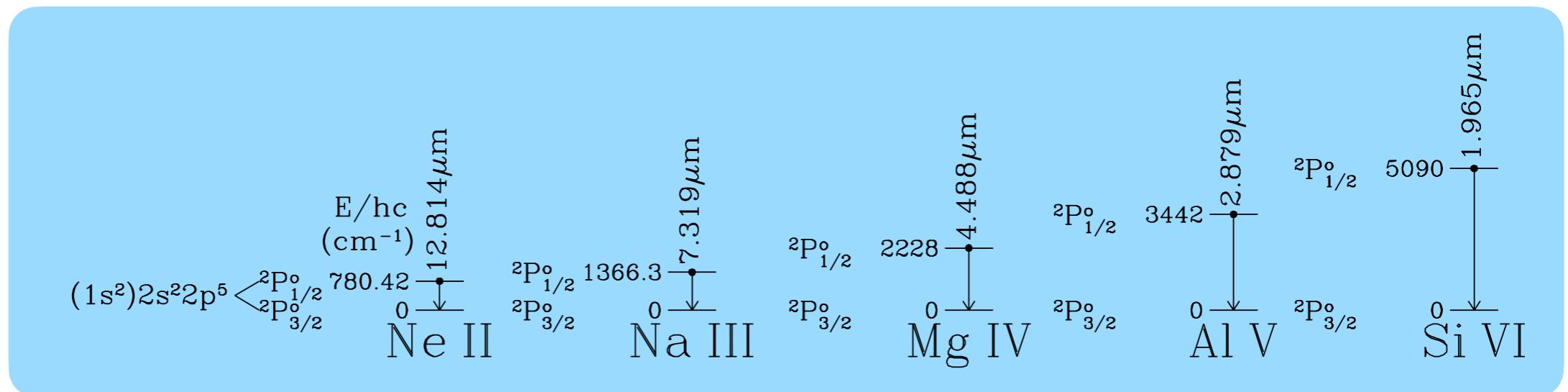
- 9 electrons

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

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

9 electrons

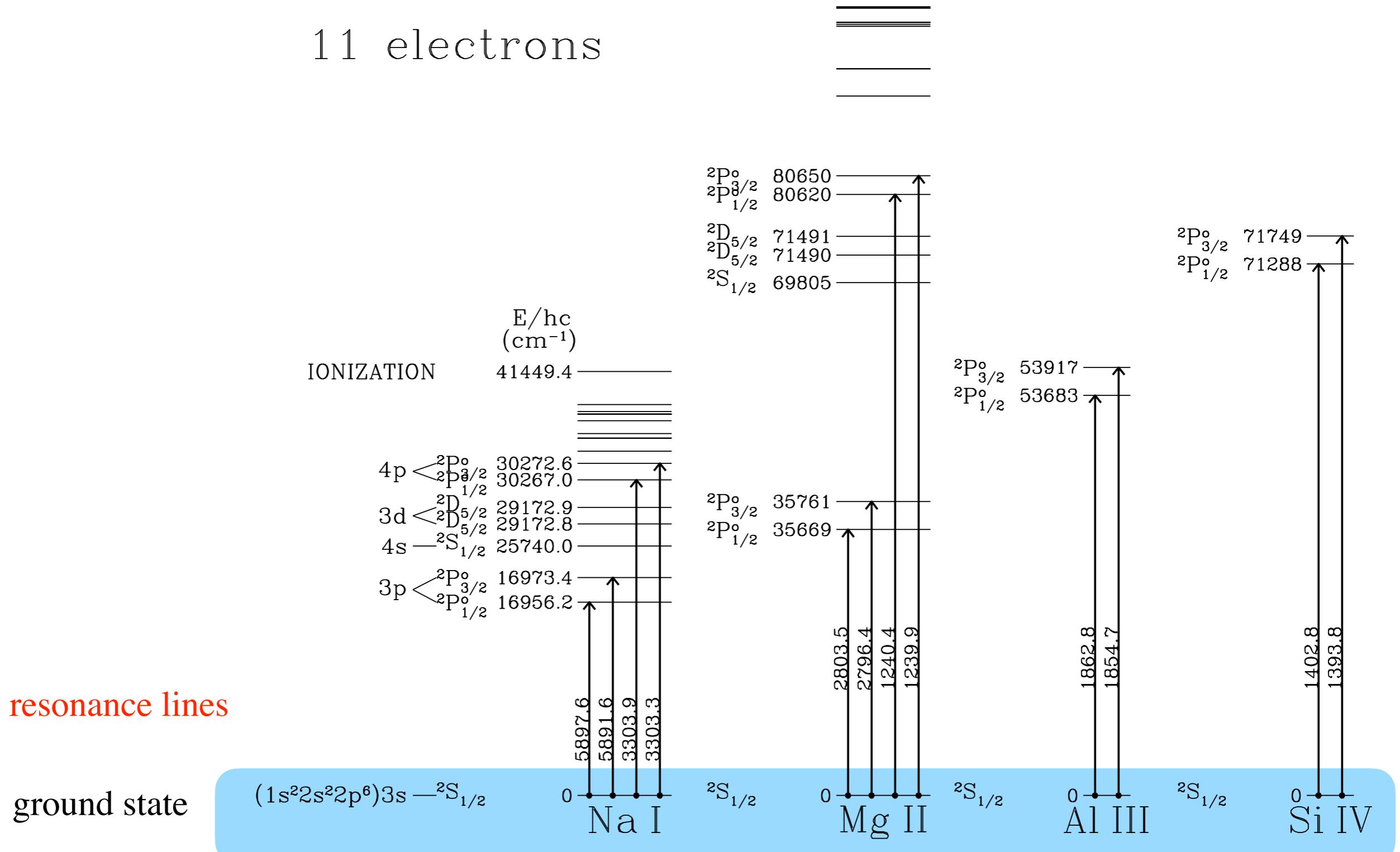
forbidden
lines



- 11 electrons

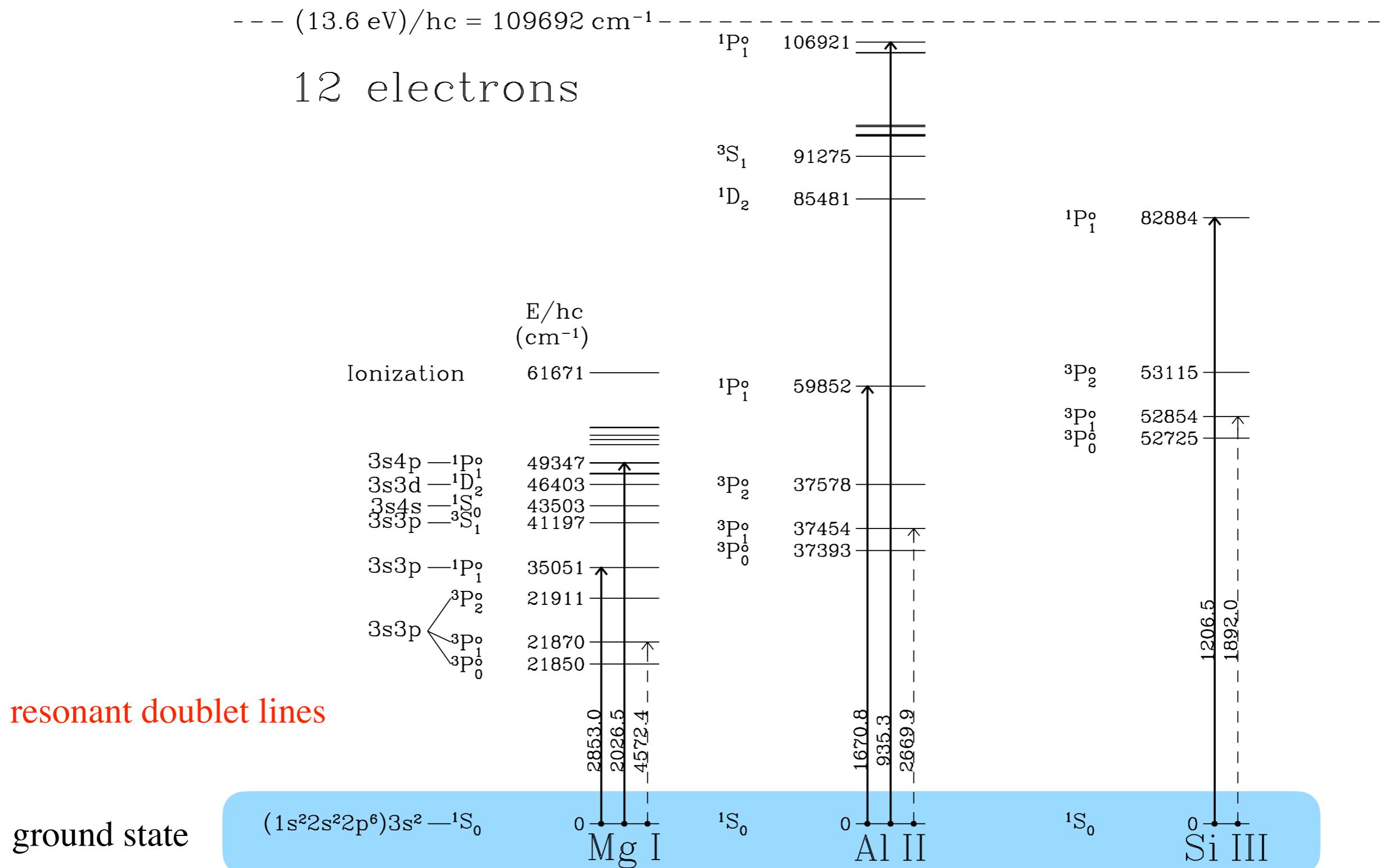
$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{ --- }$$

11 electrons



- 12 electrons

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

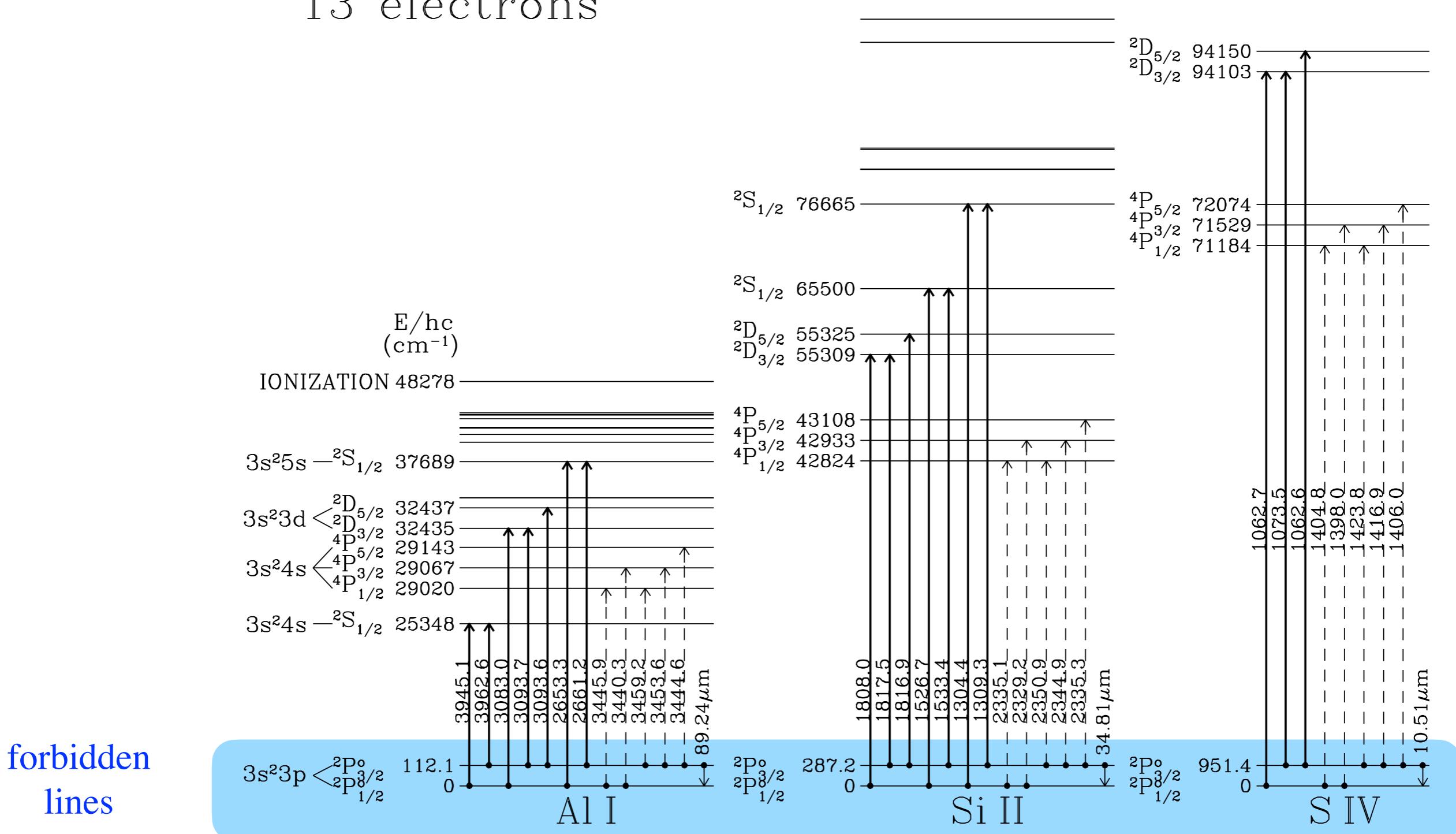


- 13 electrons

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

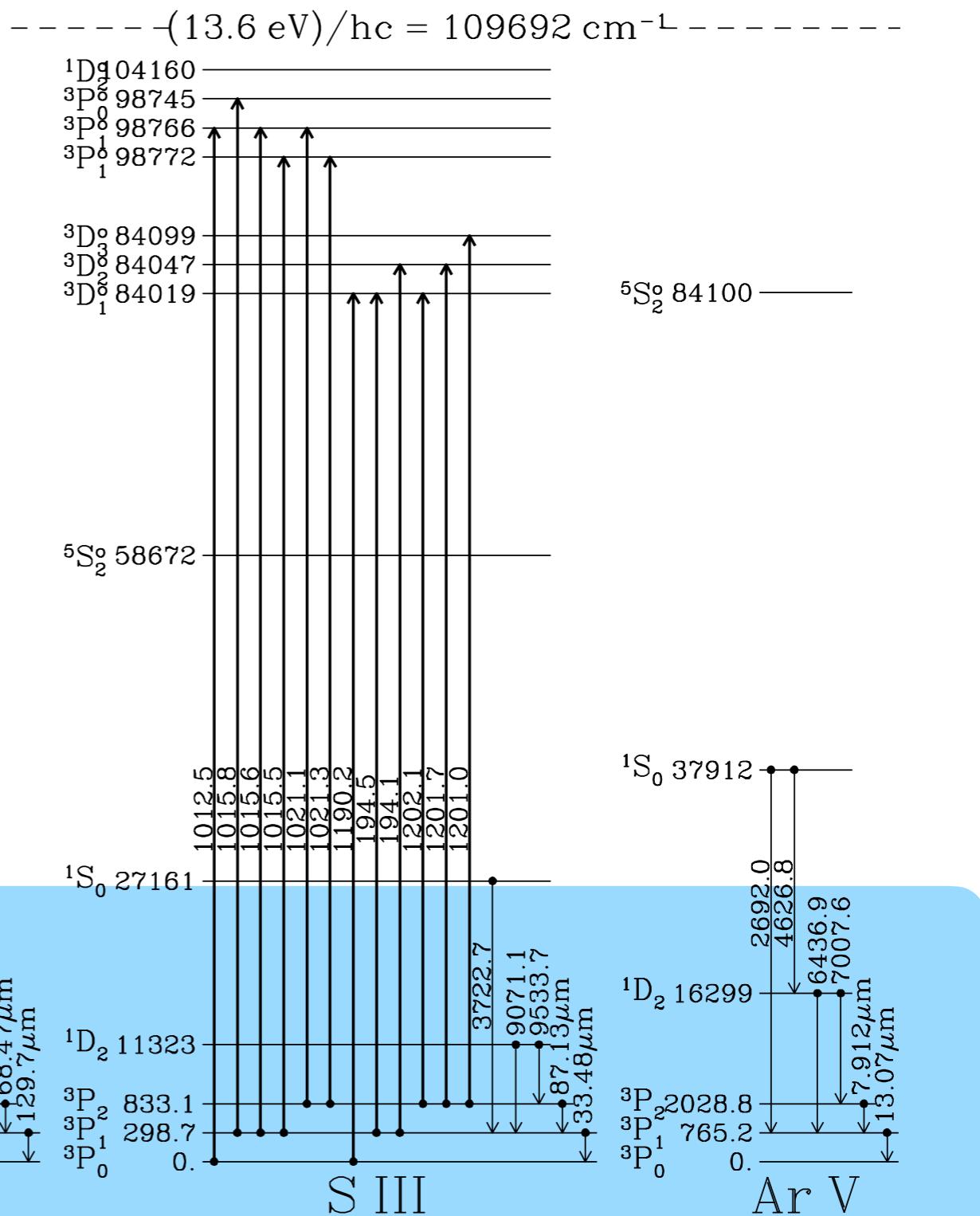
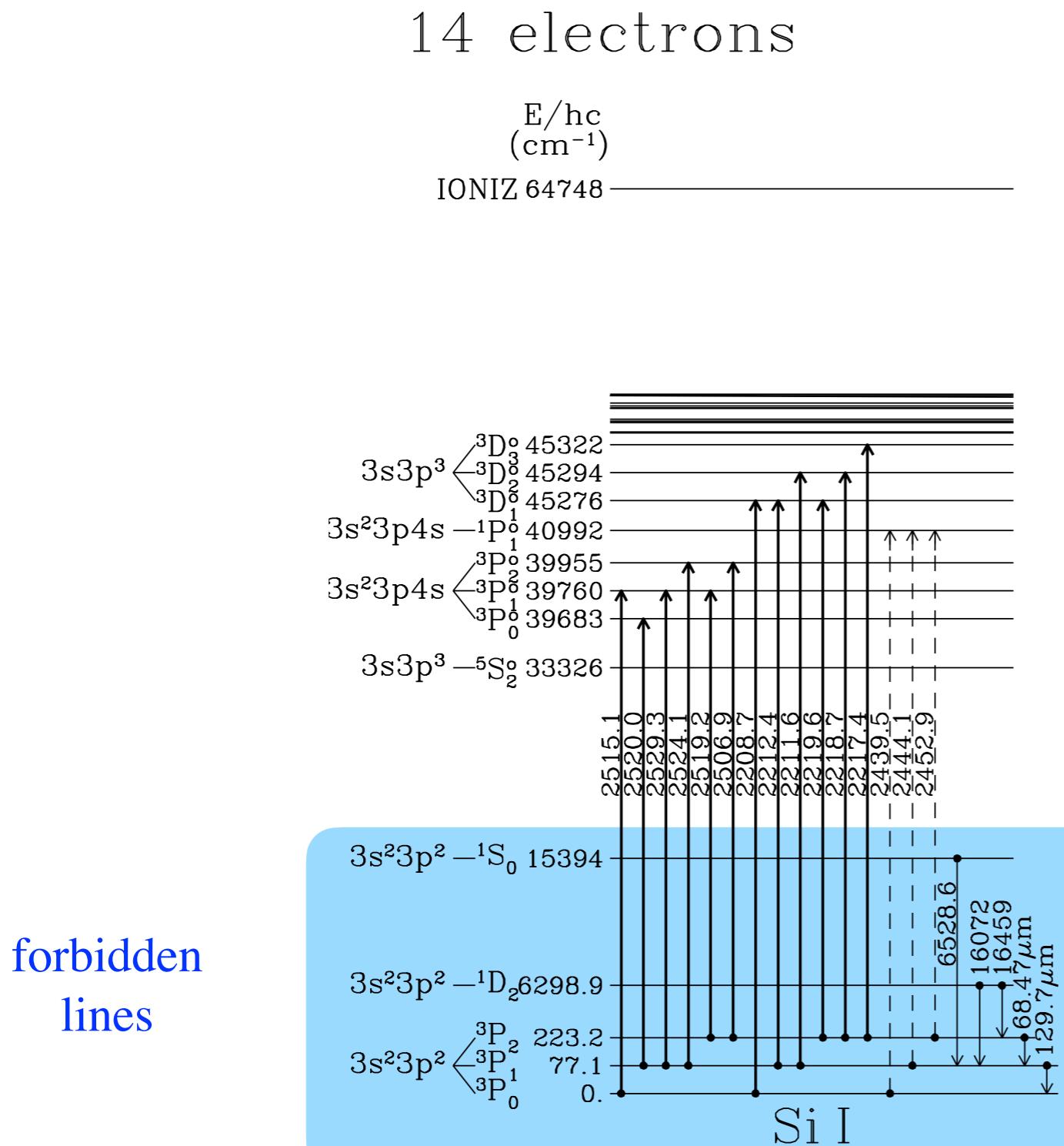
$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1}$$

13 electrons



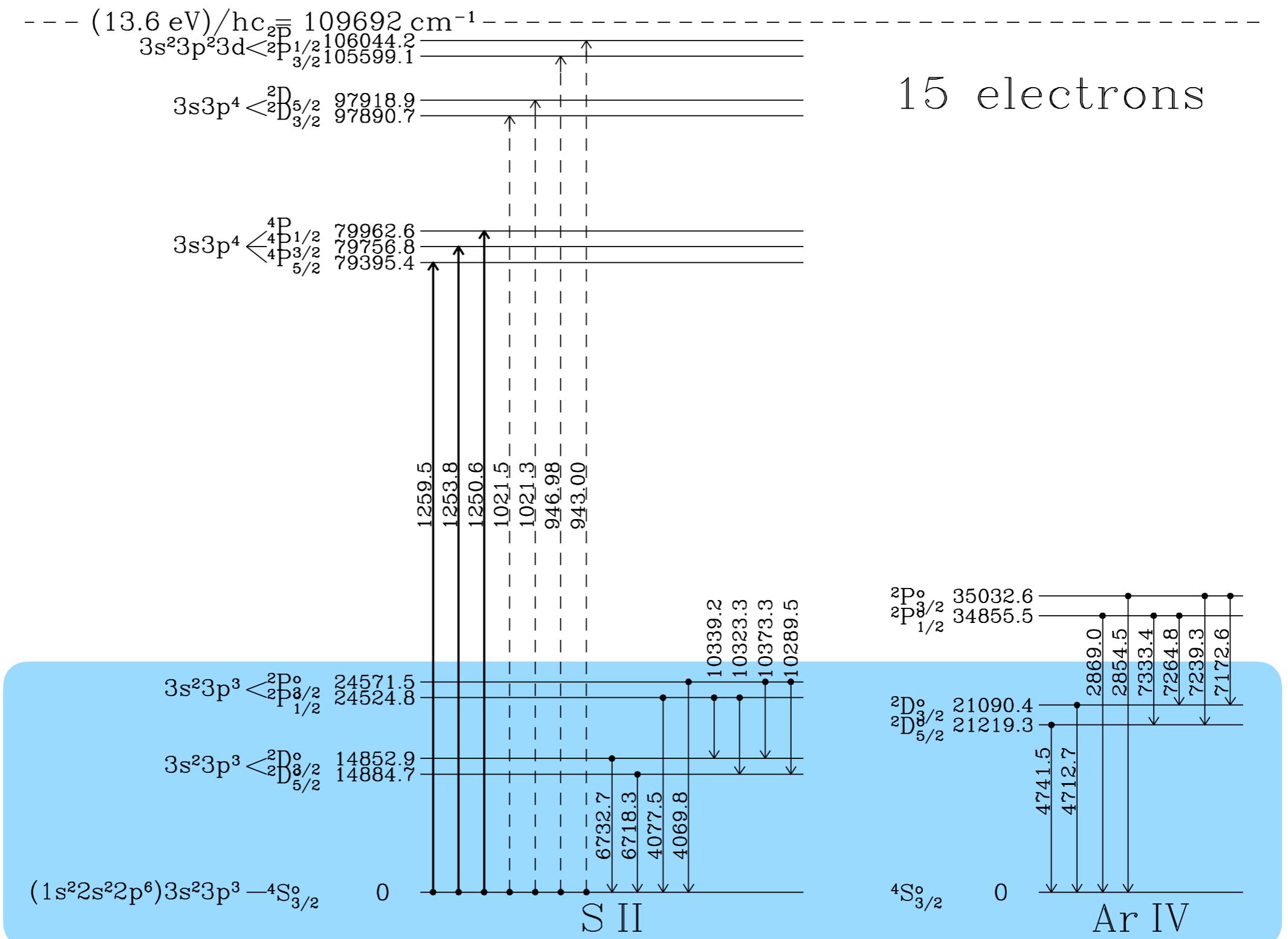
- 14 electrons

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



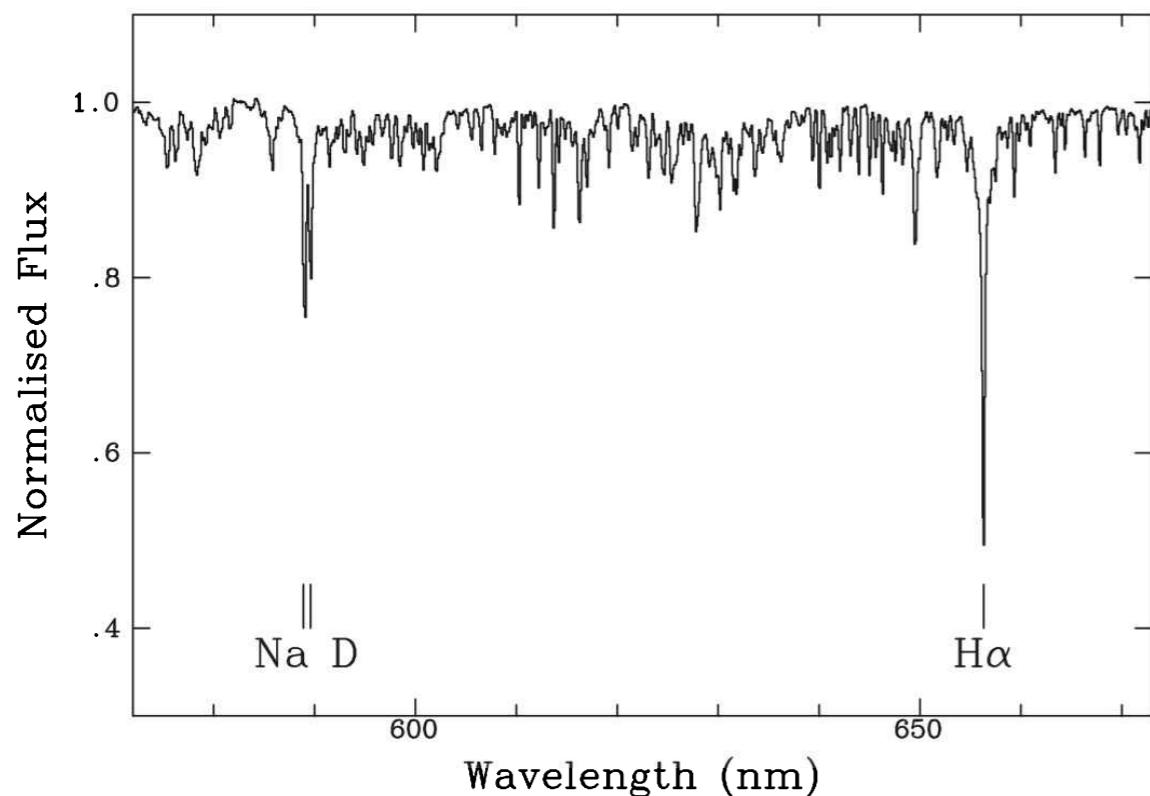
- 15 electrons

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

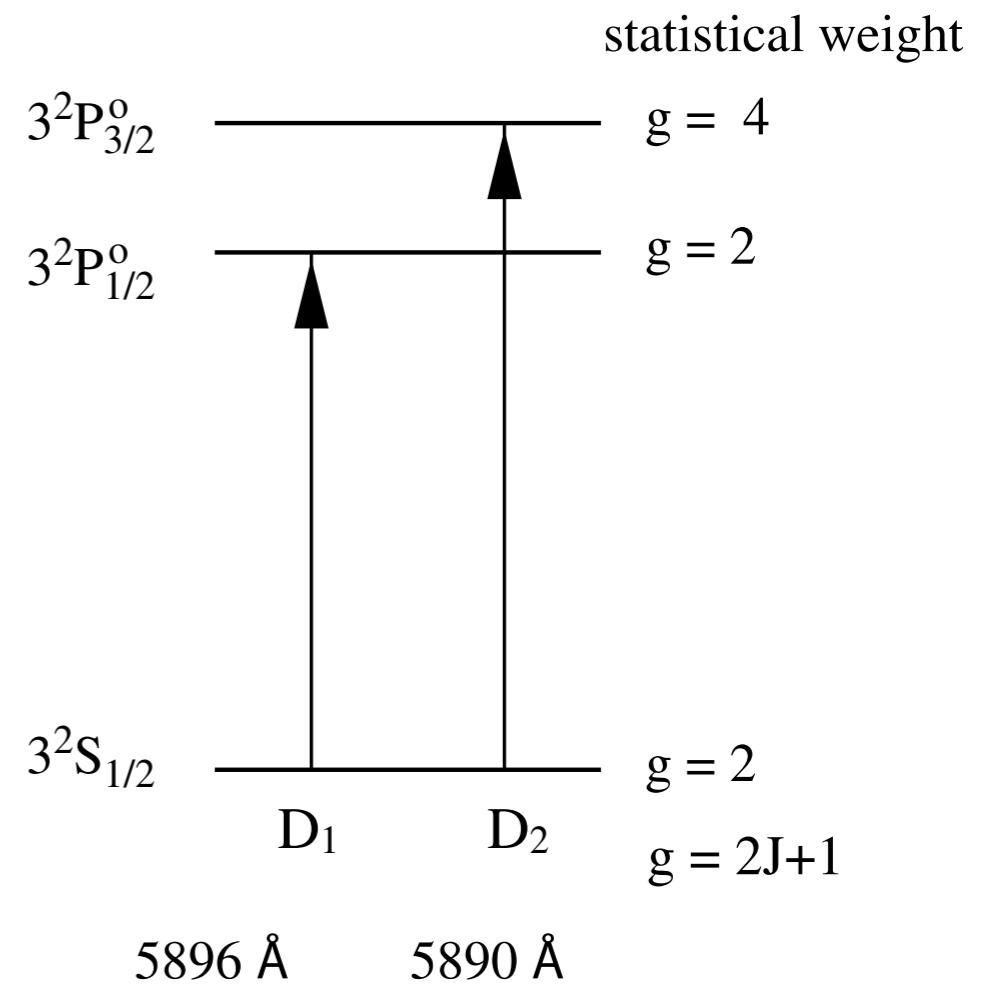


[Alkali Atoms]

- 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 a ground state configuration of $1s^2 2s^2 2p^6 3s^1$.



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:

$$\begin{aligned} D_1 \text{ } 5896 \text{ } \text{\AA} \text{ line} &: 3^2S_{1/2} - 3^2P_{1/2} \\ D_2 \text{ } 5890 \text{ } \text{\AA} \text{ line} &: 3^2S_{1/2} - 3^2P_{3/2} \end{aligned}$$

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

[Zeeman Effect]

- **Zeeman effect**

the splitting of atomic energy levels in the presence of an external magnetic field.

- **Zeeman effect at 1420MHz**

The upper level of the 1420 MHz hyperfine transition of hydrogen is the $F = 1$ state. Its angular momentum has three possible projections onto a given axis. The three states are

$$F_z = m_F \hbar \quad (m_F = -1, 0, +1)$$

The three states have the same energy (i.e., they are degenerate), but if the atoms are immersed in an external magnetic field, the three states take on different energies. This is a consequence of the interaction of the magnetic moment of the hydrogen atom with the external field.

$$\begin{aligned} E_{\text{pot}} &= -\mu \cdot \mathbf{B} \simeq g_e \frac{e}{2m_e} \mathbf{F} \cdot \mathbf{B} \\ &= g_2 \frac{e\hbar}{2m_e} m_F B \end{aligned}$$

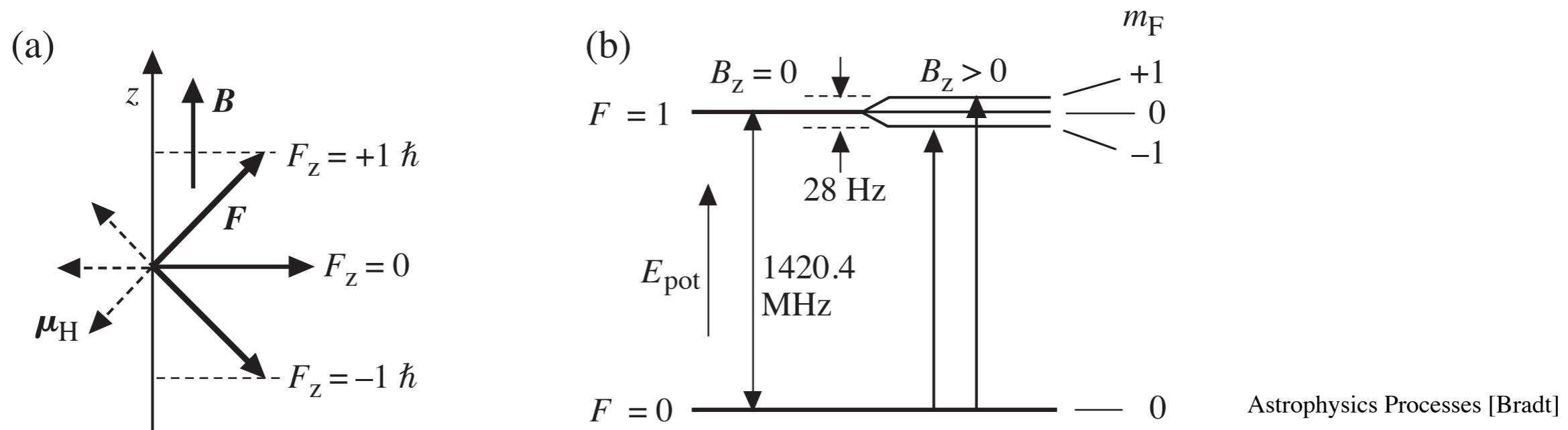
$\mu \simeq \mu_e$ because μ arises almost totally from the electron.

The separation between the +1 and -1 levels is

$$\Delta E_{\text{pot}} = E_{\text{pot}}(m_F = +1) - E_{\text{pot}}(m_F = -1) = g_e \frac{e\hbar}{m_e} B$$

In the $F = 0$ ground state, the total angular momentum is zero. Therefore, the magnetic moment is zero and no Zeeman splitting occurs in the ground state.

Photons carry one unit of angular momentum \mathbf{J} . The allowed transitions are from the $F = 0$ ($m_F = 0$) to the $F = 1$ ($m_F = +1$) or $F = 1$ ($m_F = -1$).

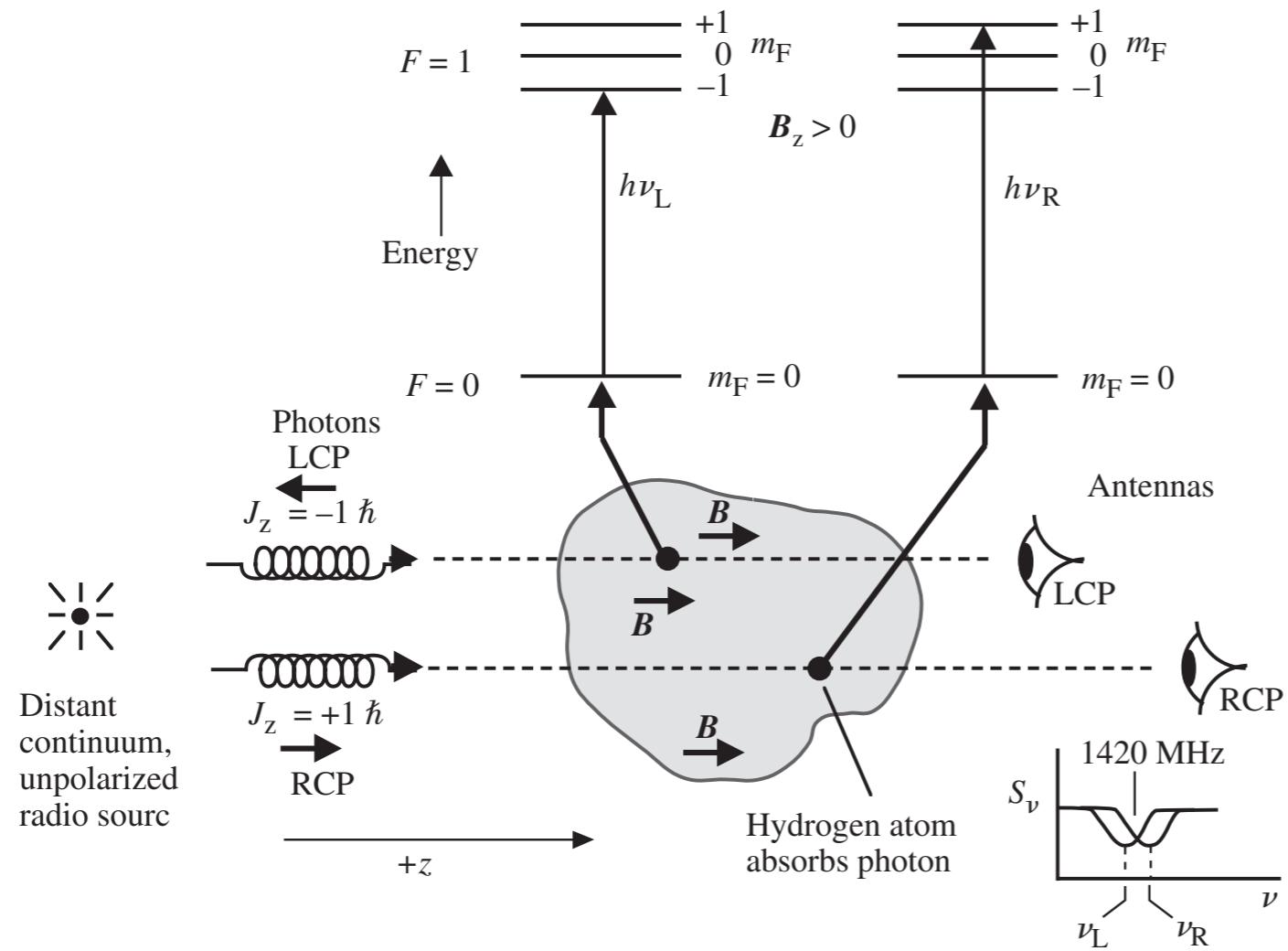


Energy levels for Zeeman absorption by hydrogen atom in an external magnetic field \mathbf{B} . The z-axis is taken to be in the direction of \mathbf{B} .

- (a) The three allowed projections ($m_F = +1, 0, -1$) of the angular momentum for the $F = 1$ state. The atomic magnetic moment μ_H , which is directed opposite to the angular momentum, interacts with the magnetic field to perturb the energy state.
- (b) Energy levels showing (left) the 1420-MHz transition for $B = 0$ and (right) the Zeeman splitting of the upper energy level into the three sublevels for $B_z > 0$. The two allowed transitions to the upper states are shown; they differ in frequency by 28 Hz for $B_z = 1$ nT.

In quantum theory, a single photon is always circularly polarized with $S = \pm \hbar$ (no state with $S = 0$). Linearly polarized photon state is a superposition of a pair of circularly polarized photons.

A magnetic field of order $10 \mu\text{G}$ shifts the frequency by about one part in 10^8 of the hyperfine splitting. This shift is much smaller than the frequency shift $v/c \sim 10^{-5}$ due to a radial velocity of a few km s^{-1} , and it would be nearly impossible to detect, except that it leads to a shift in frequency between two circular polarization modes. The Zeeman effect in H I 21 cm can therefore be detected by taking the difference of the two circular polarization signals. This technique has been used to measure the magnetic field strength in a number of H I regions.



$$\nu_R - \nu_L = \frac{eB_z}{2\pi m_e} = 28.0 \left(\frac{B_z}{1.0 \text{nT}} \right) \text{ Hz}$$

Left circularly polarized (LCP) photons are absorbed at a slightly lower frequency.

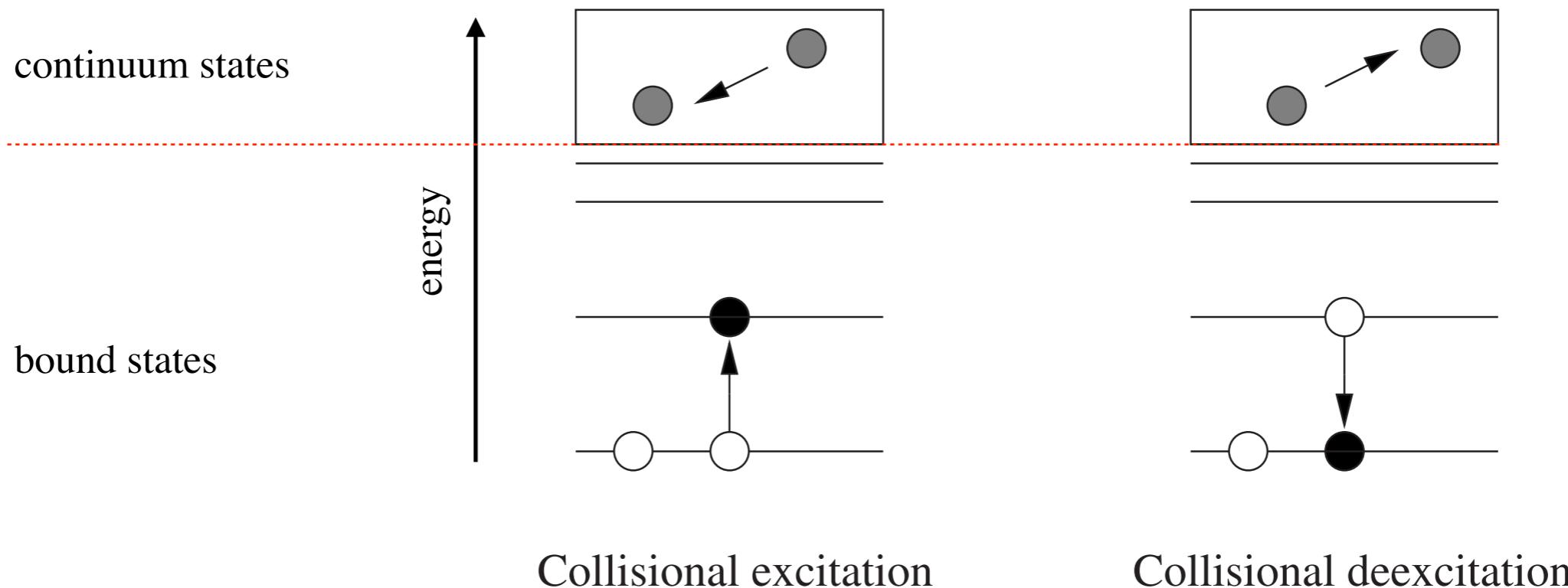
Right circularly polarized (RCP) photons are absorbed at a slightly higher frequency.

[Electron-Ion Collisional Processes]

- To predict the emergent spectra of astrophysical plasmas, we need to understand the details of how excited atomic levels are populated. For the most part, it involves the study of electron-ion collisional processes in gas.
- Each electron-ion collisional process is accompanied by a quantum mechanical inverse, which can be viewed as the same process time-reversed.
- There are essentially four (+1) key electron-ion collisional processes.
 - Collisional Excitation / Deexcitation
 - Collisional Ionization / 3-Body Recombination
 - Radiative Recombination / Photoionization
 - Dielectronic Capture / Autoionization
- + Charge Exchange

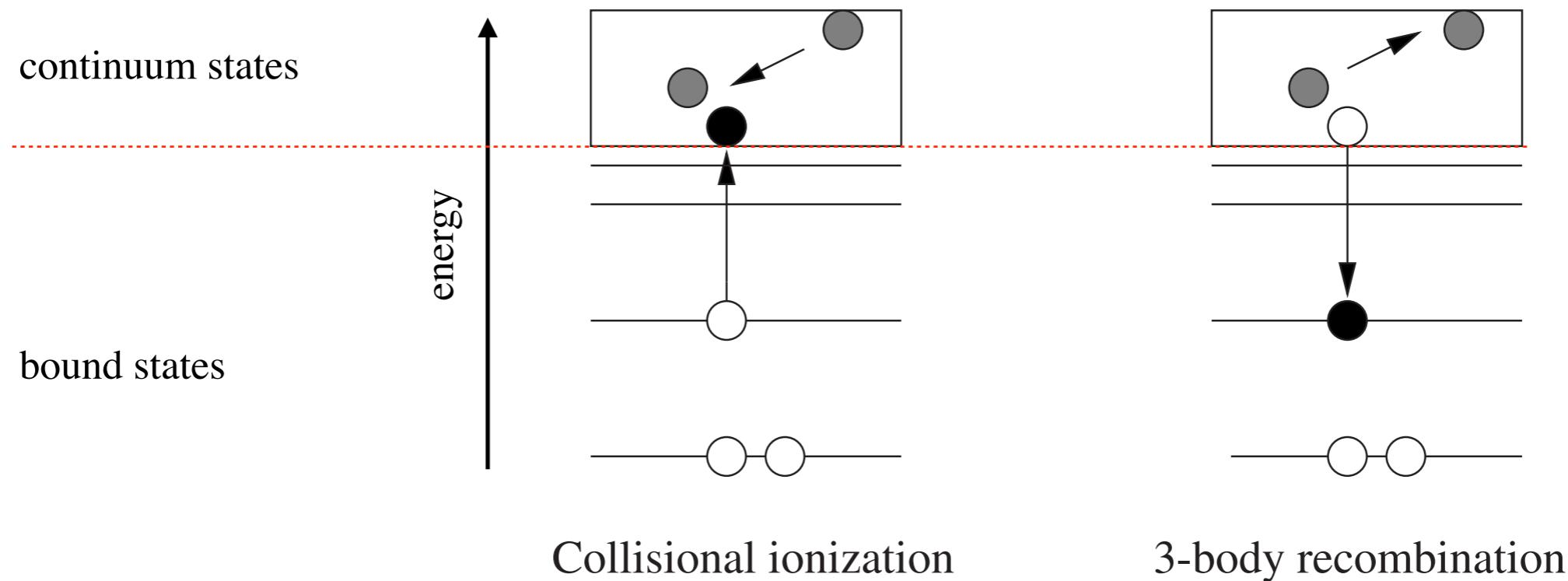
(1) Collisional Excitation / Deexcitation

- In collisional excitation, the interaction between a passing electron in a continuum state and a bound electron in a discrete state result in the excitation of the bound electron to a higher energy discrete level.
- To conserve energy, the colliding electron gives up a fraction of its energy and thus “falls” into a lower continuum state.
- The inverse process is collisional deexcitation, where a passing electron interacting with an excited atom actually gains energy as a result of the collisions.



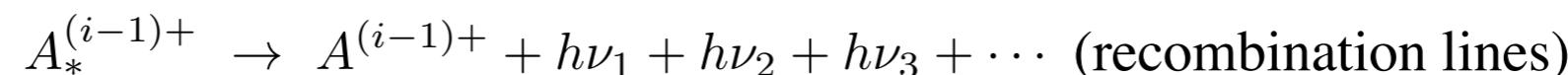
(2) Collisional ionization / 3-body recombination

- Collisional ionization is similar to collisional excitation, except that in this case, the final state of the initially bound electron is also a continuum state.
- The inverse process if 3-body recombination. Here, two initially free electrons interact with the ion in the same collision. One of the two gets captured into a bound discrete level, while the other carries off the excess energy in a higher continuum state.

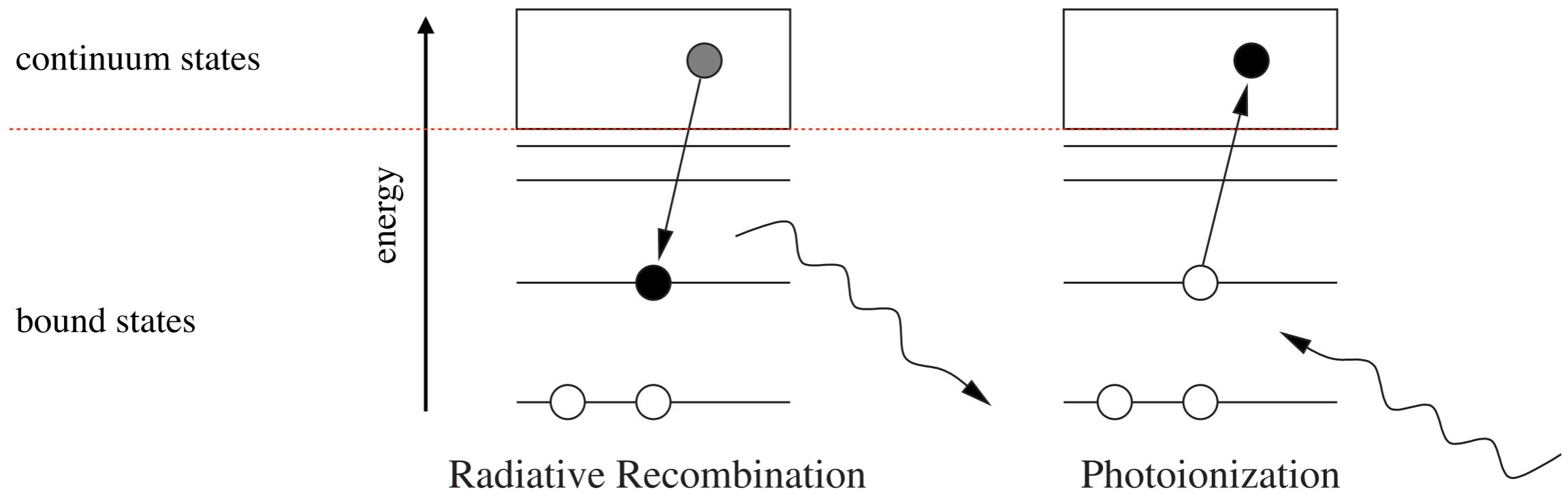


(3) Radiative Recombination / Photoionization

- In radiative recombination a free electron in a continuum state decays into a bound discrete state through the emission of a photon. This is actually a form of a spontaneous emission, similar to the radiative decay between two bound levels.

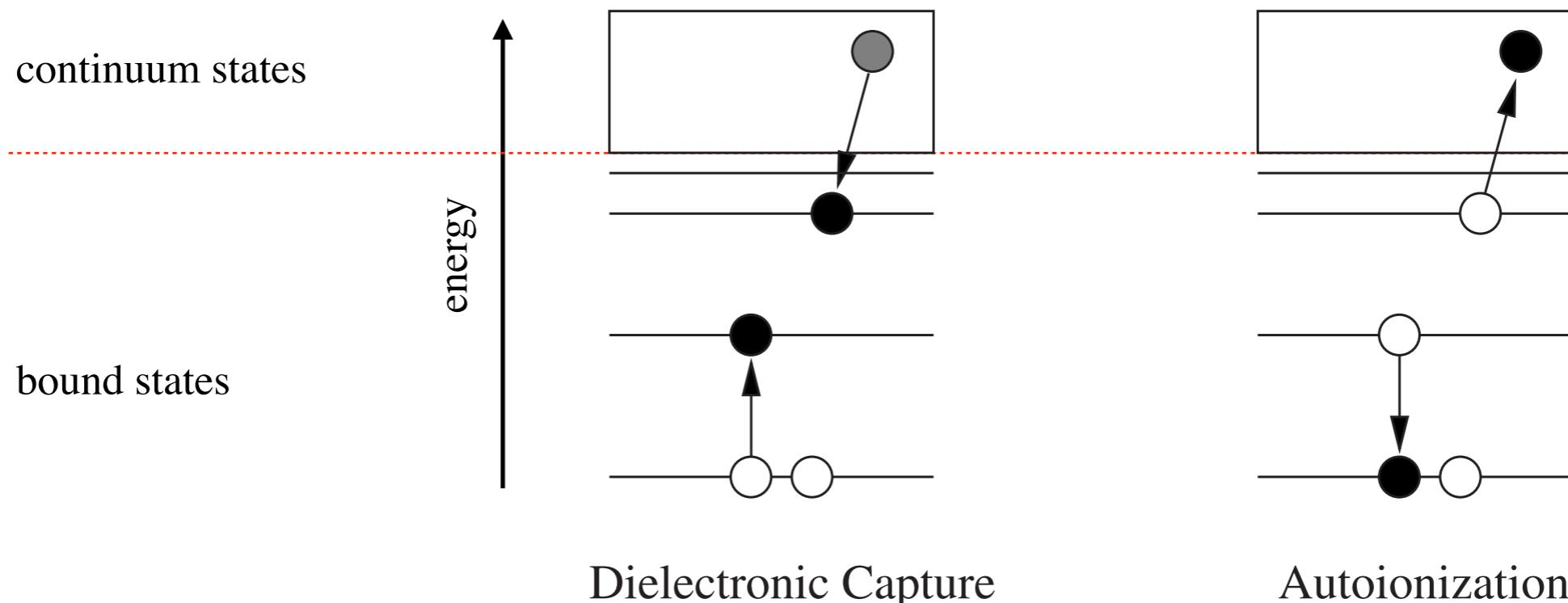


- The inverse process is photoionization or bound-free absorption.
 - Interstellar medium (ISM) is transparent to $h\nu < 13.6 \text{ eV}$ photons, but is very opaque to ionizing photons. In fact, the ISM does not become transparent until $h\nu \sim 1 \text{ keV}$. Sources of ionizing photons include massive, hot young stars, hot white dwarfs, and supernova remnant shocks.



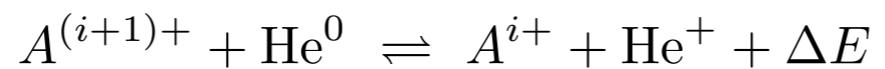
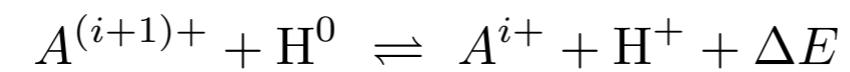
(4) Dielectronic Capture / Autoionization

- Dielectronic capture (recombination) is a resonant radiationless process in which the decay of an electron from a continuum state to a bound state is accompanied by the elevation of a core electron into an excited state. The resulting atom is doubly excited, and it has a total energy above the ionization potential of the initial ion.
- The inverse process is autoionization, where a doubly excited atom decays via the emission of a weakly bound outer electron. If the core excitation is associated with a “hole”, in one of the orbitals of an inner shell, this process is usually called Auger decay.



(5) Charge Exchange

- During the collision of two ionic species, the charge clouds surrounding each interact, and it is possible that an electron is exchanged between them.
- Since, in virtually all diffuse astrophysical plasmas, hydrogen and helium are overwhelmingly the most abundant species, the charge-exchange reactions which are significant to the ionization balance of the plasma are



[Ionization Equilibrium]

- **Collisional Ionization Equilibrium (CIE) or coronal equilibrium**
 - dynamic balance at a given temperature between collisional ionization from the ground states of the various atoms and ions, and the process of recombination from the higher ionization stages.
 - In this equilibrium, effectively, all ions are in their ground state.
 - Software: **Chianti** (<https://www.chiantidatabase.org/>)
- **Photoionization Equilibrium**
 - dynamic balance between photo-ionization and the process of recombination.
 - Software: **Cloudy** (<https://trac.nublado.org/>), **MAPPINGS** (<https://mappings.anu.edu.au/>), **MOCASSIN** (<https://github.com/mocassin>, <https://mocassin.nebulosresearch.org/>)
- **Ionization balance under conditions of Local Thermodynamic Equilibrium (LTE)**
 - The ionization equilibrium in LTE is described by the Saha equation.

$$\frac{n_{r+1} n_e}{n_r} = \frac{G_{r+1} g_e}{G_r} \frac{(2\pi m_e k T)^{3/2}}{h^3} \exp\left(-\frac{\chi_r}{kT}\right)$$

n_{r+1} : density of atoms in ionization state $r + 1$
 n_r : density of atoms in ionization state r
 n_e : density of electrons
 G_{r+1} : partition function of ionization state $r + 1$
 G_r : partition function of ionization state r
 g_e : statistical weight of the electron, $g_e = 2$
 χ_r : ionization potential of state r (to reach state $r + 1$)

$$G_r = \sum_j g_{r,k} \exp\left(-\frac{E_{r+1,j}}{kT}\right)$$