

Interstellar Medium (ISM)

Week 4

2025 March 24 (Monday), 9AM

updated 03/22, 22:14

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Hydrogen Atom : Allowed Transitions

- **Selection Rules**

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

Δn any  selection rule for configuration

$\Delta l = \pm 1$

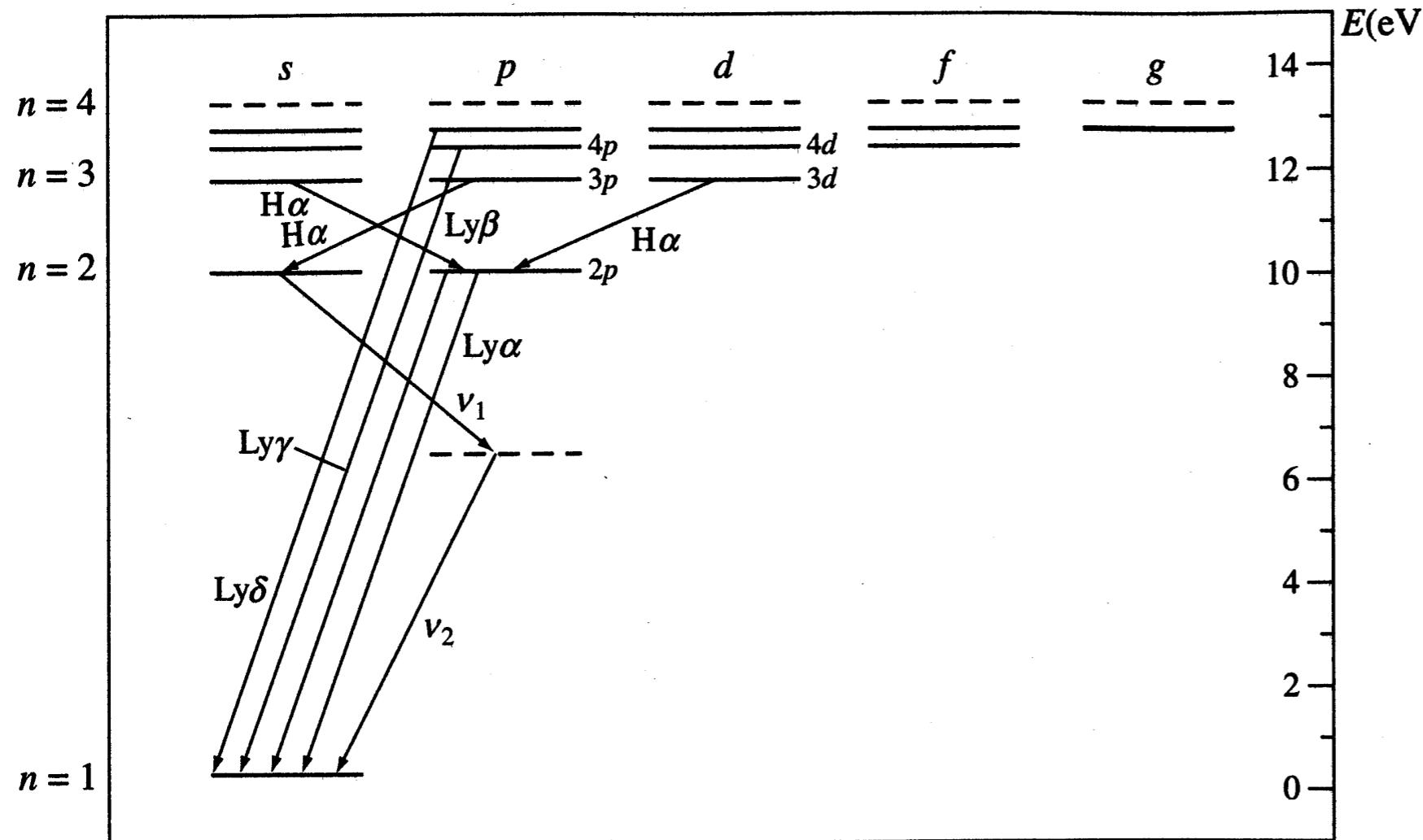
$\Delta S = 0$  For H atom, this is always satisfied as $S = 1/2$ for all states.

$\Delta L = 0, \pm 1$ (not $L = 0 - 0$; $^xS \rightarrow ^{x'}S$)

$\Delta J = 0, \pm 1$ (not $J = 0 - 0$; $^xL_0 \rightarrow ^{x'}L_0$)

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.

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

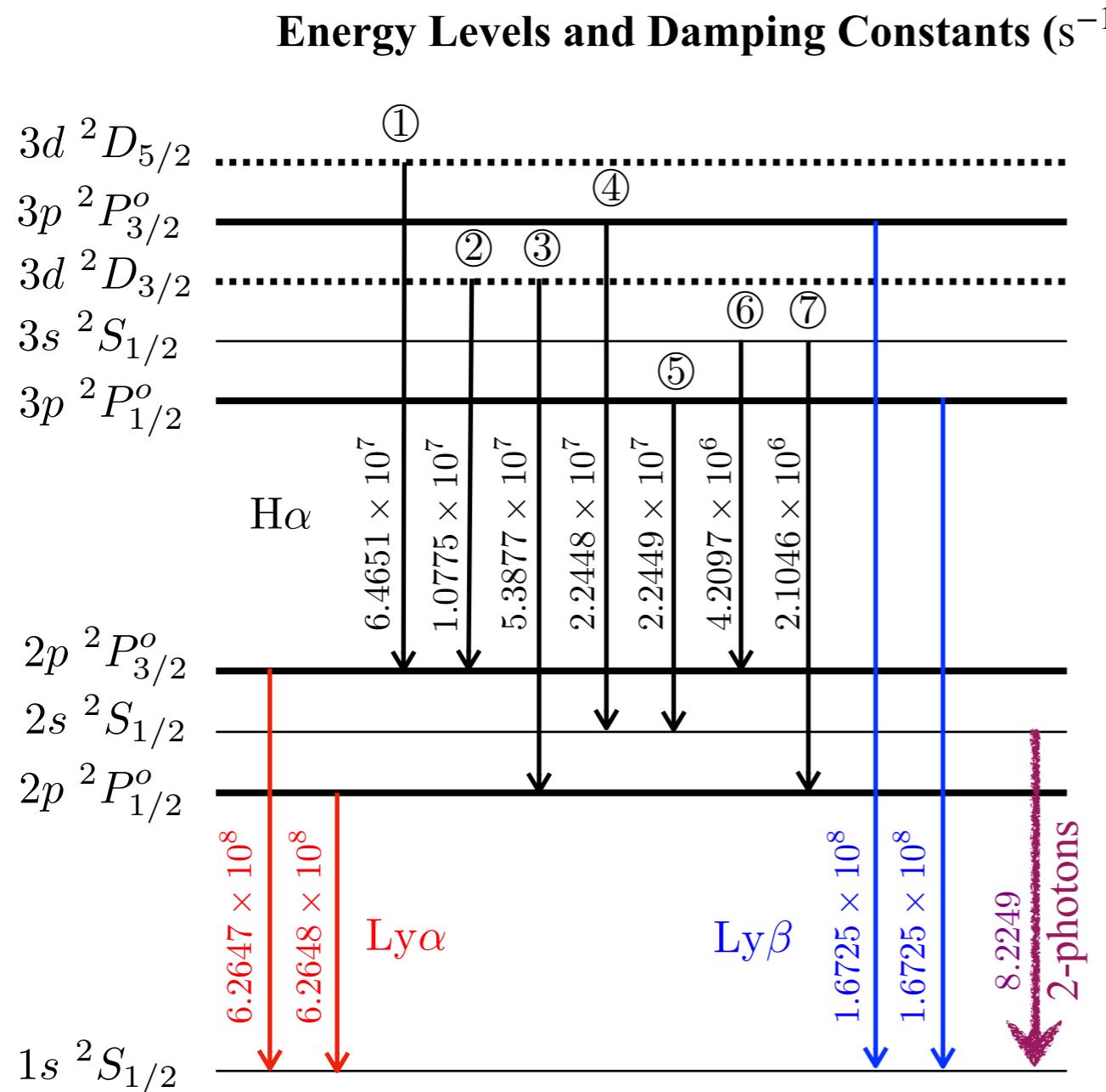
$- 3d_{\frac{3}{2}}$ is allowed;

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

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

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

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



Energy Levels of Neutral Hydrogen (NIST)

Configuration	Term	J	Level (cm^{-1})	Ref.
$1s$	2S	$1/2$	0.0000	MK00a
$2p$	$^2P^o$	$1/2$	82258.9191	MK00a
		$3/2$	82259.2850	MK00a
$2s$	2S	$1/2$	82258.9544	MK00a
$3p$	$^2P^o$	$1/2$	97492.2112	MK00a
		$3/2$	97492.3196	MK00a
$3s$	2S	$1/2$	97492.2217	MK00a
$3d$	2D	$3/2$	97492.3195	MK00a
		$5/2$	97492.3556	MK00a
$4p$	$^2P^o$	$1/2$	102823.8486	MK00a
		$3/2$	102823.8943	MK00a
$4s$	2S	$1/2$	102823.8530	MK00a
$4d$	2D	$3/2$	102823.8942	MK00a
		$5/2$	102823.9095	MK00a
$4f$	$^2F^o$	$5/2$	102823.9095	MK00a
		$7/2$	102823.9171	MK00a
$5p$	$^2P^o$	$1/2$	105291.6287	MK00a
		$3/2$	105291.6521	MK00a
$5s$	2S	$1/2$	105291.6309	MK00a
$5d$	2D	$3/2$	105291.6520	MK00a
		$5/2$	105291.6599	MK00a
$5f$	$^2F^o$	$5/2$	105291.6598	MK00a
		$7/2$	105291.6637	MK00a
$5g$	2G	$7/2$	105291.6637	MK00a
		$9/2$	105291.6661	MK00a
H	<i>Limit</i>		109678.7717	MK00a

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

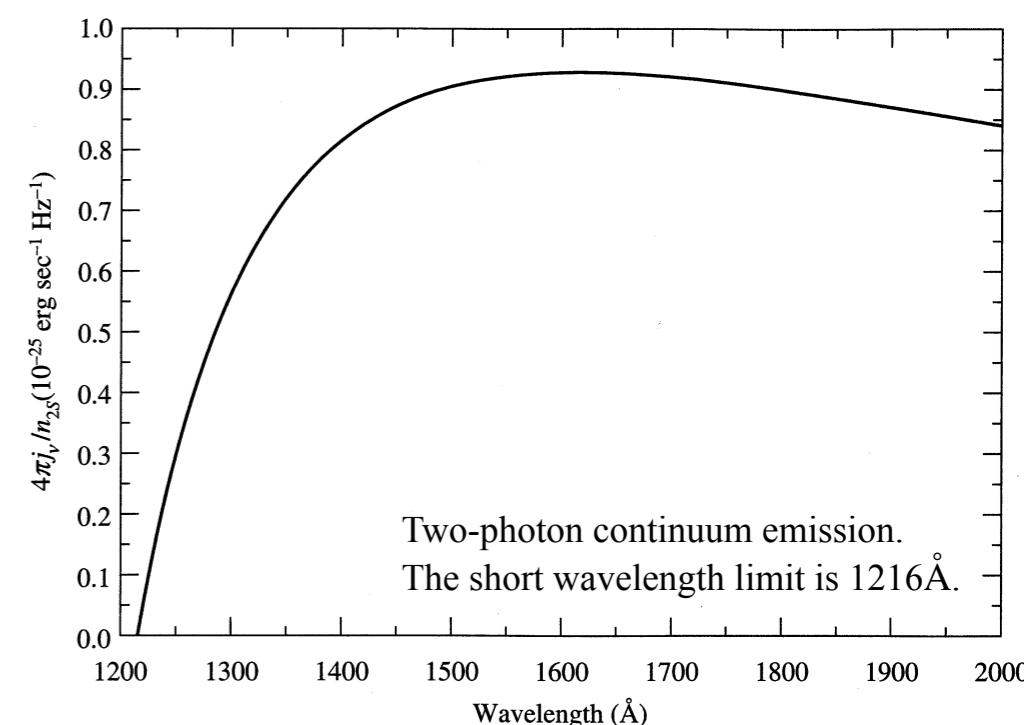
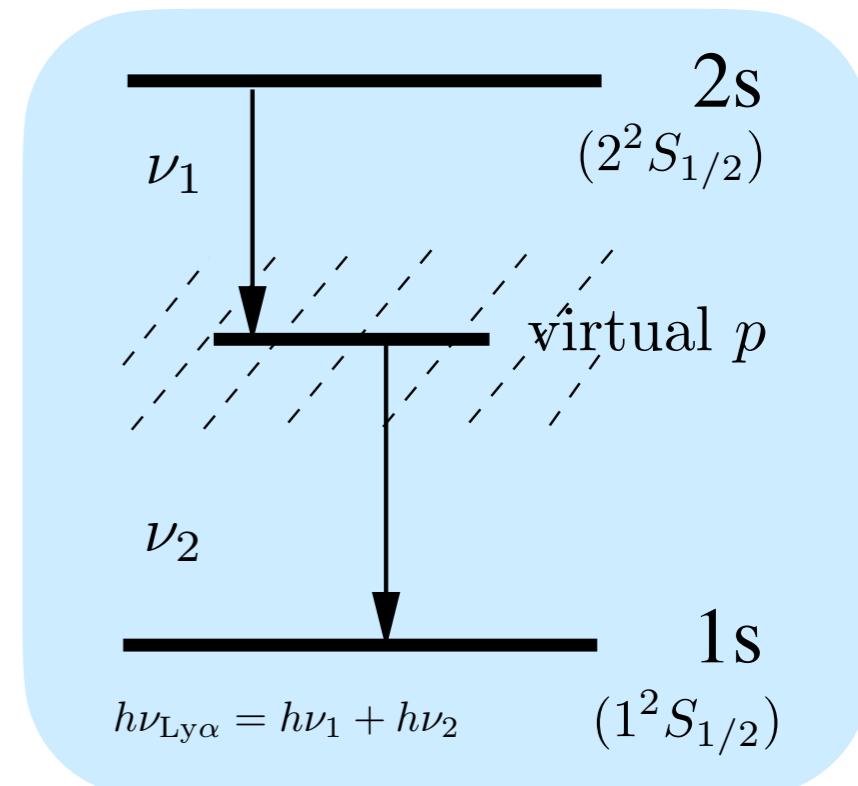
$$\tau_i = \left(\sum_j A_{ij} \right)^{-1} \quad \text{where } A_{ij} \text{ is the Einstein A coefficient}$$

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 .

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.

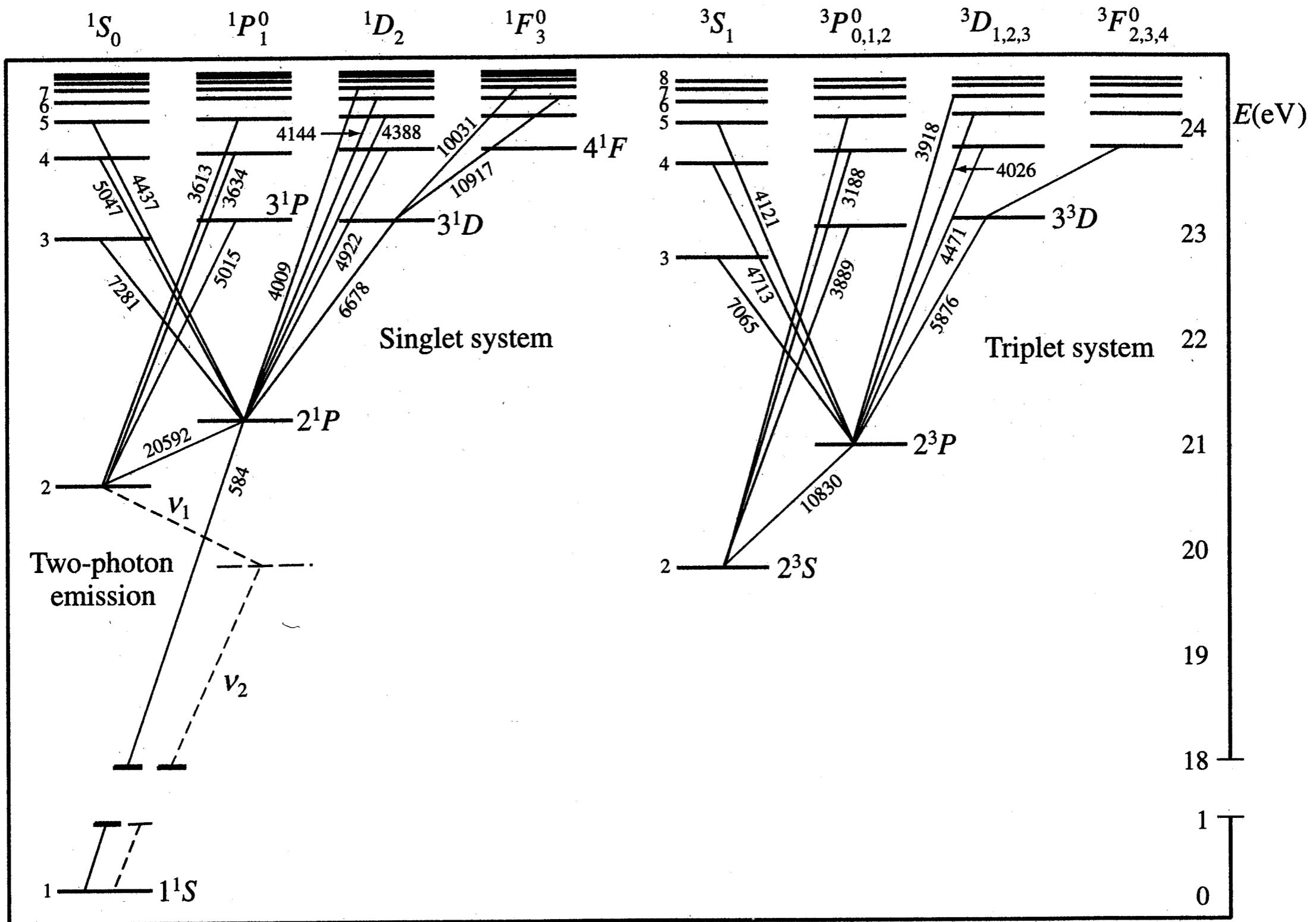
S	L	J
0	1	1
1	1	0, 1, 2

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

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

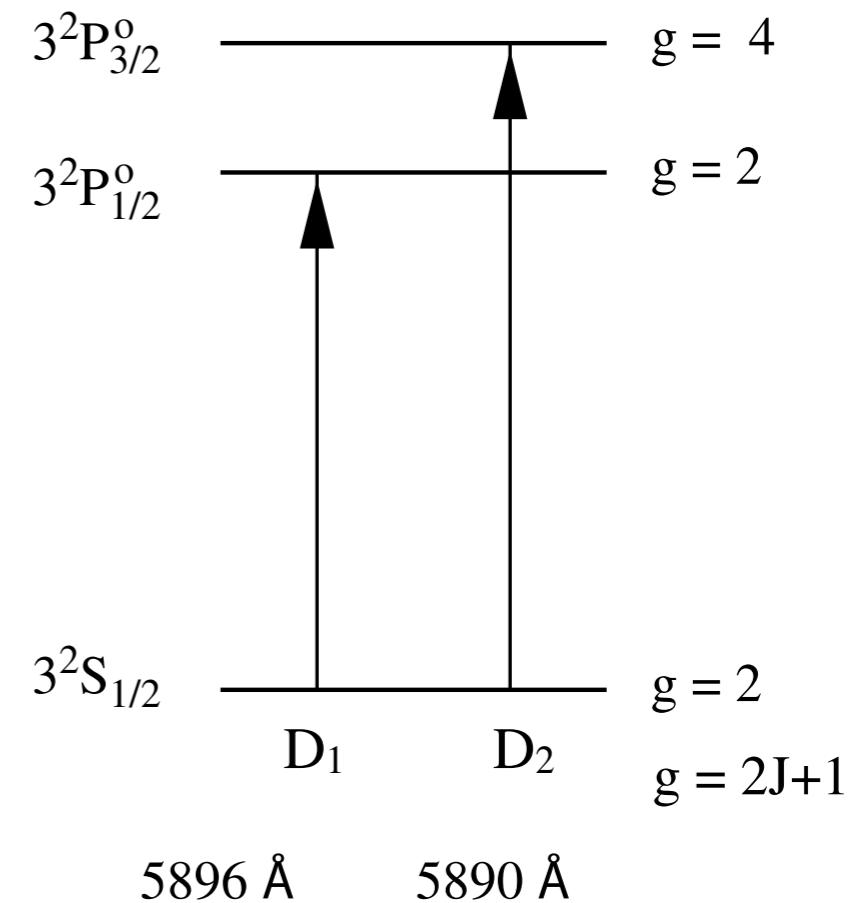
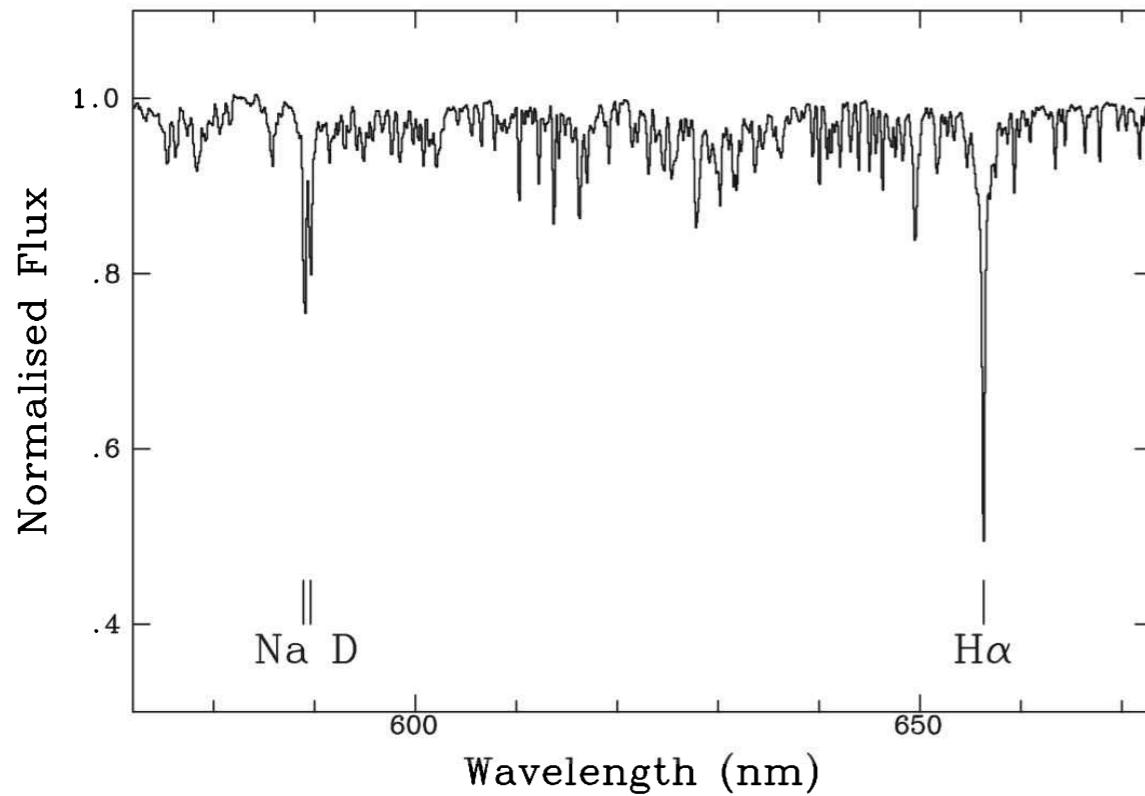
Parity is calculated as $(-1)^{l_1+l_2+\dots}$.

- Helium (Grotrian diagram)



LS coupling: Alkali Atoms

- Alkali atoms: Lithium (Li, Z=3), sodium (Na, Z=11), potassium (K, Z=19) and rubidium (Rb, Z=37) 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 $1s^2 2s^2 2p^6 3p^1$.



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

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

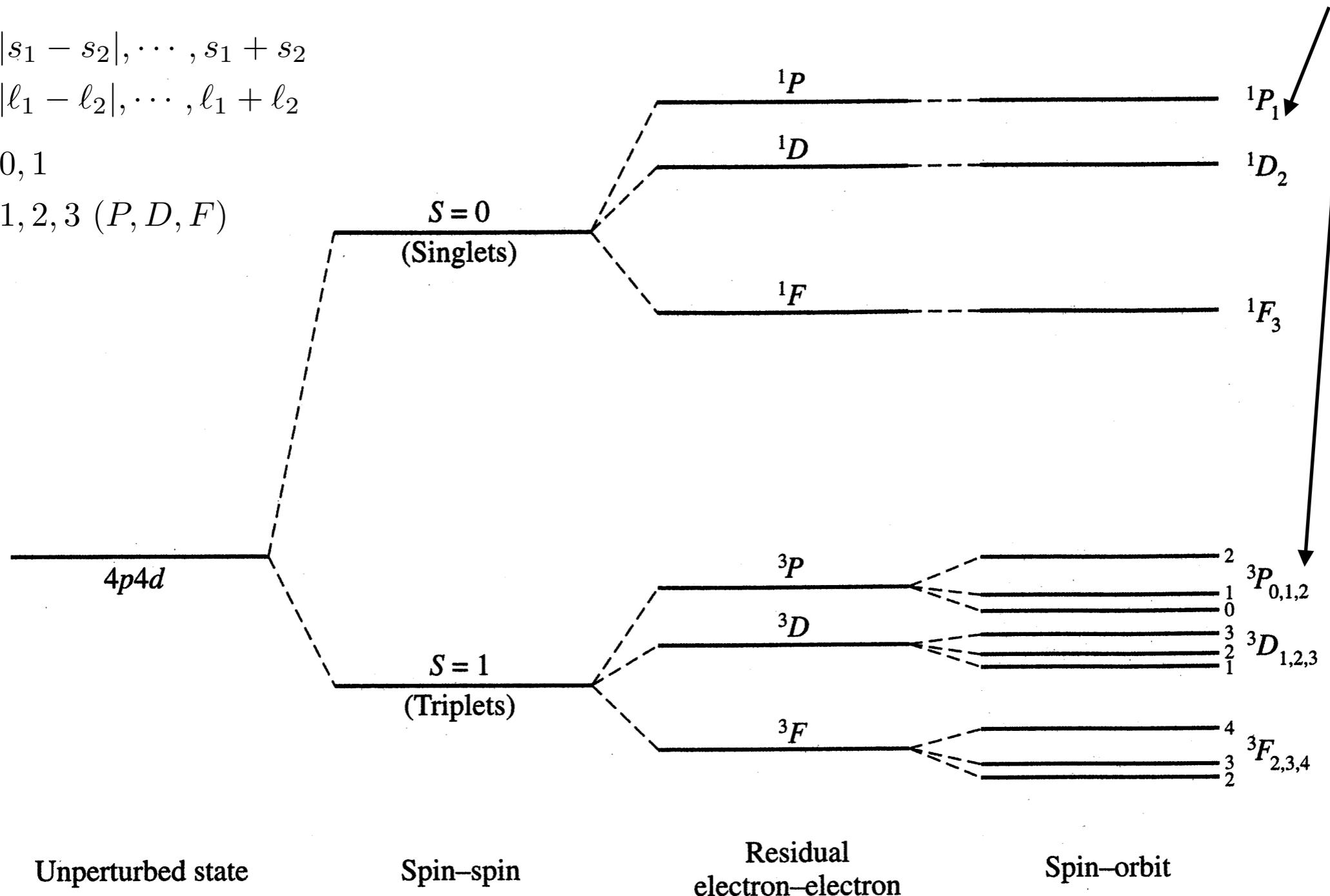
$$J = |L - S|, \dots, L + S$$

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

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

$$S = 0, 1$$

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



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.

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

In other words, 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 ($n = n'$)

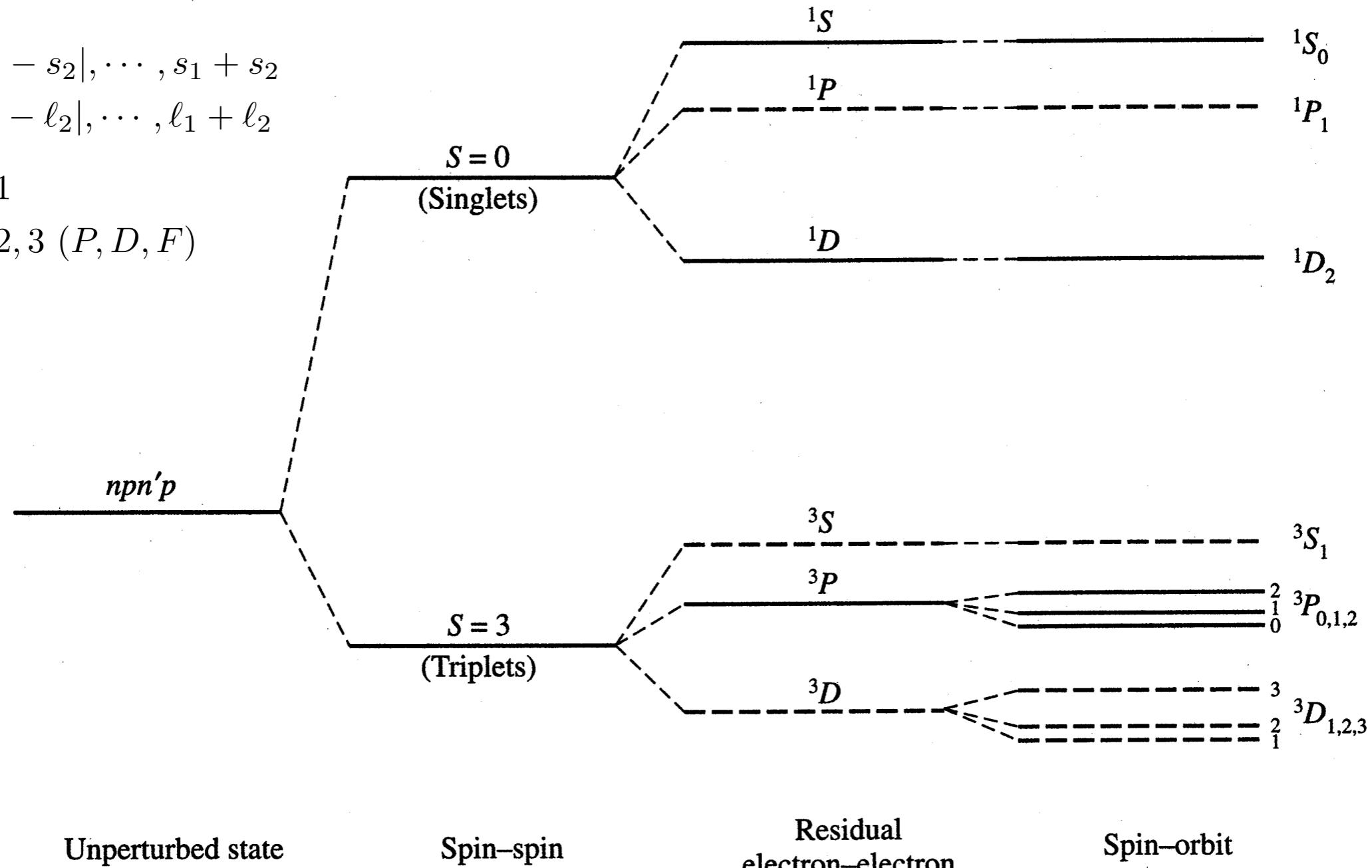
The levels for $n = n'$ will be explained in the next slides.

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

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

$$S = 0, 1$$

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



(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

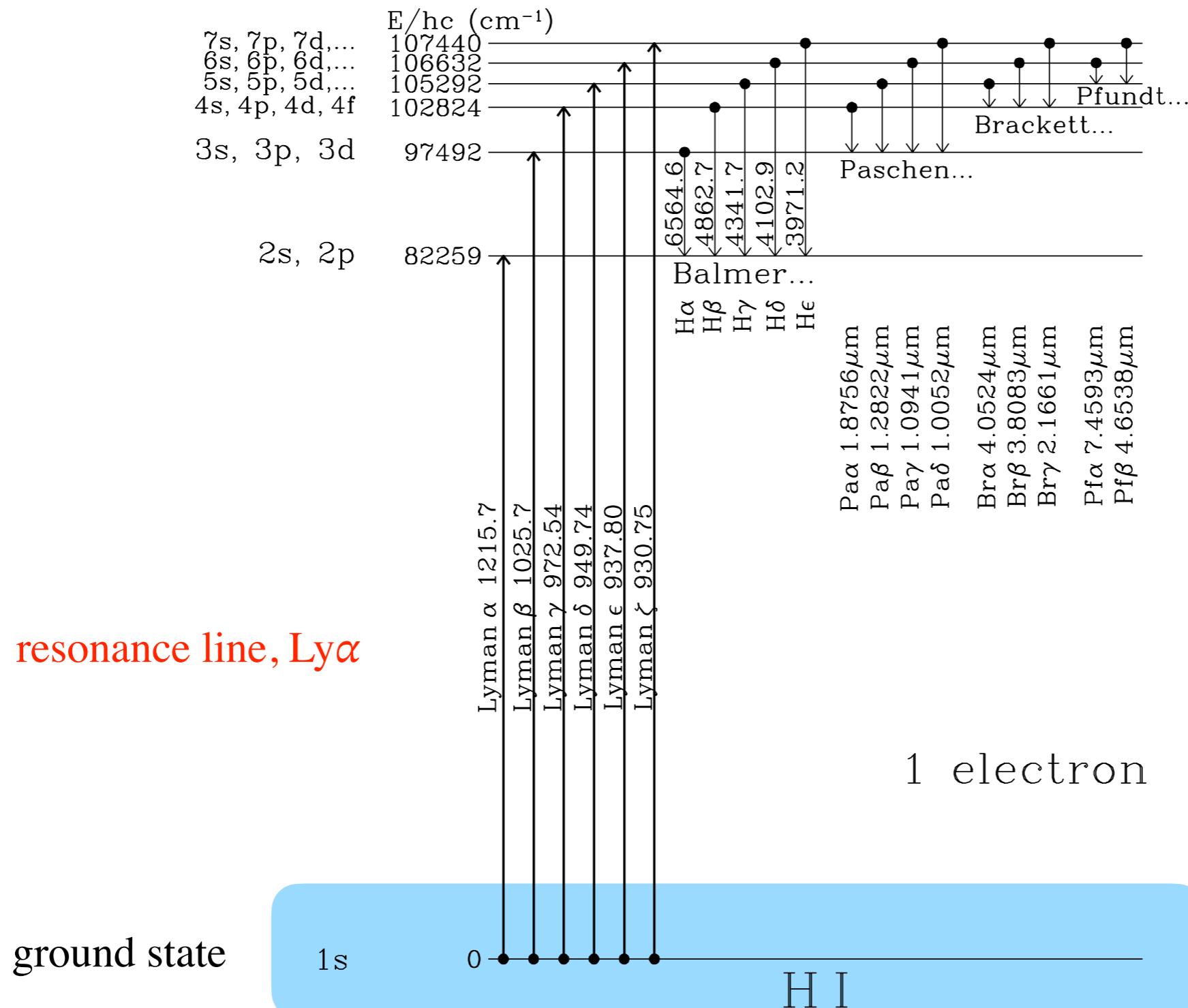
- In addition to the above two rules, we can recognize that every “negative” values have always their “positive” counterparts.
 - Therefore, it is more convenient to remove the states with negative values. This gives us Table 3, which contains only 8 states.
- Now, we pick the states starting with the 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 .**

Ionization Potentials (eV)

Element		I→II	II→III	III→IV	IV→V	V→VI	VI→VII	VII→VIII
1	H	13.5984						
2	He	24.5874	54.418					
3	Li	5.3917	75.640	122.454				
4	Be	9.3227	18.211	153.896	217.719			
5	B	8.2980	25.155	37.931	259.375	340.226		
6	C	11.2603	24.385	47.888	64.494	392.091	489.993	
7	N	14.5341	29.601	47.445	77.474	97.890	552.067	667.046
8	O	13.6181	35.121	54.936	77.414	113.899	138.119	739.327
9	F	17.4228	34.971	62.708	87.175	114.249	157.163	185.187
10	Ne	21.5645	40.963	63.423	97.190	126.247	157.934	207.271
11	Na	5.1391	47.286	71.620	98.936	138.404	172.23	208.504
12	Mg	7.6462	15.035	80.144	109.265	141.33	186.76	225.02
13	Al	5.9858	18.829	28.448	119.992	153.825	190.49	241.76
14	Si	8.1517	16.346	33.493	45.142	166.767	205.267	246.32
15	P	10.4867	19.769	30.203	51.444	65.025	220.430	263.57
16	S	10.3600	23.338	34.86	47.222	72.595	88.053	280.954
17	Cl	12.9676	23.814	39.80	53.24	67.68	96.94	114.201
18	Ar	15.7596	27.630	40.735	59.58	74.84	91.290	124.41
19	K	4.3407	31.625	45.806	60.913	82.66	99.4	117.6
20	Ca	6.1132	11.872	50.913	67.273	84.34	108.78	127.21
21	Sc	6.5615	12.800	24.757	73.489	91.95	110.68	137.99
22	Ti	6.8281	13.576	27.492	43.267	92.299	119.533	140.68
23	V	6.7462	14.618	29.311	46.709	65.282	128.125	150.72
24	Cr	6.7665	16.486	30.959	49.16	69.46	90.635	160.29
25	Mn	7.4340	15.640	33.668	51.2	72.41	95.604	119.203
26	Fe	7.9025	16.199	30.651	54.91	75.0	98.985	124.98
27	Co	7.8810	17.084	33.50	51.27	79.50	102.0	128.9
28	Ni	7.6399	18.169	35.187	54.92	76.06	108.0	132.0
29	Cu	7.7264	20.292	36.841	57.38	79.8	103.0	139.0
30	Zn	9.3942	17.964	39.723	59.573	82.6	108.0	133.9

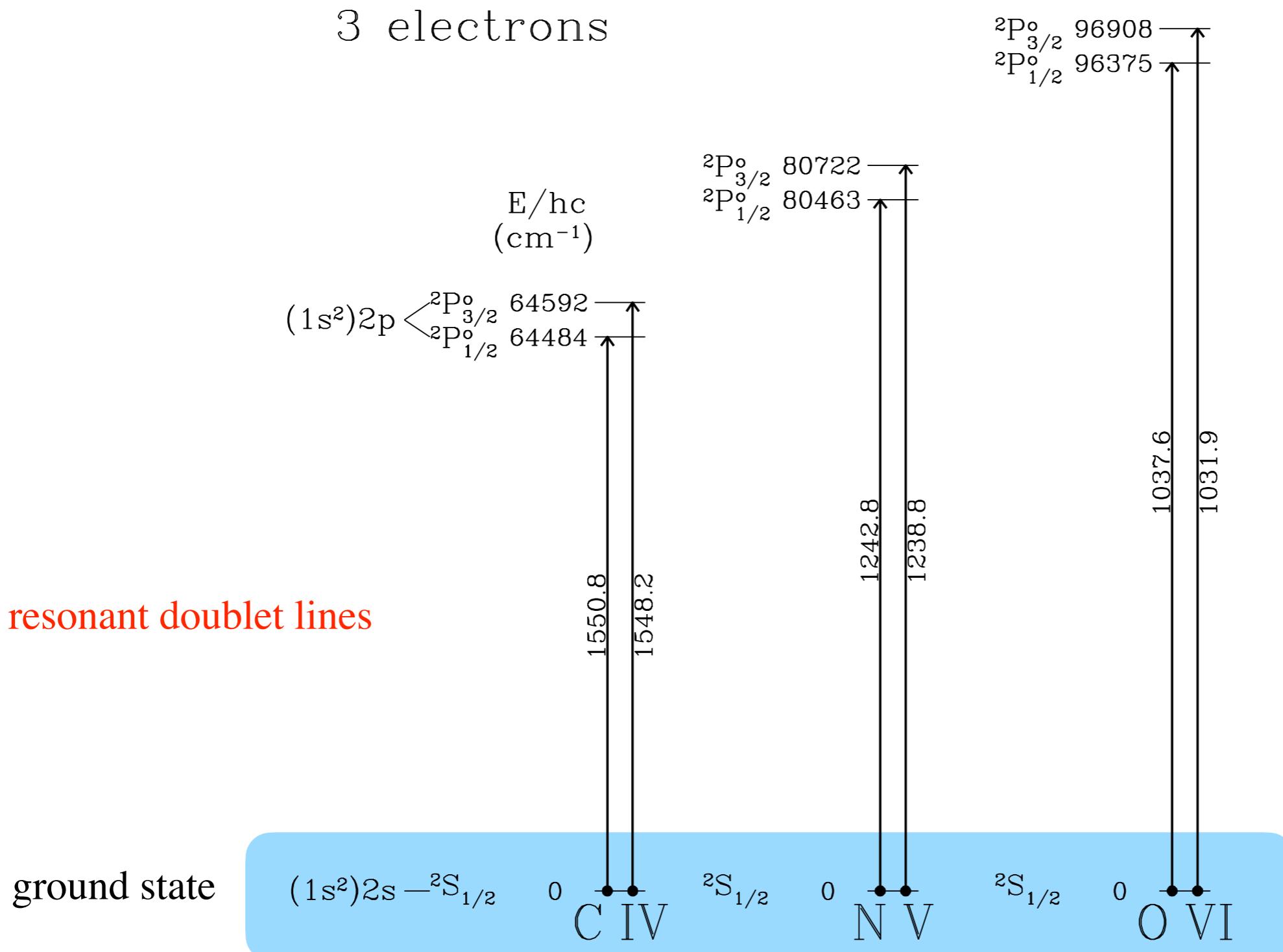
Energy Level Diagrams

- 1 electron



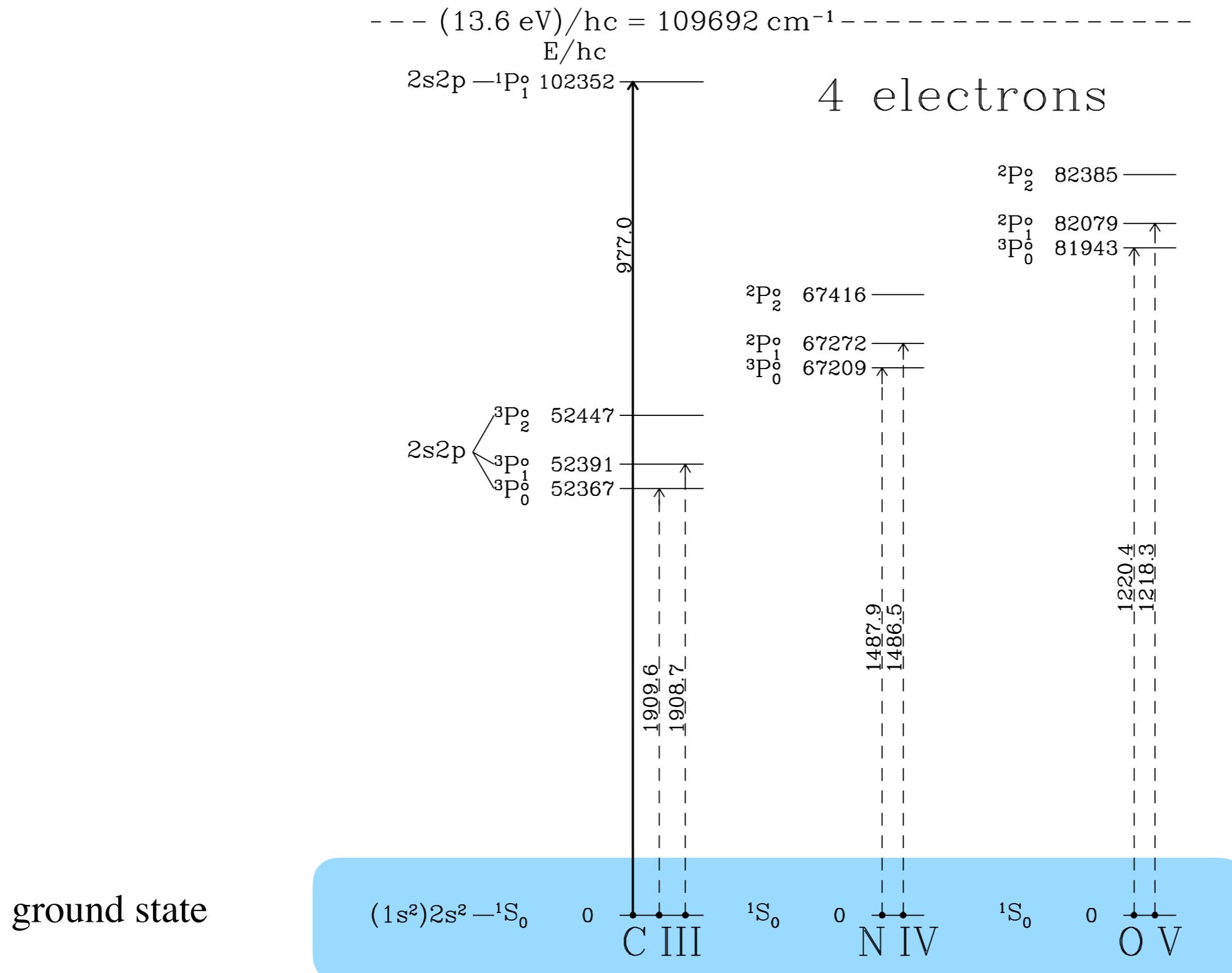
- 3 electrons (Lithium-like ions)

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



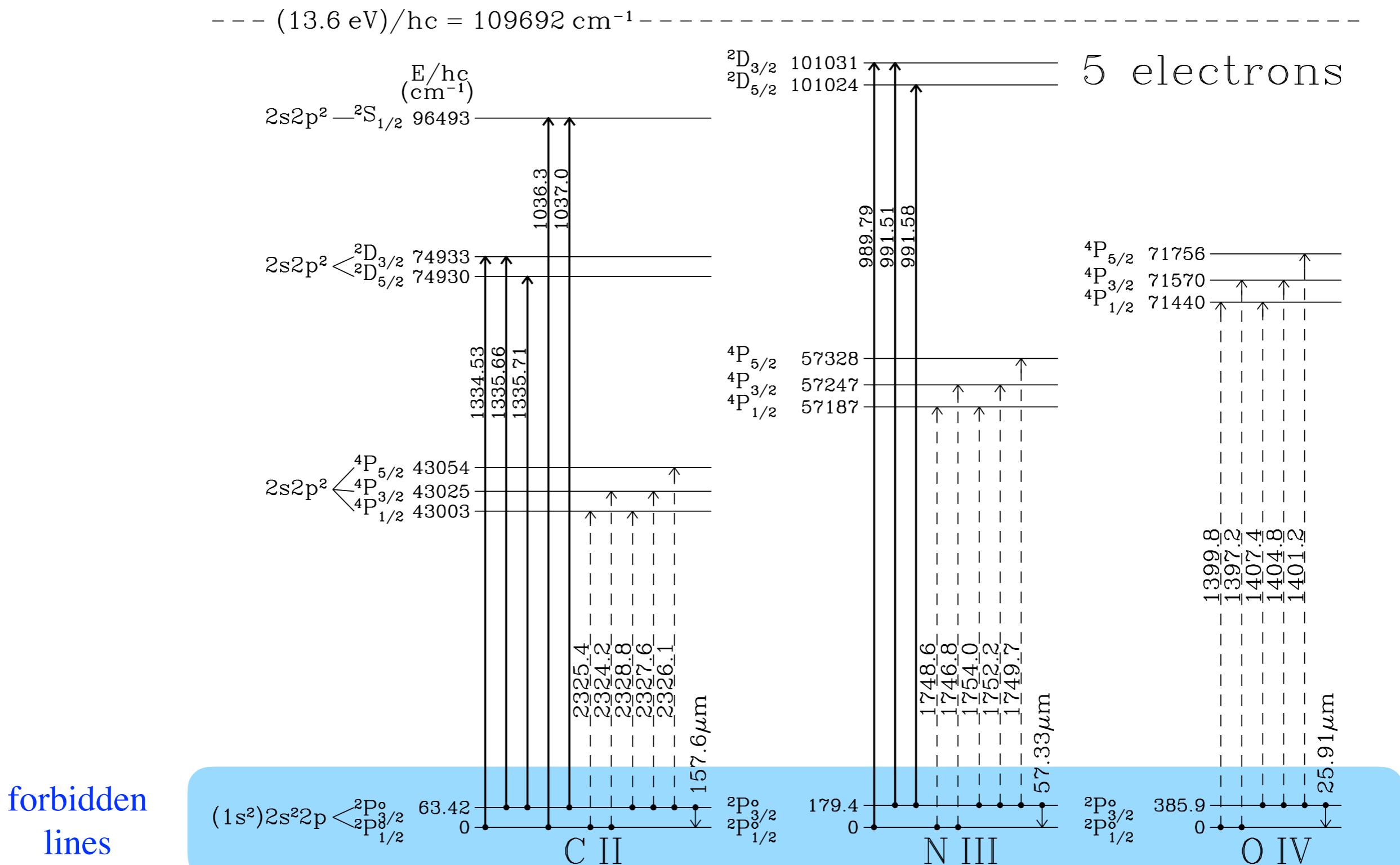
- 4 electrons

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



- 5 electrons

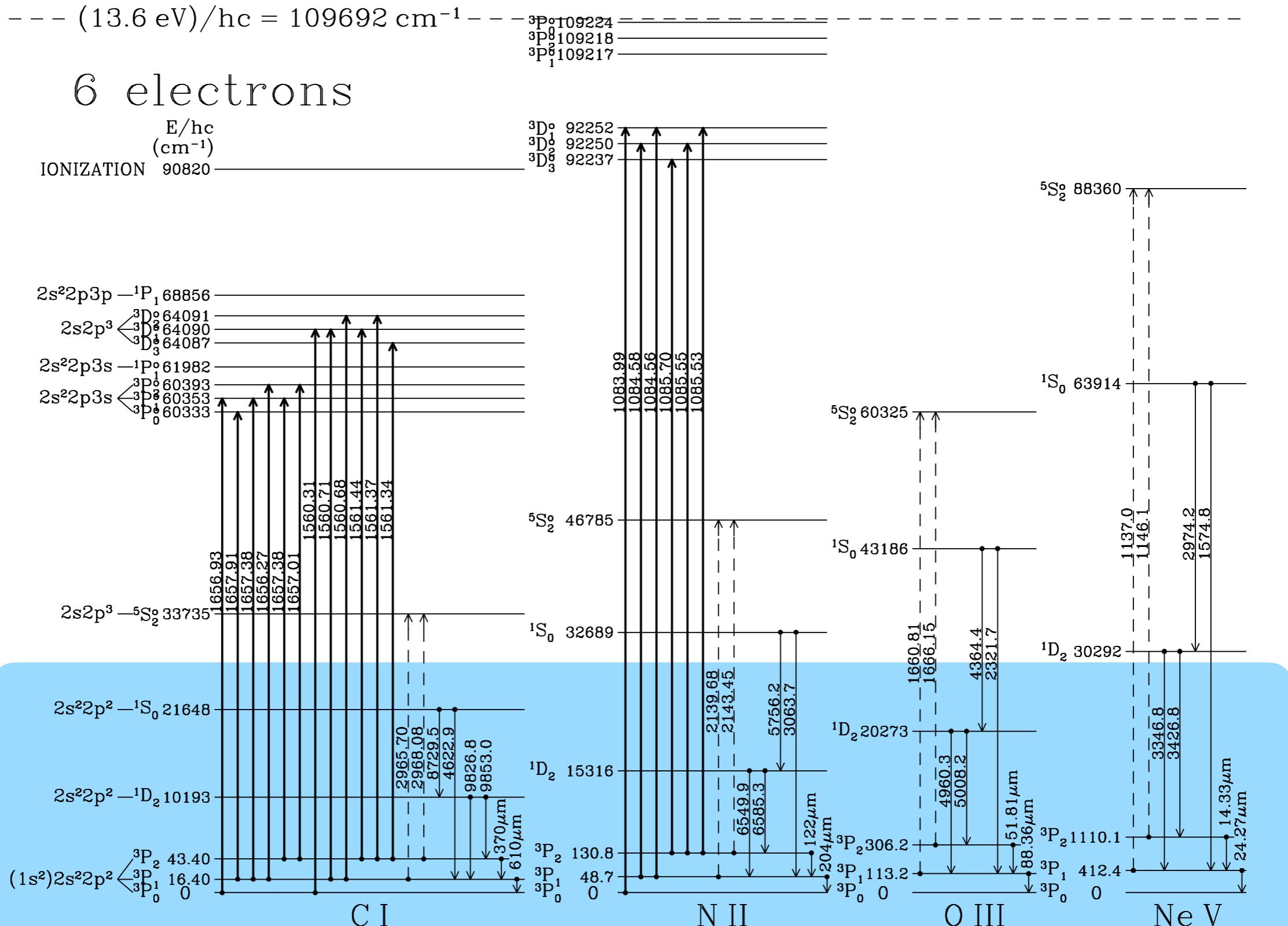
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



forbidden
lines

- 6 electrons

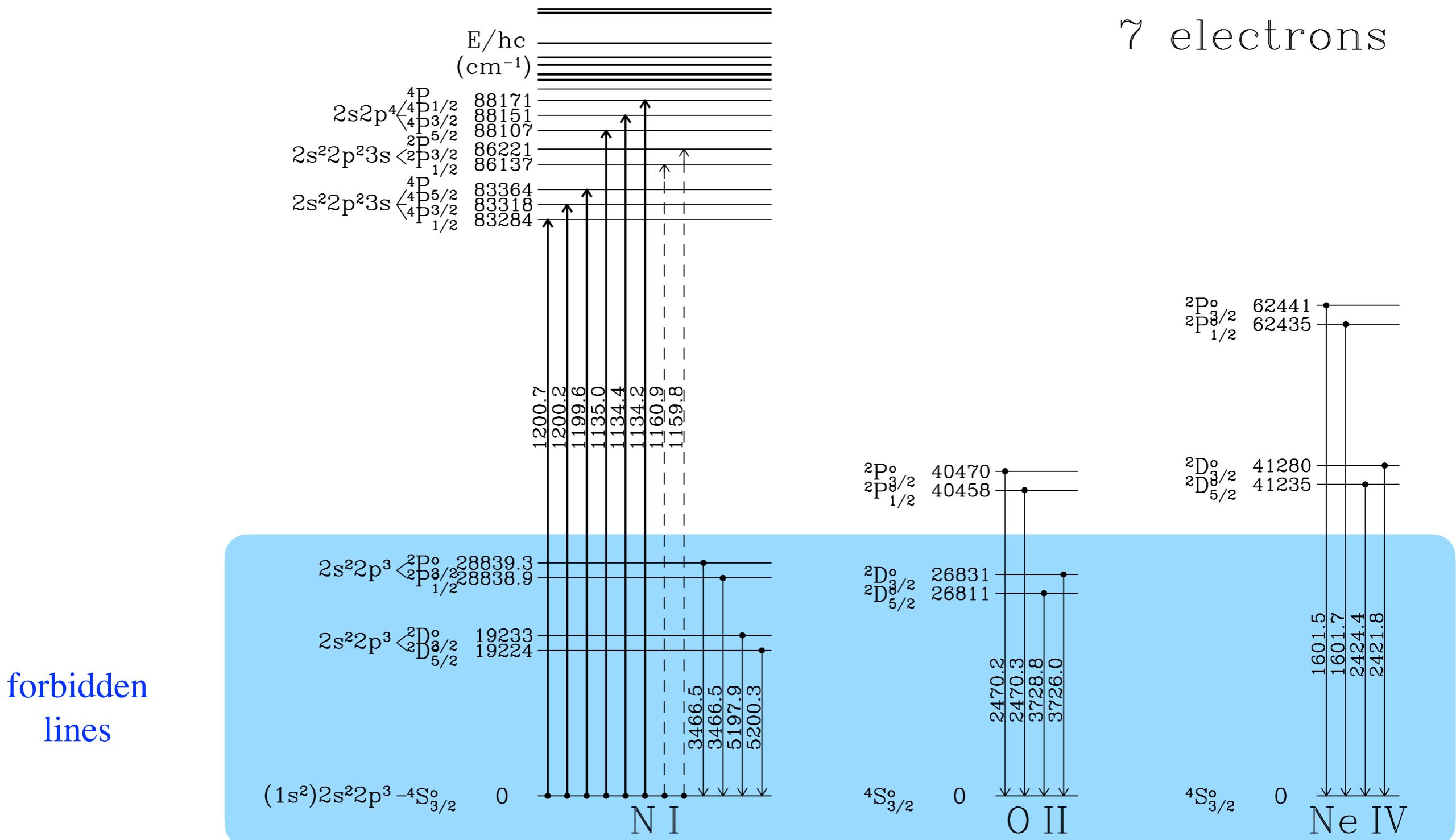
Upward heavy: resonance, Upward Dashed: intercombination
Downward solid: forbidden



- 7 electrons

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

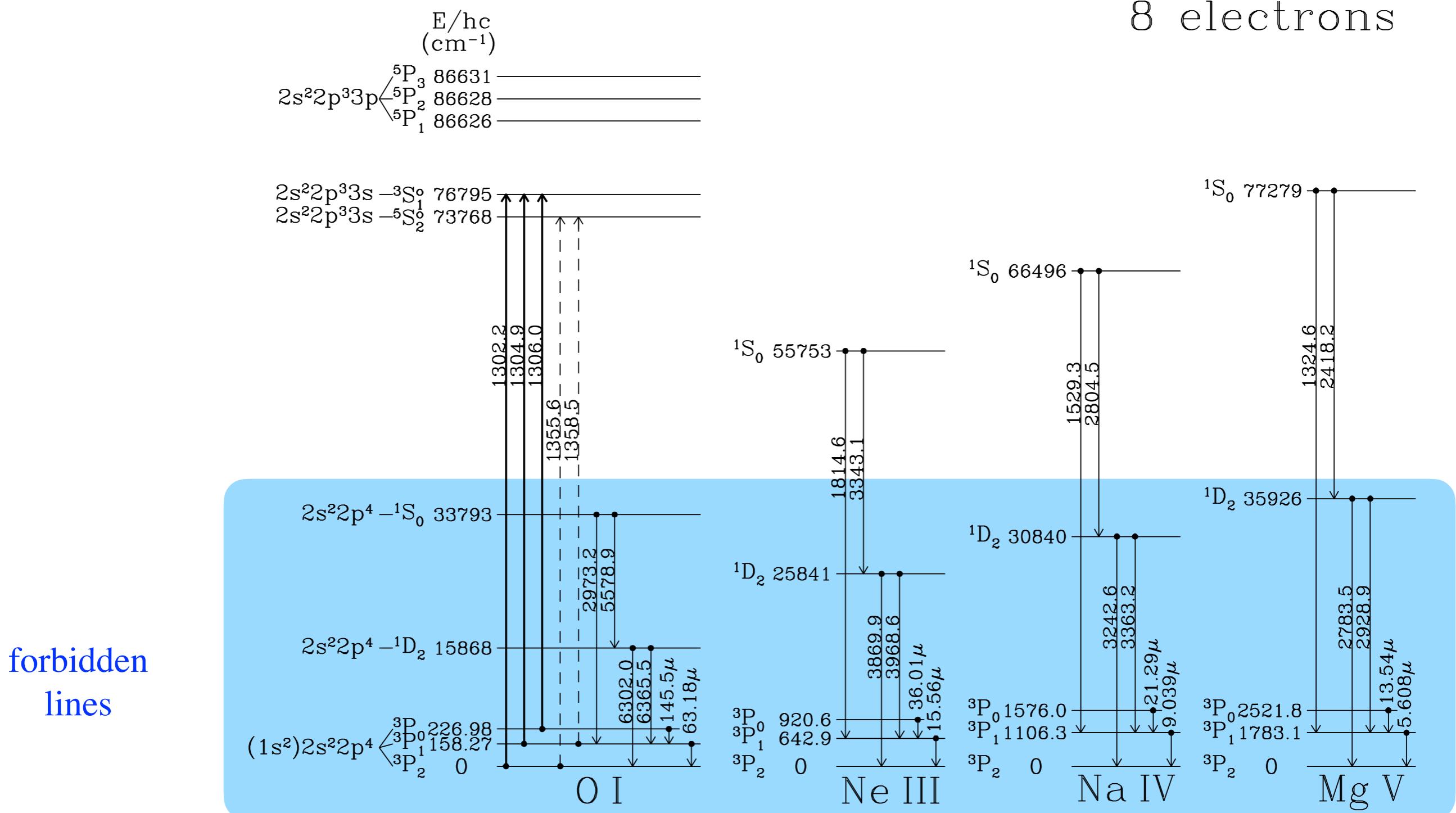
$$\text{---} (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{---} \text{---} \text{---}$$



- 8 electrons

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

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



forbidden
lines

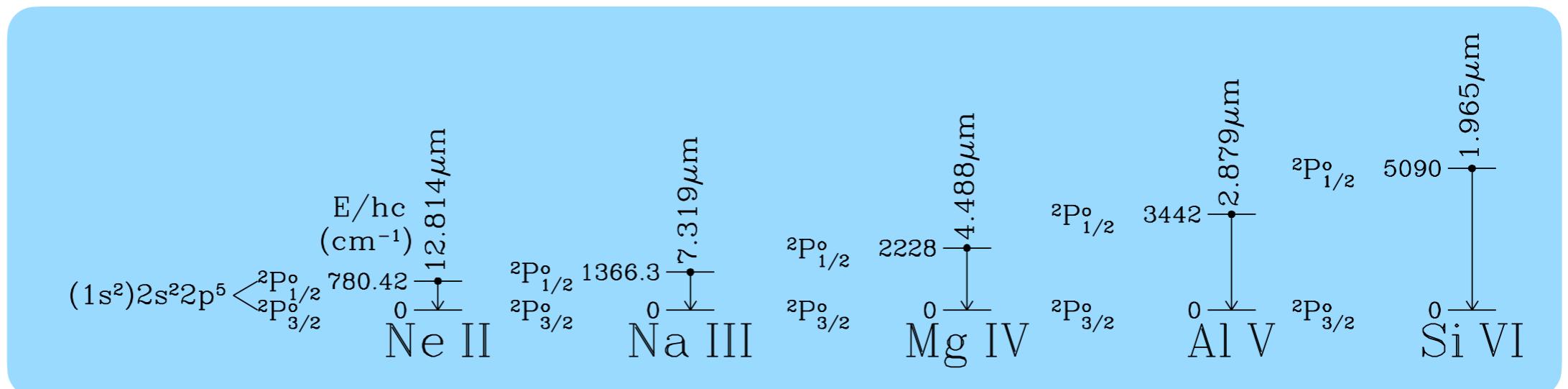
- 9 electrons

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

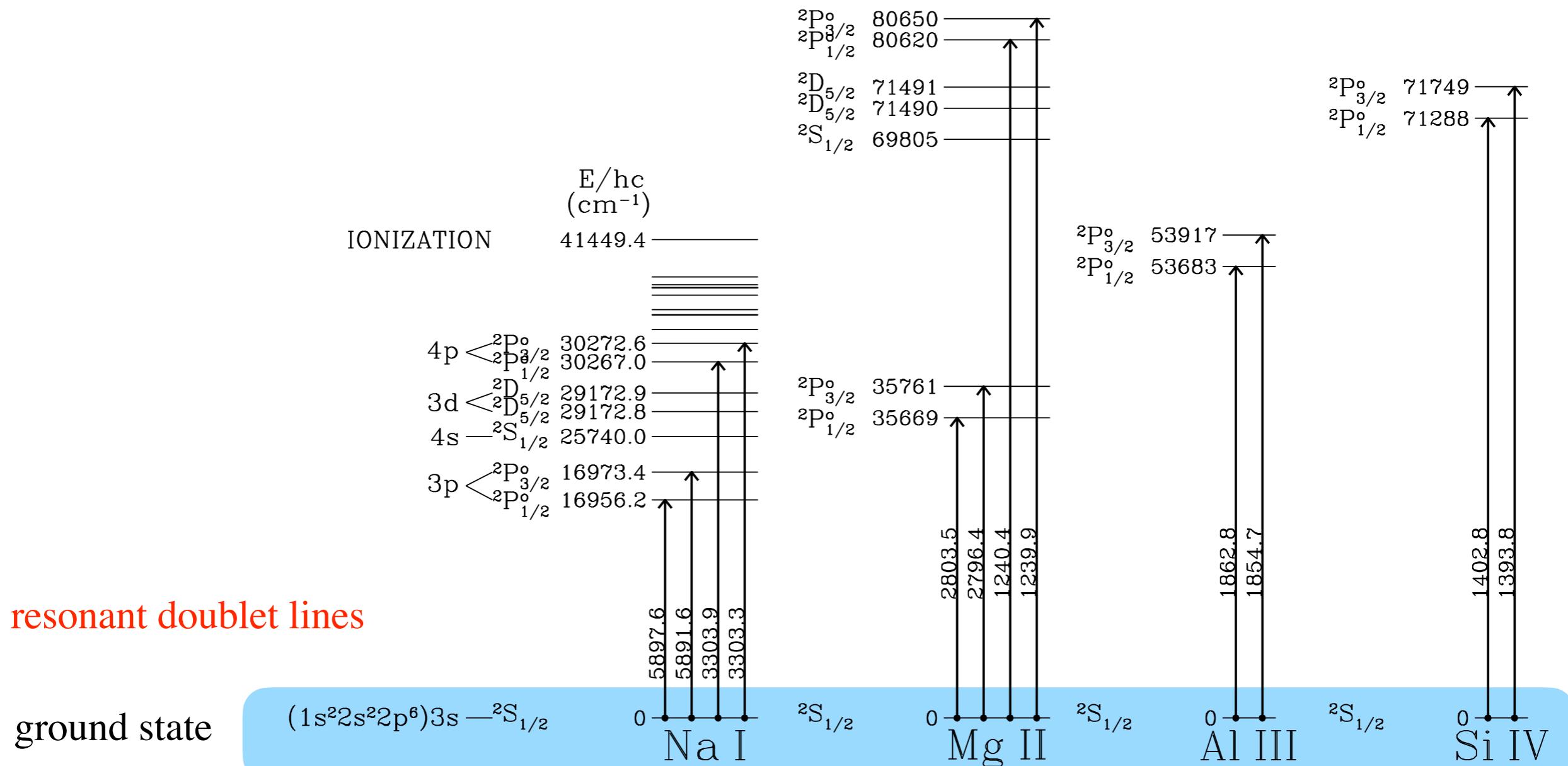


- 11 electrons

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

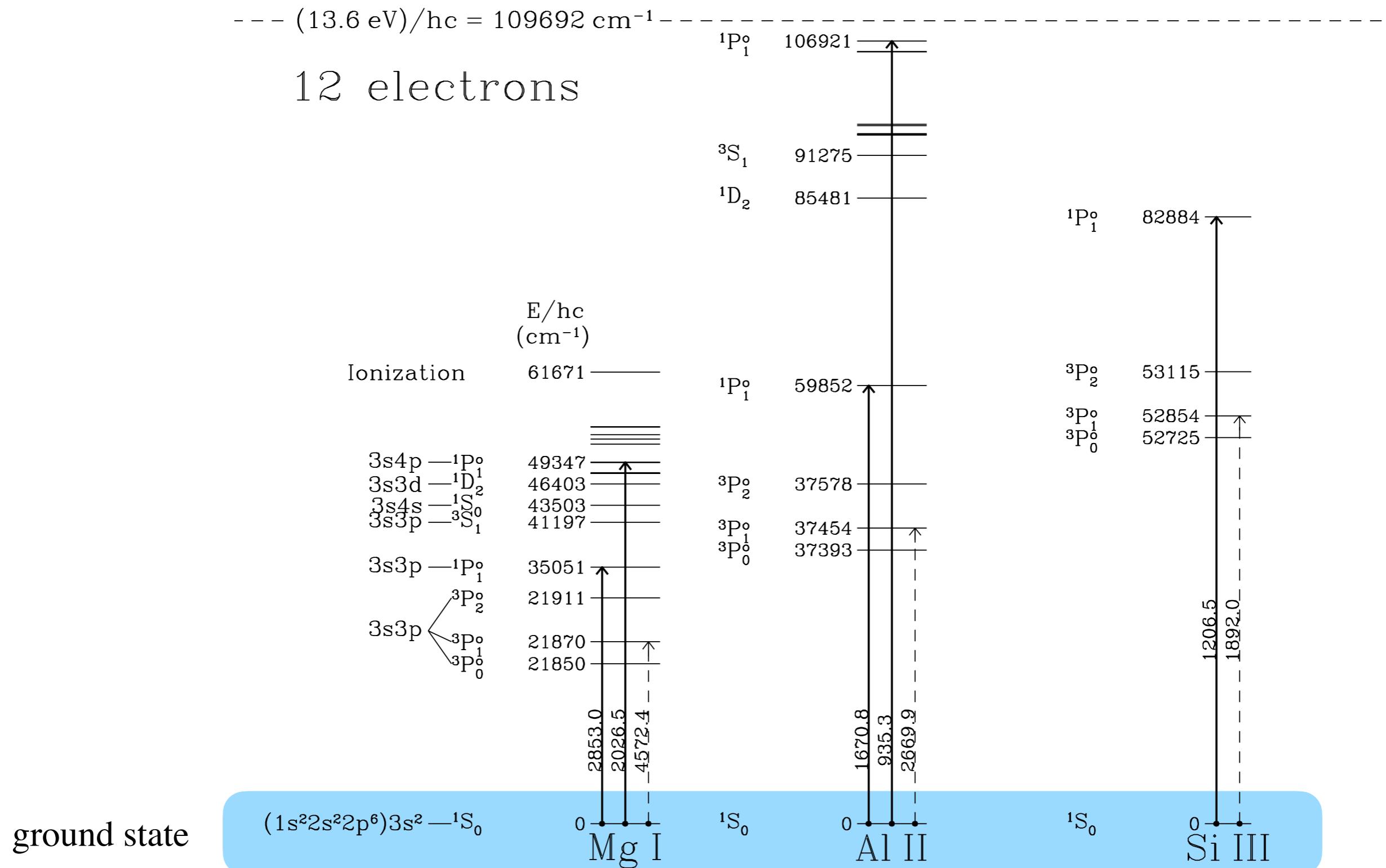
$$\text{---} (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1} \text{---} \text{---} \text{---}$$

11 electrons



- 12 electrons

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

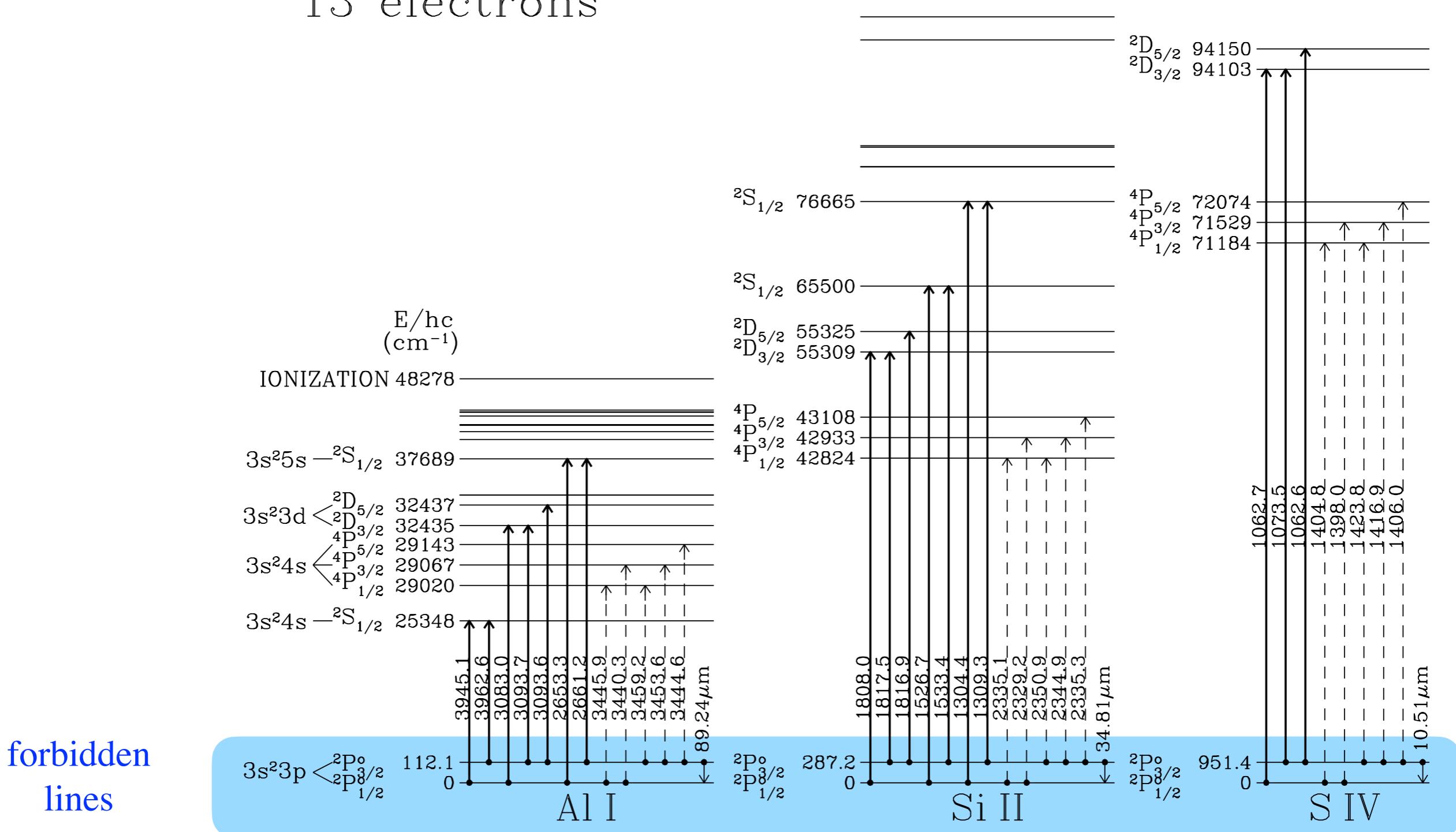


- 13 electrons

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

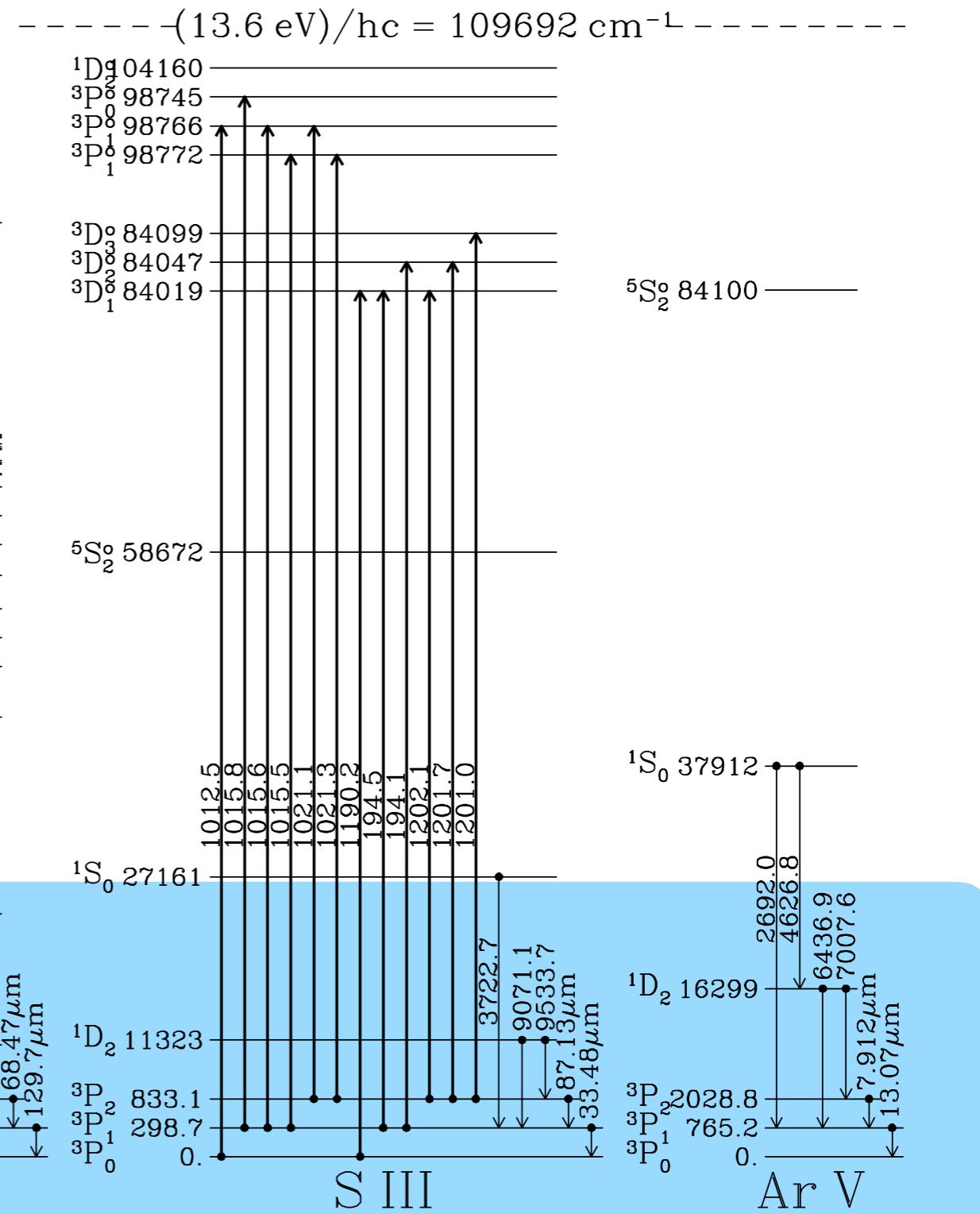
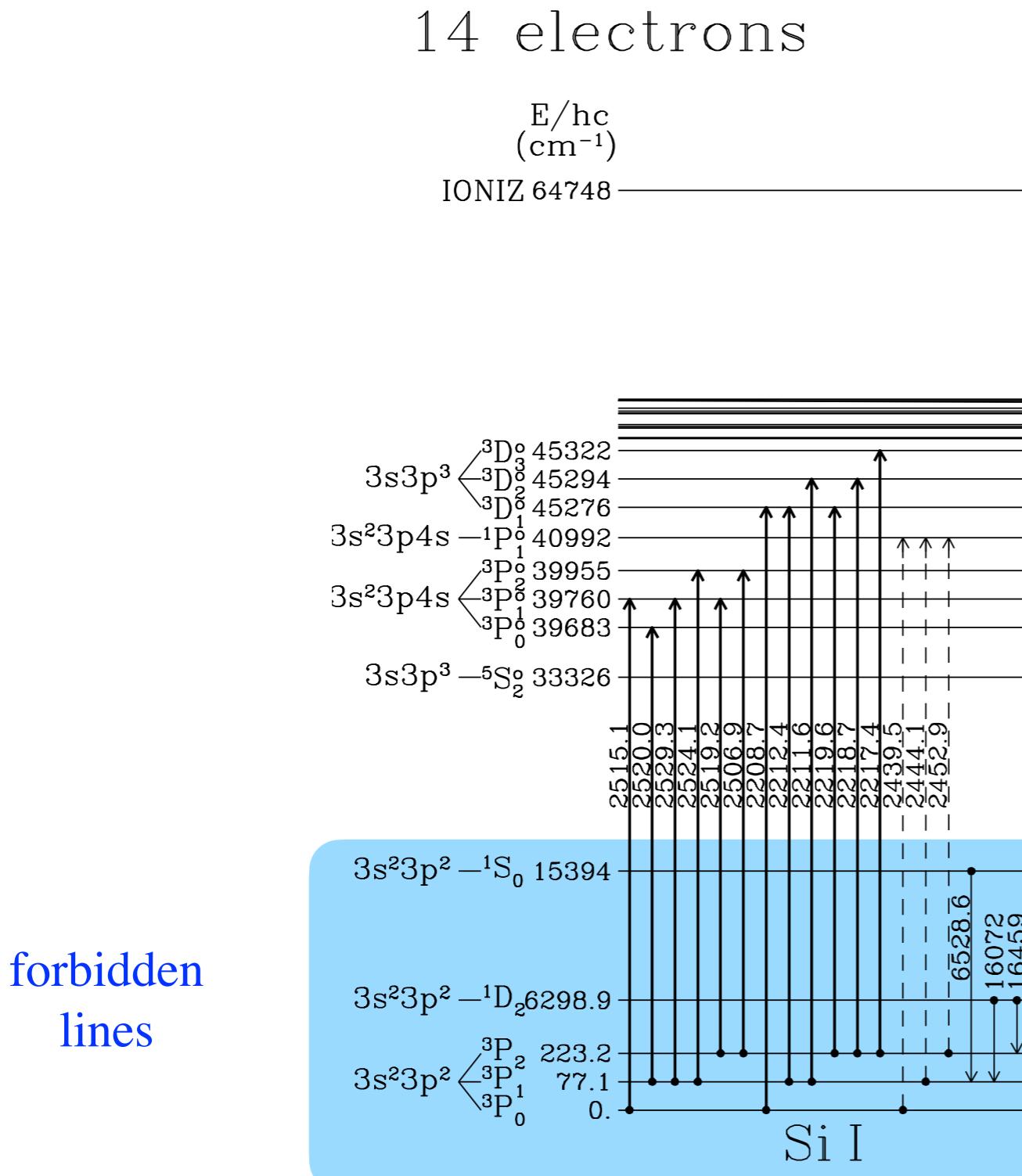
$$\text{--- } (13.6 \text{ eV})/\hbar c = 109692 \text{ cm}^{-1}$$

13 electrons



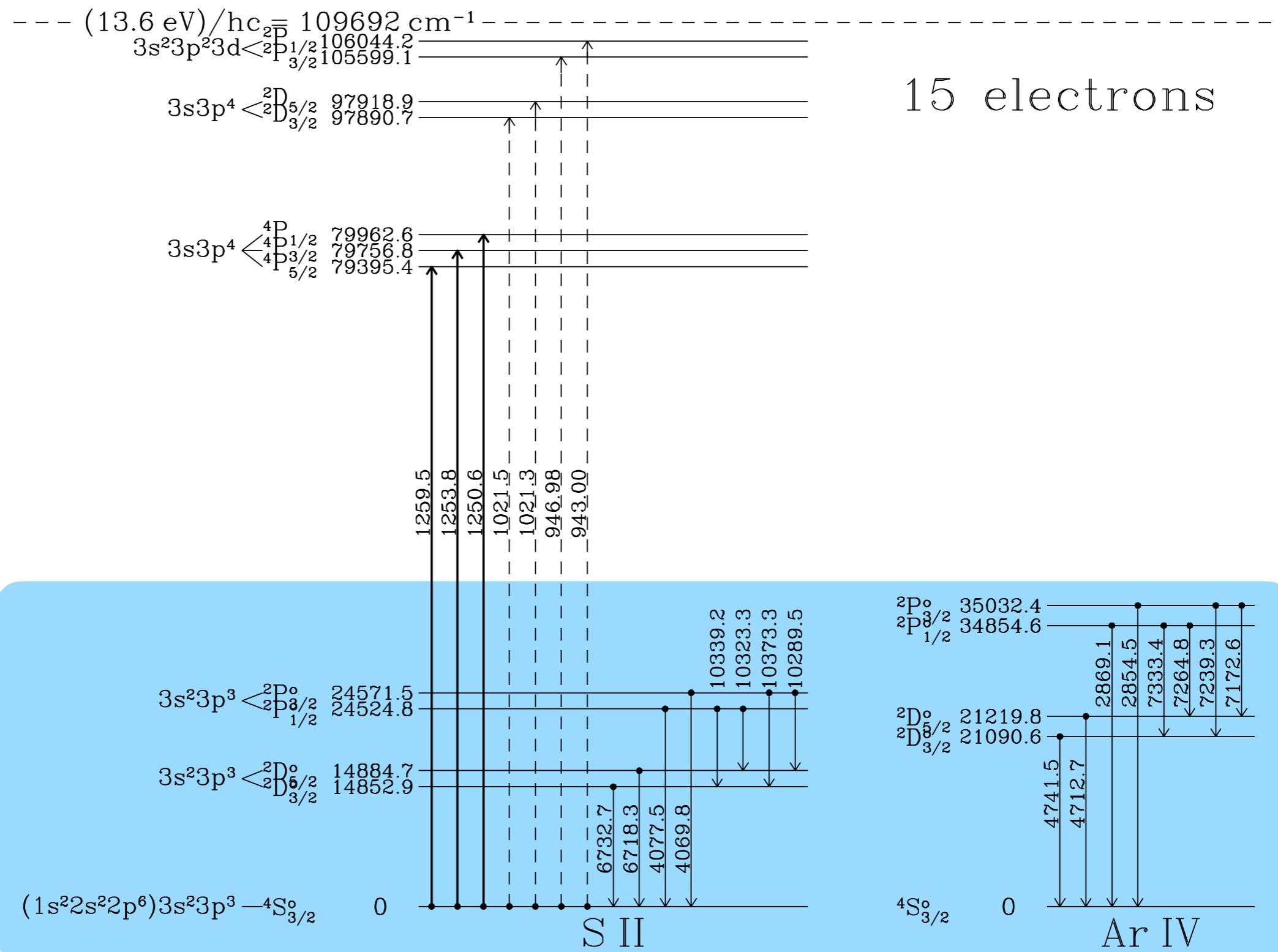
- 14 electrons

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



- 15 electrons

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



Neutral Medium

- Intrinsic Line Profile
- Excitation & De-excitation
- Optical/UV Absorption Line
 - Curve of Growth
 - H I 21 cm line
- Cold Neutral Medium & Warm Neutral Medium

< Line Profile > Classical model

- **Lorentz Oscillator Model** to describe the interaction between atoms and electric fields
 - The electron (with a small mass) is bound to the nucleus of the atom (with a much larger mass) by a force that behaves according to Hooke's Law (a spring-like force).
 - An applied electric field would then interact with the charge of the electron, causing “stretching” or “compression” of the spring.
 - ***The electron's equation of motion:***

$$m\ddot{\mathbf{x}} = -k\mathbf{x} + \mathbf{F}_{\text{ext}} + \mathbf{F}_{\text{rad}}$$

Here, m = electron mass

$k = m\omega_0^2$, where k = spring constant

ω_0 = natural (fundamental or resonant) frequency

\mathbf{F}_{ext} = external force, driving force, or external electric field

\mathbf{F}_{rad} = radiation reaction force (radiation damping)
the damping of a charge's motion which arises because of
the emission of radiation

[1] Spontaneous Emission : Damping, Free Oscillator

- **Undriven Harmonically Bound Particles** (free oscillator)
 - Since an oscillating electron represents a continuously accelerating charge, the electron will radiate energy.
 - The energy radiated away must come from the particle's own energy (energy conservation). In other words, **there must be a force acting on a particle by virtue of the radiation it produces. This is called the *radiation reaction force*.**
 - Let's derive the formula for the radiation reaction force from the fact that the energy radiated must be compensated for by the work done against the radiation reaction force.
 - (1) The radiative loss rate of energy, averaged over one cycle of the oscillating dipole, can be represented by the radiative reaction force:

$$\boxed{\frac{dW}{dt} = \langle \mathbf{F}_{\text{rad}} \cdot \dot{\mathbf{x}} \rangle}$$

- (2) From the *Larmor's formula* for a dipole, the radiative loss will be:

$$\boxed{\frac{dW}{dt} = -\frac{2e^2 \langle |\ddot{\mathbf{x}}|^2 \rangle}{3c^3}}$$

$$\frac{dW}{d\omega} = \frac{8\pi\omega^4}{3c^3} e^2 |\bar{x}(\omega)|^2$$

angular frequency : $\omega = 2\pi\nu$

[1] Spontaneous Emission : Abraham-Lorentz formula

$$\therefore \langle \mathbf{F}_{\text{rad}} \cdot \dot{\mathbf{x}} \rangle = -\frac{2e^2 \langle |\ddot{\mathbf{x}}|^2 \rangle}{3c^3}$$

Here, $\langle |\ddot{\mathbf{x}}|^2 \rangle \equiv \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} \ddot{\mathbf{x}} \cdot \ddot{\mathbf{x}} dt$ where τ is the **oscillation period**.

$$= \frac{1}{\tau} \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} \Big|_{-\tau/2}^{\tau/2} - \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} dt$$

We assume that the radiation loss is very slow and thus the initial and final states are approximately the same: $\ddot{\mathbf{x}} \cdot \dot{\mathbf{x}}(-\tau/2) = \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}}(\tau/2)$

Then,

$$\langle |\ddot{\mathbf{x}}|^2 \rangle = -\frac{1}{\tau} \int_{-\tau/2}^{\tau/2} \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} dt = -\langle \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} \rangle \rightarrow \langle \mathbf{F}_{\text{rad}} \cdot \dot{\mathbf{x}} \rangle = \frac{2e^2 \langle \ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} \rangle}{3c^3}$$

Therefore, we can obtain

$$\mathbf{F}_{\text{rad}} = \frac{2e^2 \ddot{\mathbf{x}}}{3c^3} : \text{Abraham-Lorentz formula}$$

- **Abraham-Lorentz formula:**

$$\mathbf{F}_{\text{rad}} = \frac{2e^2 \ddot{\mathbf{x}}}{3c^3}$$

- This formula depends on the derivative of acceleration. This increases the degree of the equation of motion of a particle and can lead to some nonphysical behavior if not used properly and consistently.
- For a simple harmonic oscillator with a frequency ω_0 , we can avoid the difficulty by using

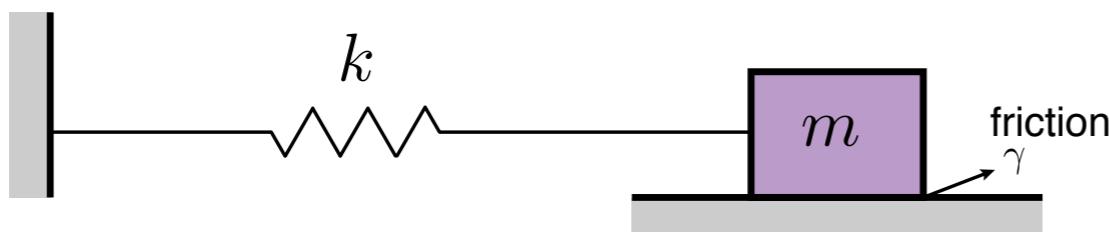
$$\ddot{\mathbf{x}} = -\omega_0^2 \dot{\mathbf{x}} \quad \leftarrow \quad \begin{aligned} x(t) &= x_0 \cos(\omega_0 t) & \ddot{x}(t) &= -\omega_0^2 x(t) \\ \dot{x}(t) &= -\omega_0 x_0 \sin(\omega_0 t) & \ddot{x}(t) &= -\omega_0^2 \dot{x}(t) \end{aligned}$$

- ***This is a good assumption as long as the energy is to be radiated on a time scale that is long compared to the period of oscillation ($\gamma \ll \omega_0$).*** In this regime, ***radiation reaction may be considered as a perturbation on the particle's motion.***

We then rewrite the radiation reaction force as

$$\mathbf{F}_{\text{rad}} = -\frac{2e^2 \omega_0^2}{3c^3} \dot{\mathbf{x}} = -m\gamma \dot{\mathbf{x}},$$

$$\gamma \equiv \frac{2e^2 \omega_0^2}{3mc^3} : \text{damping constant}$$



$$m\ddot{\mathbf{x}} + k\mathbf{x} + m\gamma \dot{\mathbf{x}} = 0$$

This is the equation for a string-mass system subject to friction damping.

- Therefore, the equation of motion of the electron in a Lorentz atom is

$$\ddot{\mathbf{x}} + \gamma \dot{\mathbf{x}} + \omega_0^2 \mathbf{x} = 0$$

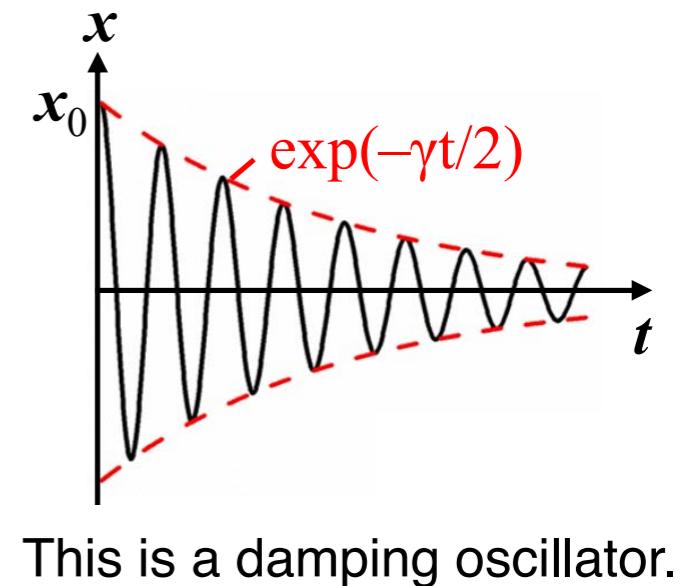
- This equation may be solved by assuming that $x(t) \propto e^{\alpha t}$.

$$\begin{aligned}\alpha^2 + \gamma\alpha + \omega_0^2 &= 0 \rightarrow \alpha = -(\gamma/2) \pm \sqrt{(\gamma/2)^2 - \omega_0^2} \\ &= -\gamma/2 \pm i\omega_0 + \mathcal{O}(\gamma^2/\omega_0^2)\end{aligned}$$

Here, we assumed $\gamma \ll \omega_0$.

- Assuming initial conditions: $x(0) = x_0$, $\dot{x}(0) = 0$ at $t = 0$
- we have

$$x(t) = \frac{1}{2}x_0 \left[e^{-(\gamma/2 - i\omega_0)t} + e^{-(\gamma/2 + i\omega_0)t} \right] = x_0 e^{-\gamma t/2} \cos \omega_0 t \quad \longrightarrow$$



- Power spectrum:

$$\bar{x}(\omega) = \frac{1}{2\pi} \int_0^\infty x(t) e^{i\omega t} dt = \frac{x_0}{4\pi} \left[\frac{1}{\gamma/2 - i(\omega + \omega_0)} + \frac{1}{\gamma/2 - i(\omega - \omega_0)} \right]$$

- This becomes large in the vicinity of $\omega = \omega_0$ and $\omega = -\omega_0$.
- We are ultimately interested only in **positive frequencies**, and only in regions in which the values become large. Therefore, we obtain

$$\bar{x}(\omega) \approx \frac{x_0}{4\pi} \frac{1}{\gamma/2 - i(\omega - \omega_0)}, \quad |\bar{x}(\omega)|^2 = \left(\frac{x_0}{4\pi} \right)^2 \frac{1}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

- Spontaneous Emission: Line profile

- Recall the Larmor's formula:

$$\frac{dW}{d\omega} = \frac{8\pi\omega^4}{3c^3} e^2 |\bar{x}(\omega)|^2$$

- Energy radiated per unit frequency:

$$\begin{aligned}\frac{dW}{d\omega} &= \frac{8\pi\omega^4}{3c^3} \frac{e^2 x_0^2}{(4\pi)^2} \frac{1}{(\omega - \omega_0)^2 + (\gamma/2)^2} = \frac{1}{2} m \left(\frac{\omega^4}{\omega_0^2} \right) x_0^2 \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2} \\ &\approx \frac{1}{2} m \omega_0^2 x_0^2 \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2}\end{aligned}$$

- For a harmonic oscillator, note that the equation of motion is $\mathbf{F} = -k\mathbf{x} = -m\omega_0^2\mathbf{x}$, spring constant is $k = m\omega_0^2$, and the potential energy (energy stored in spring) is $(1/2)kx_0^2$.

- From

$$\int_{-\infty}^{\infty} \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2} d\omega = \frac{1}{\pi} \tan^{-1} \{ 2(\omega - \omega_0)/\gamma \} \Big|_{-\infty}^{\infty} = 1$$

- Note that the total emitted energy is equal to the initial potential energy of the oscillator:

$$W = \int_0^{\infty} \frac{dW}{d\omega} d\omega = \frac{1}{2} k x_0^2$$

- Profile of the emitted spectrum:

$$\phi(\omega) = \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

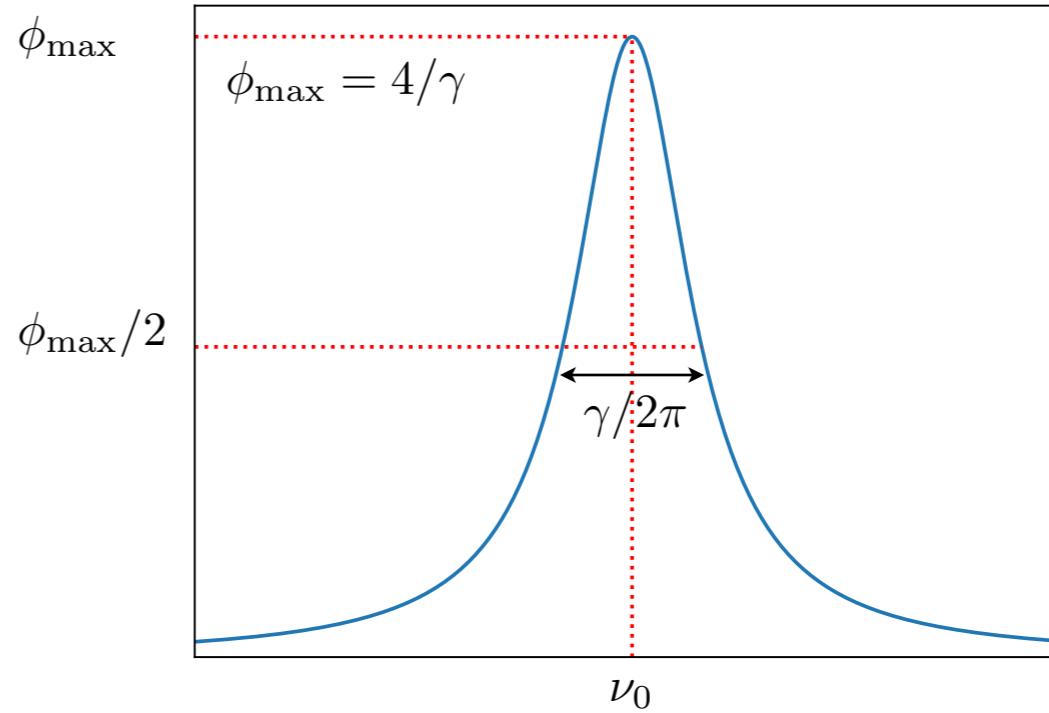
This is the Lorentz (natural) line profile.

- Damping constant is the full width at half maximum (FWHM).

$$\phi(\omega) = \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$

Note $\phi(\omega)d\omega = \phi(\nu)d\nu$



- In this solution, *the line width $\Delta\omega = \gamma$ is a universal constant* when expressed in terms of wavelength:

$$\lambda = \frac{2\pi c}{\omega} \quad (\omega = 2\pi\nu)$$

$$\begin{aligned} \Delta\lambda &= 2\pi c \frac{\Delta\omega}{\omega^2} = 2\pi c \frac{2}{3} \frac{r_e}{c} \quad \leftarrow \quad \left(\Delta\omega = \gamma = \frac{2}{3} r_e \frac{\omega_0^2}{c} \right) \\ &= \frac{4}{3} \pi r_e \\ &= 1.2 \times 10^{-4} \text{\AA} \end{aligned}$$

However, **in Quantum Mechanics, the line width is not a universal constant.**

[2] Absorption/Scattering : Driven Oscillator

- **Driven Harmonically Bound Particles** (forced oscillators)

- Electron's equation of motion (electric charge = $-e$): $\mathbf{F}_{\text{ext}} = -e\mathbf{E}_0 e^{i\omega t}$

$$\ddot{\mathbf{x}} + \gamma \dot{\mathbf{x}} + \omega_0^2 \mathbf{x} = -\frac{e\mathbf{E}_0}{m} e^{i\omega t}$$



- A particular solution for this inhomogeneous differential equation:

$$\mathbf{x} = \mathbf{x}_0 e^{i\omega t} \equiv |\mathbf{x}_0| e^{i(\omega t + \delta)} \rightarrow (-\omega^2 + i\omega\gamma + \omega_0^2) \mathbf{x}_0 e^{i\omega t} = -\frac{e\mathbf{E}_0}{m} e^{i\omega t}$$

$$\mathbf{x}_0 = \frac{(e/m)\mathbf{E}_0}{(\omega^2 - \omega_0^2) - i\omega\gamma}$$

$$\mathbf{x}_0 = |\mathbf{x}_0| e^{i\delta} \propto (\omega^2 - \omega_0^2) + i\omega\gamma \rightarrow \delta = \tan^{-1} \left(\frac{\omega\gamma}{\omega^2 - \omega_0^2} \right)$$

The response is slightly out of phase with respect to the imposed field.

- Time-averaged total power radiated is given by

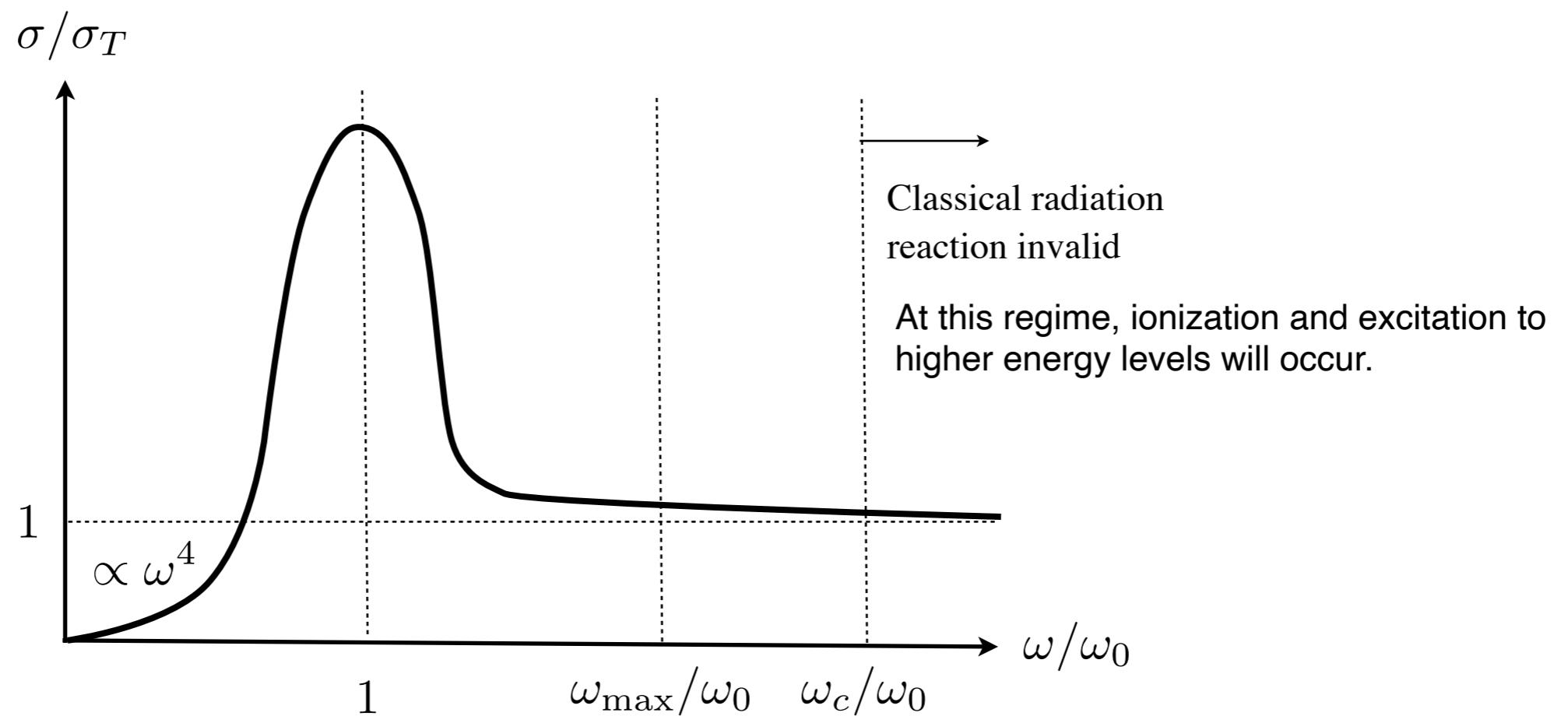
$$\begin{aligned} P &= \left\langle \frac{dW}{dt} \right\rangle = \frac{2e^2 \langle |\ddot{\mathbf{x}}|^2 \rangle}{3c^3} = \frac{e^2 \omega^4 |\mathbf{x}_0|^2}{3c^3} \\ &= \frac{e^4 E_0^2}{3m^2 c^3} \frac{\omega^4}{(\omega^2 - \omega_0^2)^2 + (\omega\gamma)^2} \end{aligned}$$

- Scattering cross section:

Poynting flux:

$$\sigma_{\text{sca}} \equiv \frac{\langle P \rangle}{\langle S \rangle}, \quad \langle S \rangle = \frac{c}{8\pi} E_0^2 \quad \longrightarrow \quad \sigma_{\text{sca}}(\omega) = \frac{8\pi e^4}{3m^2 c^4} \frac{\omega^4}{(\omega^2 - \omega_0^2)^2 + (\omega\gamma)^2}$$

$$= \sigma_T \frac{\omega^4}{(\omega^2 - \omega_0^2)^2 + (\omega\gamma)^2}$$



- Limiting Cases of Interest

(a) $\omega \gg \omega_0$ (Thomson scattering by free electron)

$$\sigma_{\text{sca}} = \sigma_T = \frac{8\pi}{3} r_e^2$$

- ▶ At high incident energies, the binding becomes negligible. Therefore, this corresponds to the case of a free electron.

(b) $\omega \ll \omega_0$ (Rayleigh scattering by bound electron)

$$\sigma_{\text{sca}} = \sigma_T \left(\frac{\omega}{\omega_0} \right)^4 = \sigma_T \left(\frac{\lambda_0}{\lambda} \right)^4$$

- ▶ Rayleigh scattering refers to the ***scattering of light by particles smaller than the wavelength of the light.***
- ▶ The strong wavelength dependence of the scattering means that shorter (blue) wavelengths are scattered more strongly than longer wavelengths.
- ▶ (blue color of the sky) This dependence results in the indirect blue light coming from all regions of the sky.
- ▶ (red color of the sun at sunset) Conversely, glancing toward the Sun, the colors that were not scattered away - the longer wavelengths such as red and yellow light - are directly visible, giving the Sun itself a slightly yellowish color.
- ▶ However, viewed from space, the sky is black and the Sun is white.

- Absorption/Scattering : Line Profile

(c) $\omega \approx \omega_0$ (resonance scattering of line radiation)

$$\begin{aligned}\sigma_{\text{sca}}(\omega) &\approx \sigma_T \frac{\omega_0^4}{(\omega - \omega_0)^2(2\omega_0)^2 + (\omega_0\gamma)^2} \\ &= \sigma_T \frac{\omega_0^2/4}{(\omega - \omega_0)^2 + (\gamma/2)^2} \\ \sigma_T \frac{\omega_0^2}{4} &= \frac{8\pi}{3} \left(\frac{e^2}{mc^2} \right)^2 \times \frac{1}{4} \times \left(\gamma \frac{3}{2} \frac{mc^3}{e^2\omega_0^2} \right) = 2\pi^2 \frac{e^2}{mc} (\gamma/2\pi)\end{aligned}$$

Note that $\nu = \omega/2\pi$ and $\sigma_\nu = 2\pi\sigma_\omega$.

$$\boxed{\begin{aligned}\sigma_\omega &= \frac{2\pi^2 e^2}{m_e c} \frac{\gamma/2\pi}{(\omega - \omega_0)^2 + (\gamma/2)^2} \\ \sigma_\nu &= \frac{\pi e^2}{m_e c} \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}\end{aligned}}$$

- ▶ In the neighborhood of the resonance, ***the shape of the absorption/scattering cross-section is the same as the (spontaneous) emission line profile from the free oscillator. This conclusion can also be obtained from the argument about the Einstein coefficients.***
- ▶ Total scattering cross section is
- **Resonance line**
 - A spectral line caused by an electron jumping ***between the “ground” state and the “first excited” energy level in an atom or ion.*** It is the longest wavelength line produced by a jump to or from the ground state.
 - Because the majority of electrons are in the ground state in many astrophysical environments, and because the energy required to reach the first excited level is the least needed for any transition, resonance lines are the strongest lines in the spectrum for any given atom or ion.

- ***In the quantum theory of spectral lines,***

we obtain similar formulas, which are conveniently stated in terms of the classical results as

$$\sigma_\nu = f_{nn'} \frac{\pi e^2}{m_e c} \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$

$$\int_0^\infty \sigma_\nu d\nu = f_{nn'} \frac{\pi e^2}{m_e c}$$

where $f_{nn'}$ is called the **oscillator strength** or **f-value** for the transition between states n and n' .

Selected Resonance Lines^a with $\lambda < 3000 \text{ \AA}$

	Configurations	ℓ	u	$E_\ell/hc(\text{ cm}^{-1})$	$\lambda_{\text{vac}}(\text{ \AA})$	$f_{\ell u}$
C IV	$1s^2 2s - 1s^2 2p$	$^2S_{1/2}$	$^2P_{1/2}^o$	0	1550.772	0.0962
		$^2S_{1/2}$	$^2P_{3/2}^o$	0	1548.202	0.190
N V	$1s^2 2s - 1s^2 2p$	$^2S_{1/2}$	$^2P_{1/2}^o$	0	1242.804	0.0780
		$^2S_{1/2}$	$^2P_{3/2}^o$	0	1242.821	0.156
O VI	$1s^2 2s - 1s^2 2p$	$^2S_{1/2}$	$^2P_{1/2}^o$	0	1037.613	0.066
		$^2S_{1/2}$	$^2P_{3/2}^o$	0	1037.921	0.133
C III	$2s^2 - 2s 2p$	1S_0	$^1P_1^o$	0	977.02	0.7586
C II	$2s^2 2p - 2s 2p^2$	$^2P_{1/2}^o$	$^2D_{3/2}^o$	0	1334.532	0.127
		$^2P_{3/2}^o$	$^2D_{5/2}^o$	63.42	1335.708	0.114
N III	$2s^2 2p - 2s 2p^2$	$^2P_{1/2}^o$	$^2D_{3/2}^o$	0	989.790	0.123
		$^2P_{3/2}^o$	$^2D_{5/2}^o$	174.4	991.577	0.110
CI	$2s^2 2p^2 - 2s^2 2p 3s$	3P_0	$^3P_1^o$	0	1656.928	0.140
		3P_1	$^3P_2^o$	16.40	1656.267	0.0588
		3P_2	$^3P_2^o$	43.40	1657.008	0.104
N II	$2s^2 2p^2 - 2s 2p^3$	3P_0	$^3D_1^o$	0	1083.990	0.115
		3P_1	$^3D_2^o$	48.7	1084.580	0.0861
		3P_2	$^3D_3^o$	130.8	1085.701	0.0957
NI	$2s^2 2p^3 - 2s^2 2p^2 3s$	$^4S_{3/2}^o$	$^4P_{5/2}$	0	1199.550	0.130
		$^4S_{3/2}^o$	$^4P_{3/2}$	0	1200.223	0.0862
OI	$2s^2 2p^4 - 2s^2 2p^3 3s$	3P_2	$^3S_1^o$	0	1302.168	0.0520
		3P_1	$^3S_1^o$	158.265	1304.858	0.0518
		3P_0	$^3S_1^o$	226.977	1306.029	0.0519
Mg II	$2p^6 3s - 2p^6 3p$	$^2S_{1/2}$	$^2P_{1/2}^o$	0	2803.531	0.303
		$^2S_{1/2}$	$^2P_{3/2}^o$	0	2796.352	0.608
Al III	$2p^6 3s - 2p^6 3p$	$^2S_{1/2}$	$^2P_{1/2}^o$	0	1862.790	0.277
		$^2S_{1/2}$	$^2P_{3/2}^o$	0	1854.716	0.557

Table 9.4 in [Draine]

See also Table 9.3

[3] Line Broadening Mechanisms

- ***Atomic levels are not infinitely sharp***, nor are the lines connecting them.
 - (1) Doppler (Thermal) Broadening
 - (2) Natural Broadening
 - (3) Collisional Broadening
 - (4) Thermal Doppler + Natural Broadening
- **[1] Doppler (Thermal) Broadening**
 - The simplest mechanism for line broadening in the Doppler effect. An atom is in thermal motion, so that the frequency of emission or absorption in its own frame corresponds to a different frequency for an observer.
 - Each atom has its own Doppler shift, so that the net effect is to spread the line out, but not to change its total strength.
 - The change in frequency associated with an atom with velocity component v_z along the photon propagation direction (say, z axis) is, to lowest order in v_z/c , given by

$$\nu - \nu_0 = \nu_0 \frac{v_z}{c}$$

Recall Doppler shift: $\left[\frac{\nu}{\nu_0} = \frac{1}{\gamma(1 - \beta \cos \theta)} \rightarrow \nu \approx \nu_0 (1 + \beta \cos \theta) \rightarrow \nu - \nu_0 = \frac{\nu_0 v_z}{c} \right]$

- Here, ν_0 is the rest-frame frequency.

-
- We need to consider the velocity distribution of atoms. The number of atoms having velocities in the range $(v_z, v_z + dv_z)$ is proportional to

$$f(v_z)dv_z = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mv_z^2}{2kT}\right) dv_z \quad \text{Here, } m = \text{mass of the atom}$$

- From the Doppler shift formula, we have

$$v_z = \frac{c(\nu - \nu_0)}{\nu_0} \rightarrow dv_z = \frac{cd\nu}{\nu_0}$$

- Therefore, the strength of the emission is proportional to

$$\exp\left(-\frac{mv_z^2}{2kT}\right) dv_z \propto \exp\left[-\frac{mc^2(\nu - \nu_0)^2}{2\nu_0^2 kT}\right] d\nu$$

- Then, the normalized profile function is

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-(\nu - \nu_0)^2 / (\Delta\nu_D)^2}$$

where

$\Delta\nu_D = \frac{\nu_0}{c} v_{\text{th}}$ is the Doppler width.

$v_{\text{th}} = \sqrt{\frac{2kT}{m}}$ is the thermal velocity.

$$\left(v_{\text{rms}} = \sqrt{\frac{kT}{m}} \right)$$

- Numerical value of the velocity broadening is

$$v_{\text{th}} = \left(\frac{2k_{\text{B}}T}{m} \right)^{1/2} = 1.3 \text{ km s}^{-1} \left(\frac{T}{100 \text{ K}} \right)^{1/2} \left(\frac{m}{m_{\text{H}}} \right)^{-1/2}$$

- In addition to thermal motions, there can be turbulent velocities associated with macroscopic velocity fields. The turbulent motions are accounted for by an effective Doppler width.

$$\Delta\nu_{\text{D}} = \nu_0 \frac{b}{c}$$

$$b \equiv (v_{\text{th}}^2 + v_{\text{turb}}^2)^{1/2}$$

where v_{turb} is $\sqrt{2}$ times a root-mean-square measure of the turbulent velocities. This assumes that the turbulent velocities also have a Gaussian distribution.

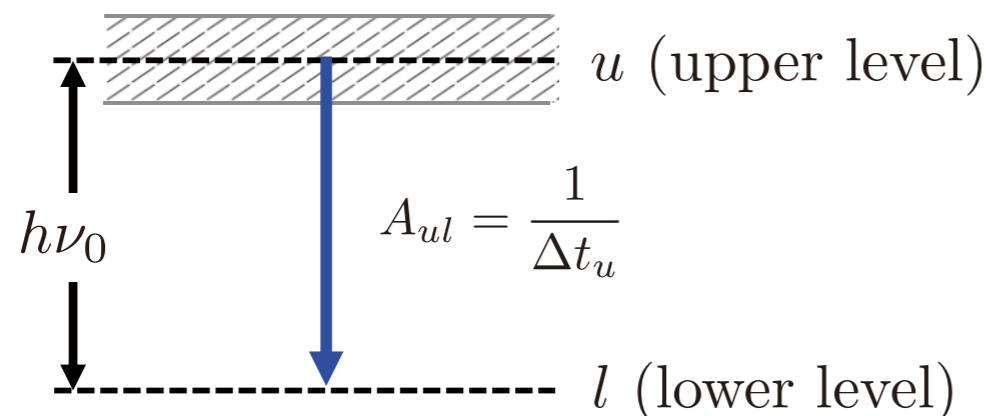
The convolution of two Gaussian functions with the widths (standard deviations) σ_1 and σ_2 is a Gaussian function with the width of σ , given by:

$$\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$$

• [2] Natural Broadening

- The intrinsic line width of a line is due to ***the Heisenberg uncertainty principle***. If an energy level u has a lifetime Δt , then uncertainty (spread) in energy ΔE must be $\Delta E \sim \hbar/\Delta t$ ($\hbar = h/2\pi$), and the resulting spread in the frequency of emitted photons is $\Delta\nu = \Delta E/h$.

(1) Line width due to the uncertainty principle:



A_{ul} = decay rate
= decay probability per unit time, Einstein A coefficient.

ΔE_u = uncertainty in energy of u

Δt_u = the uncertainty in time of occupation of u

$\Delta\nu_u$ = spread in frequency

$$= \Delta E_u/h = 1/(2\pi\Delta t_u) = A_{ul}/(2\pi)$$



(2) Line width of the Lorentz function:

$$\phi_\nu = \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$

In terms of the line width $\Delta\nu$, the normalized Lorentz profile can be rewritten as

$$\phi_\nu = \frac{1}{2\pi} \frac{\Delta\nu/2}{(\nu - \nu_0)^2 + (\Delta\nu/2)^2}$$

Hence, the FWHM of the Lorentz function: $\Delta\nu_u = \gamma/2\pi$



Comparing (1) and (2), we find that
 γ is equivalent to the Einstein A-coefficient., i.e., $\gamma = A_{ul}$.

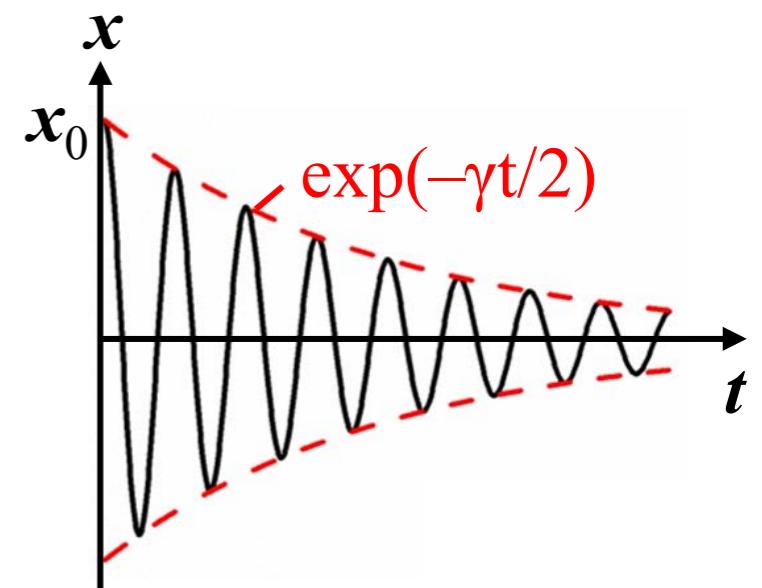
Classical physical Meaning

Suppose that the electric field is of the form $e^{-\gamma t/2}$ and then the energy decays proportional to $e^{-\gamma t}$.

We then have an emitted spectrum determined by the decaying sinusoid type of electric field.

Its Fourier transform (spectral profile) is a Lorentz (or natural, or Cauchy) profile:

$$\phi_\nu = \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$



Semiclassical (Weisskopf-Woolley) Picture of Quantum Levels

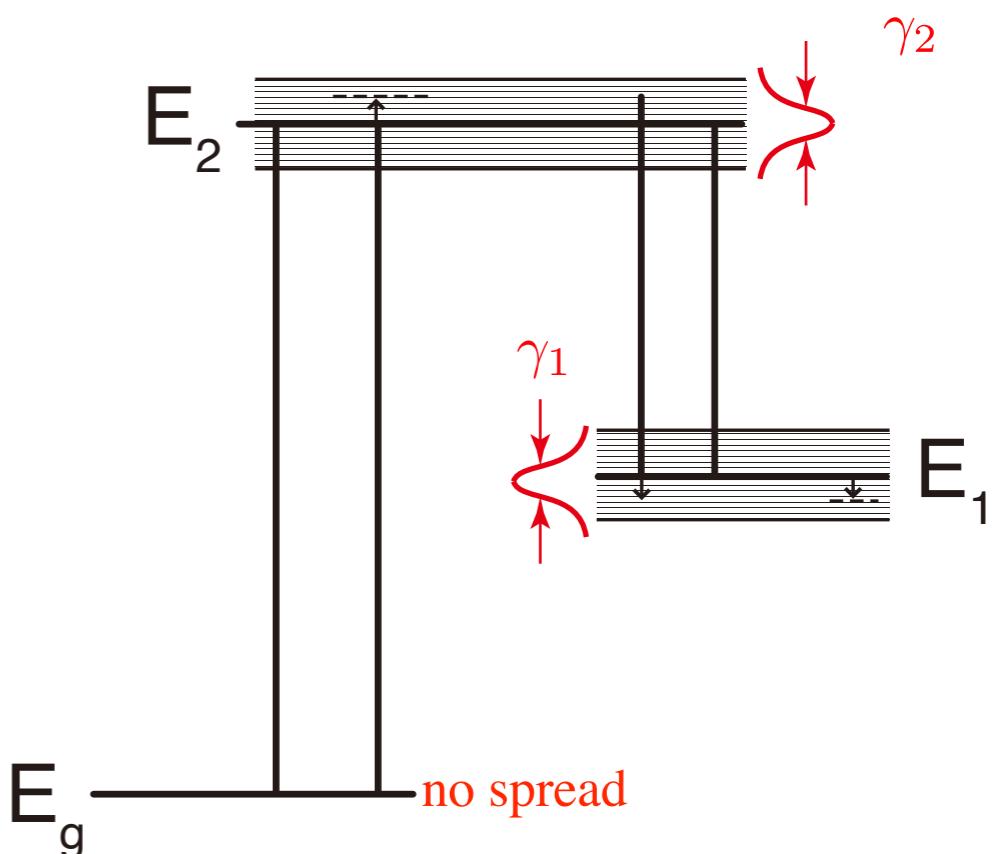
- In the semiclassical picture, each level is viewed as a continuous distribution of sublevels with energies close to the energy of the level (E_n).

The distribution of sublevels are explained by the Heisenberg Uncertainty Principle. The level has a lifetime $\Delta t = 1/A$ (A = Einstein A coefficient) and a spread in energy about $\Delta E \approx \hbar/\Delta t = \hbar A$.

$$\Delta E \Delta t \approx \hbar$$

The ground level has no spread in energy

because $\Delta t = \infty$.



The atom is in a definite sublevel of some level.

A transition in a spectral line is considered to be an **instantaneous transition** between a definite sublevel of an initial level to a definite sublevel of a final level.

- The energy spread of sublevels is described by a Lorentzian profile with the damping parameter of $\gamma = A$.*
- This picture implies that the emission line profile is the same as the absorption line profile.*

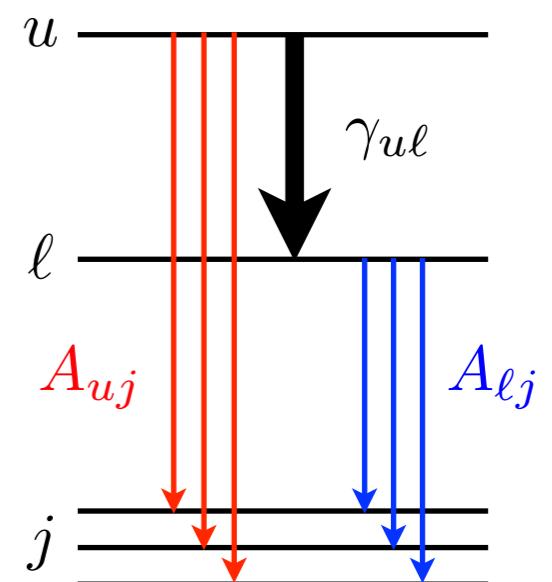
- The intrinsic line width is $\gamma = A_{ul}$.
 - This means forbidden lines are intrinsically narrower than permitted lines.
 - For instance, the permitted Ly α line has $A_{ul}/\nu_{ul} \sim 3 \times 10^{-7}$, while the forbidden [O III] 5007Å has a tiny width $A_{ul}/\nu_{ul} \sim 3 \times 10^{-17}$.
 - The intrinsic line width of [O III] 5007Å is equivalent to the Doppler broadening of

$$\Delta\nu_D = \nu_{ul} \frac{\Delta v}{c} \rightarrow \Delta v \sim 3 \times 10^{-17} c \sim 10 \text{ nm s}^{-1} \sim 30 \text{ cm yr}^{-1}$$

- For a multiple-level absorber, the upper and lower can both be broadened by transitions to other levels.

$$\gamma_{ul} = \sum_{E_j < E_u} A_{uj} + \sum_{E_j < E_\ell} A_{\ell j}$$

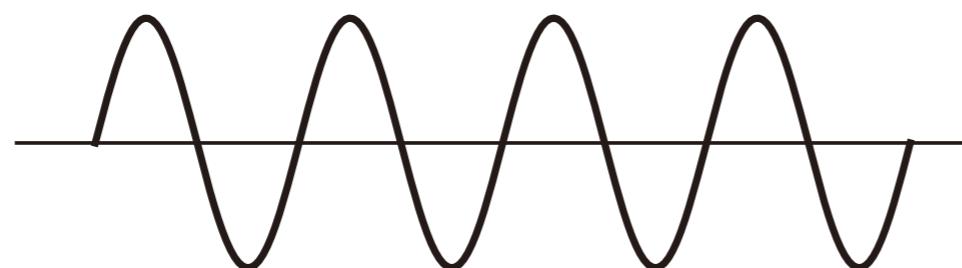
- For Ly α ($n = 1-2$), $\gamma_{ul} = A_{21} = 6.3 \times 10^8 \text{ s}^{-1}$
 $\Delta\nu/\nu = (\gamma/2\pi)/(c/\lambda) \sim 4 \times 10^{-8}$
- For H α ($n = 2-3$), $\gamma_{ul} = A_{32} + A_{31} + A_{21} = 8.9 \times 10^8 \text{ s}^{-1}$
 $\Delta\nu/\nu \sim 3 \times 10^{-7}$



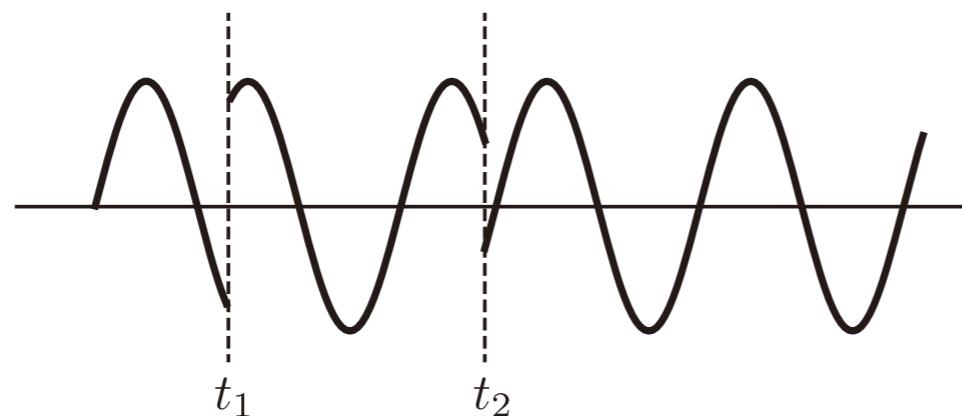
• [3] Collisional Broadening (or Pressure Broadening)

- The Lorentz profile applies even to certain types of collisional broadening mechanisms.
- If the atom suffers “*elastic*” collisions with other particles while it is emitting, the phase of the emitted radiation can be altered suddenly. If the phase changes completely randomly at the collision times, then information about the emitting frequencies is lost.
- If the collisions occur with frequency ν_{col} , that is, each atom experiences ν_{col} collisions per unit time on the average, then the profile is

$$\phi_\nu = \frac{\Gamma/4\pi^2}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \quad \text{where} \quad \Gamma = \gamma + 2\nu_{\text{col}}$$



purely sinusoidal



random phase interruptions
by atomic collisions

• [4] Voigt profile : Thermal + Natural broadening

- Atoms shows both a Lorentz profile plus the Doppler effect. In this case, we can write the profile as an average of the Lorentz profile over the various velocity states of the atom. Let's assume that the photon propagates along the z -axis.

Change of variables for the Maxwell distribution: $v_{\text{th}} \equiv \sqrt{\frac{2kT}{m}}$, $y \equiv \frac{v_z}{v_{\text{th}}}$

$$f_{v_z} = \frac{1}{\pi^{1/2} (2kT/m)^{1/2}} \exp(-mv_z^2/2kT) \longrightarrow f_y = \frac{1}{\pi^{1/2}} \exp(-y^2)$$

To interact with an atom with velocity v_z , the photon central frequency should be $\nu_0 + \nu_0(v_z/c)$. Then, the Lorentz profile at the frequency $\nu' = \nu - [\nu_0 + \nu_0(v_z/c)] = (\nu - \nu_0) - \nu_0(v_{\text{th}}/c)y$ is supposed to be multiplied with the Maxwell distribution.

Change of variables for the Lorentz function: $\phi_y^L = \phi_\nu^L \left| \frac{d\nu}{dy} \right| = \phi_\nu^L \times \left(\nu_0 \frac{v_{\text{th}}}{c} \right)$

Let $\Delta\nu_D \equiv \nu_0 \frac{v_{\text{th}}}{c}$, $u \equiv \frac{\nu - \nu_0}{\Delta\nu_D} = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_{\text{th}}}$, $a = \frac{\Gamma/4\pi}{\Delta\nu_D}$

$$\begin{aligned} \phi(\nu) &= \int_{-\infty}^{\infty} \phi_y^L f_y dy \\ &= \int_{-\infty}^{\infty} \left(\nu_0 \frac{v_{\text{th}}}{c} \right) \frac{\Gamma/4\pi^2}{[(\nu - \nu_0) - \nu_0(v_{\text{th}}/c)y]^2 + (\Gamma/4\pi)^2} \left(\frac{1}{\pi^{1/2}} \right) \exp(-y^2) dy \\ &= \frac{a}{\pi^{3/2} \Delta\nu_D} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(u - y)^2 + a^2} dy \end{aligned}$$

- The profile can be written using the Voigt function.

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} H(u, a)$$

Here, a is a ratio of the intrinsic broadening to the thermal broadening.

u is a measure of how far you are from the line center, in units of thermal broadening parameter.

In terms of Doppler velocity, u can be expressed as

$$u = \frac{\nu - \nu_0}{\Delta\nu_D} = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_{\text{th}}}$$

In the velocity term,

$$u = \frac{v}{v_{\text{th}}}, \text{ where } v = \frac{\nu - \nu_0}{\nu_0} c$$

Voigt-Hjerting function:

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_D}$$

$$u \equiv \frac{\nu - \nu_0}{\Delta\nu_D}$$

$$\Delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}}$$

Including the turbulent motion,

$$\Delta\nu_D = \nu_0 \frac{v_{\text{th}}}{c} \rightarrow \Delta\nu_D = \nu_0 \frac{b}{c} = \frac{b}{\lambda_0}$$

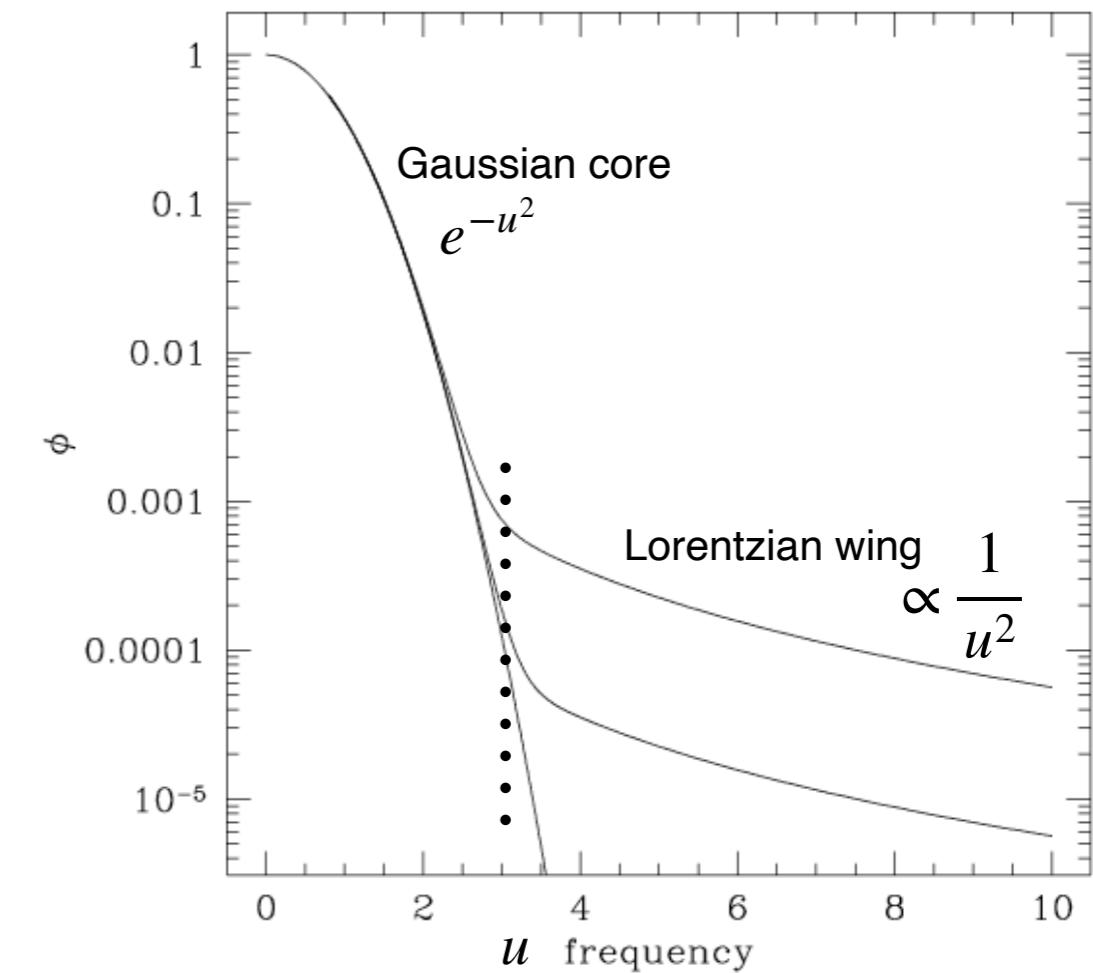
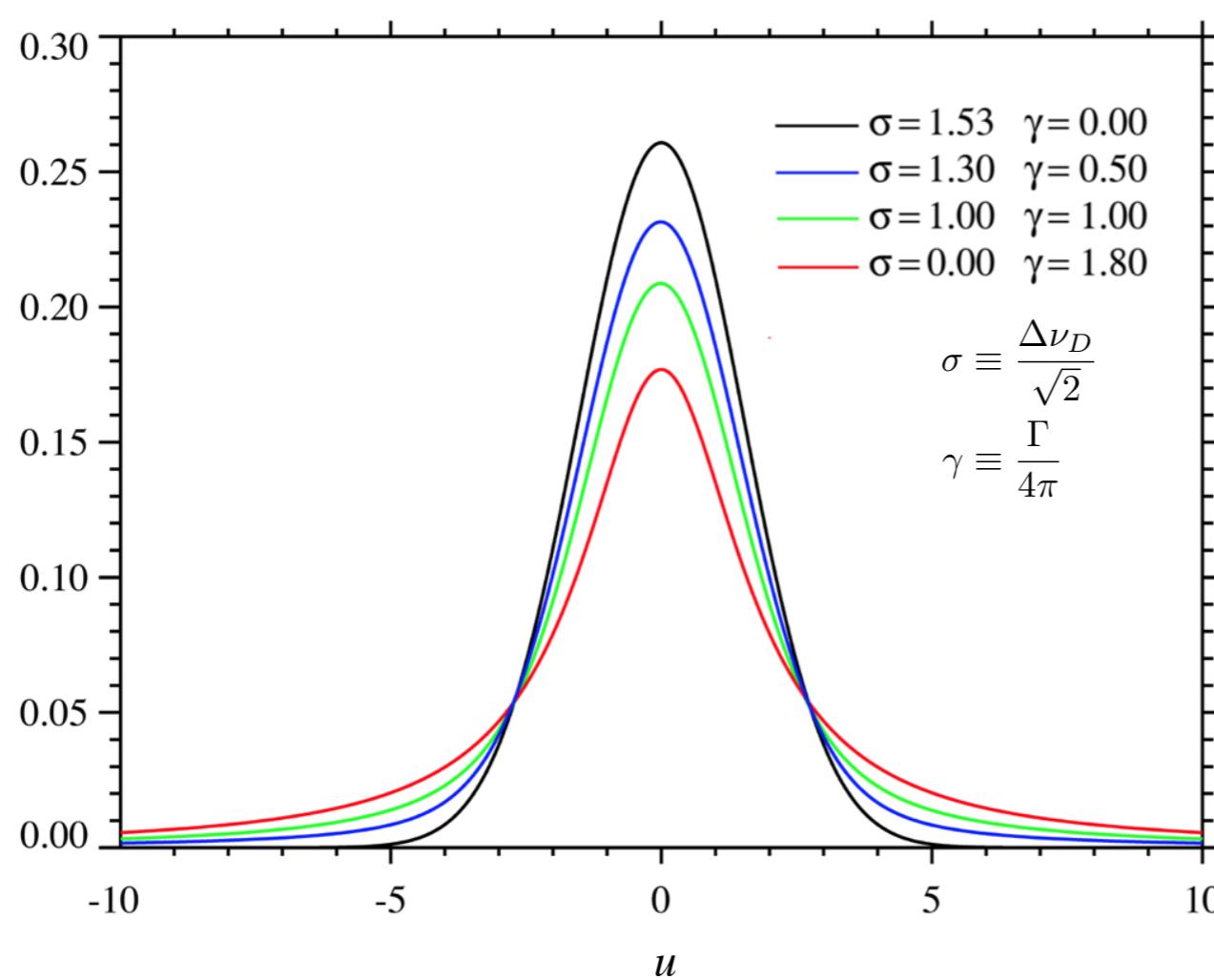
where $b = \sqrt{v_{\text{th}}^2 + v_{\text{turb}}^2}$, $v_{\text{th}} = \sqrt{\frac{2kT}{m}}$, $v_{\text{turb}} = \sqrt{2}\sigma_{\text{turb}}^{\text{rms}}$

$$u = \frac{v}{b}$$

Properties of Voigt Function

- For small a , the “core” of the line is dominated by the Gaussian (Doppler) profile, whereas the “wings” are dominated by the Lorentz profile.

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$



- In most case, $a \ll 1$. For Ly α at $T = 10^4$ K, $a \sim 0.005$.

- Line center:

$$H(0, a) = \exp(a^2) \operatorname{Erfc}(a) \approx 1 - \frac{2}{\sqrt{\pi}}a + a^2 - \mathcal{O}(a^3)$$

- Taylor series expansion of the Voigt function :

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$

- Near the line center ($u \rightarrow 0$), the contribution to the integral is dominated by $y = u$. Therefore,

$$H(u, a) \simeq \frac{a}{\pi} e^{-u^2} \int_{-\infty}^{\infty} \frac{dy}{y^2 + a^2} = e^{-u^2}$$

which is known as the Doppler core.

- In the line wings away from the core ($u \gg 1$), the integral is dominated by $y \sim 0$ because of the rapidly decreasing function in the numerator.

$$H(u, a) \simeq \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{u^2} = \frac{a}{\pi} \frac{\sqrt{\pi}}{u^2} = \frac{a}{\sqrt{\pi} u^2}$$

- In summary, we obtain the Voigt function in a Taylor series expansion around $a = 0$.

$$H(u, a) \approx H(u, 0) + a \left. \frac{dH}{da} \right|_{a=0} \approx e^{-u^2} + a \frac{1}{\sqrt{\pi} u^2}$$

- The first term represents the Gaussian core, provided by the thermal broadening, and the second term represents the Lorentzian damping wing.
- Transition from Doppler core to damping wing can be found by solving:

$$e^{u^2} = \frac{\sqrt{\pi}}{a} u^2 \quad \rightarrow \quad u^2 = \ln \left(\frac{\sqrt{\pi}}{a} \right) + \ln u^2$$

for hydrogen

$$b = 13 \text{ km s}^{-1} (T/10^4 \text{ K})^{1/2}$$

- The solution for this transcendental equation for Ly α is

$$u^2 \approx 10.31 + \ln \left[\left(\frac{6.265 \times 10^8 \text{ s}^{-1}}{\gamma_{ul}} \right) \left(\frac{1215.67 \text{ \AA}}{\lambda_{ul}} \right) \left(\frac{b}{10 \text{ km s}^{-1}} \right) \right]$$

provided that the quantity in square brackets is not very large or very small. The damping wing for $|u| \gtrsim 3.2$ or velocity shifts $|v| \gtrsim 3.2 (b/10 \text{ km s}^{-1})$.

Homework (due date: 04/07)

[Q5] Voigt profile

- We want to derive an approximate formula for the transition point from the Gaussian core to the Lorentz wing, which is defined by

$$u^2 = \ln(\sqrt{\pi}/a) + \ln u^2 \quad \text{or} \quad x = \ln(\sqrt{\pi}/a) + \ln x, \text{ where } x \equiv u^2$$

The above equation can be expressed in the form:

$$x = g(x) \text{ where } g(x) = \ln x + \ln(\sqrt{\pi}/a)$$

This equation can be solved using “**Fixed Point Iteration Method.**” Starting from any initial point x_0 , the following recursive process gives an approximate solution of the equation.

$$x_{n+1} = g(x_n)$$

- (2) Calculate $a = \Gamma/(4\pi\nu_D)$ for Ly α and $b = 10 \text{ km s}^{-1}$, which is appropriate for Ly α in the warm neutral medium (WNM) with $T \sim 10000 \text{ K}$. Note that $\Gamma = \gamma_{u\ell} = 6.265 \times 10^8 \text{ s}^{-1}$ and $\lambda_{u\ell} = 1215.67 \text{ \AA}$.

-
- (2) Plot two graphs, $f(x) = x$ and $g(x) = \ln(x) + \ln\left(\sqrt{\pi}/a\right)$.
- (3) By looking at the two graphs, choose an approximate solution of $x = g(x)$. In other words, choose an approximate value where $y = x$ and $y = g(x)$ intersect.

Let this approximate solution be x_0 , and then find the numerical solution of $x = g(x)$ using the fixed point iteration method, as follows:

$$x_1 = g(x_0)$$

$$x_2 = g(x_1)$$

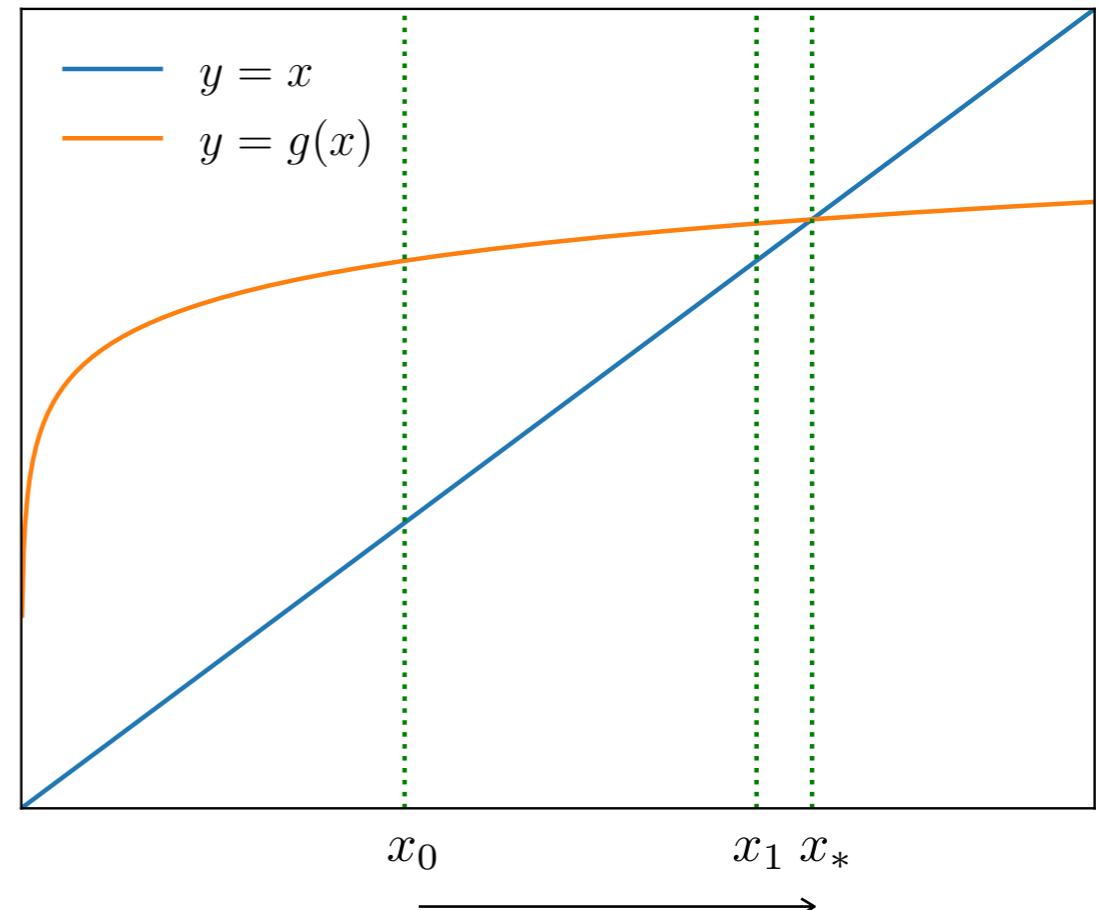
$$x_3 = g(x_2)$$

...

Denote the solution as x_* .

$$x_* = x_n \text{ as } n \rightarrow \infty$$

What is the value of x_* that you have found?



- (4) Let's denote the width parameter a for Ly α and $b = 10 \text{ km s}^{-1}$ as a_* . This means that

$$x_* = \ln x_* + \ln (\sqrt{\pi}/a_*)$$

Now, for any parameter a which is slightly different from a_* , you may express the constant term in $g(x)$ as follows:

$$\ln (\sqrt{\pi}/a) = \ln (a_*/a) + \ln (\sqrt{\pi}/a_*)$$

To find the solution for $a \neq a_*$ (but, still close to a_* , i.e., $a \approx a_*$), choose an initial guess for this case as $x_0 = x_*$.

Show that the solution for any a can be expressed, after a single iteration, as follow:

$$x_1 = x_* + \ln (a_*/a)$$

Insert numerical values into the above equation, and confirm that your solution is equivalent with or the same as the results in this lecture note and Eq. (6.42) in Draine's book.

- (5) Compare your solution with Eq. (2.39) in Ryden's book (our textbook). Does the equation in Ryden's book is equivalent with that of yours?