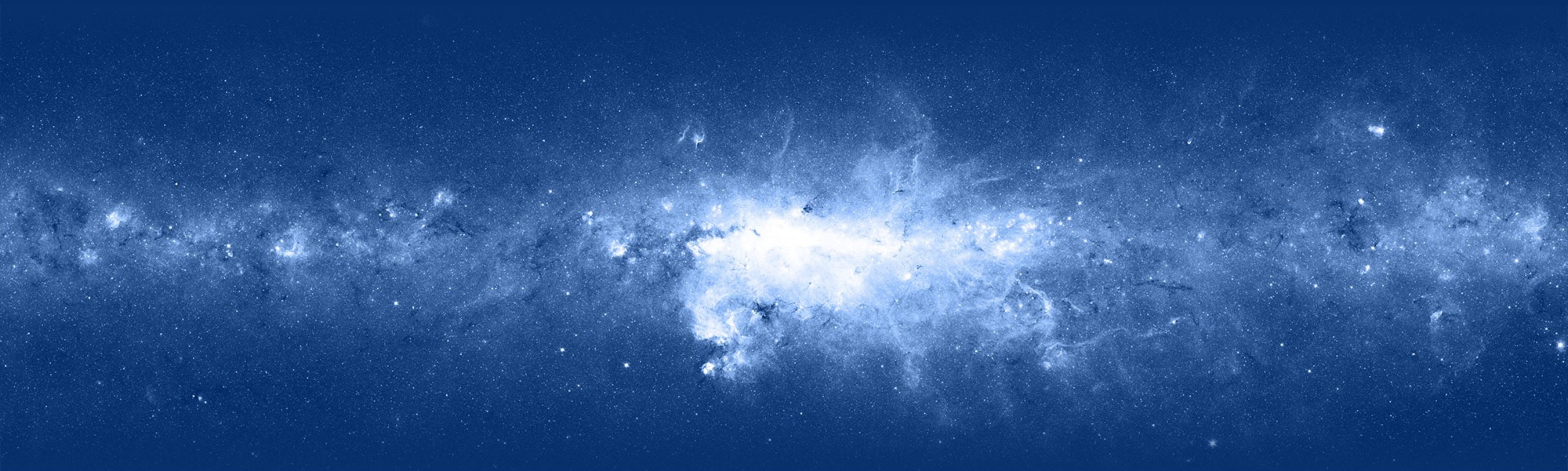
ASTR 670: Interstellar medium and gas dynamics

Prof. Benedikt Diemer



Chapter 3 • Atomic physics I: Energy levels and transitions

§3.1 • Energy levels of atoms

Chapter Four

Energy Levels of Atoms and Ions

This chapter reviews the energy-level structure of atoms and ions, together with the nomenclature for referring to those levels. It is probably an understatement to say that the material in this chapter is not electrically exciting; it should be regarded as reference material that can be returned to as needed.

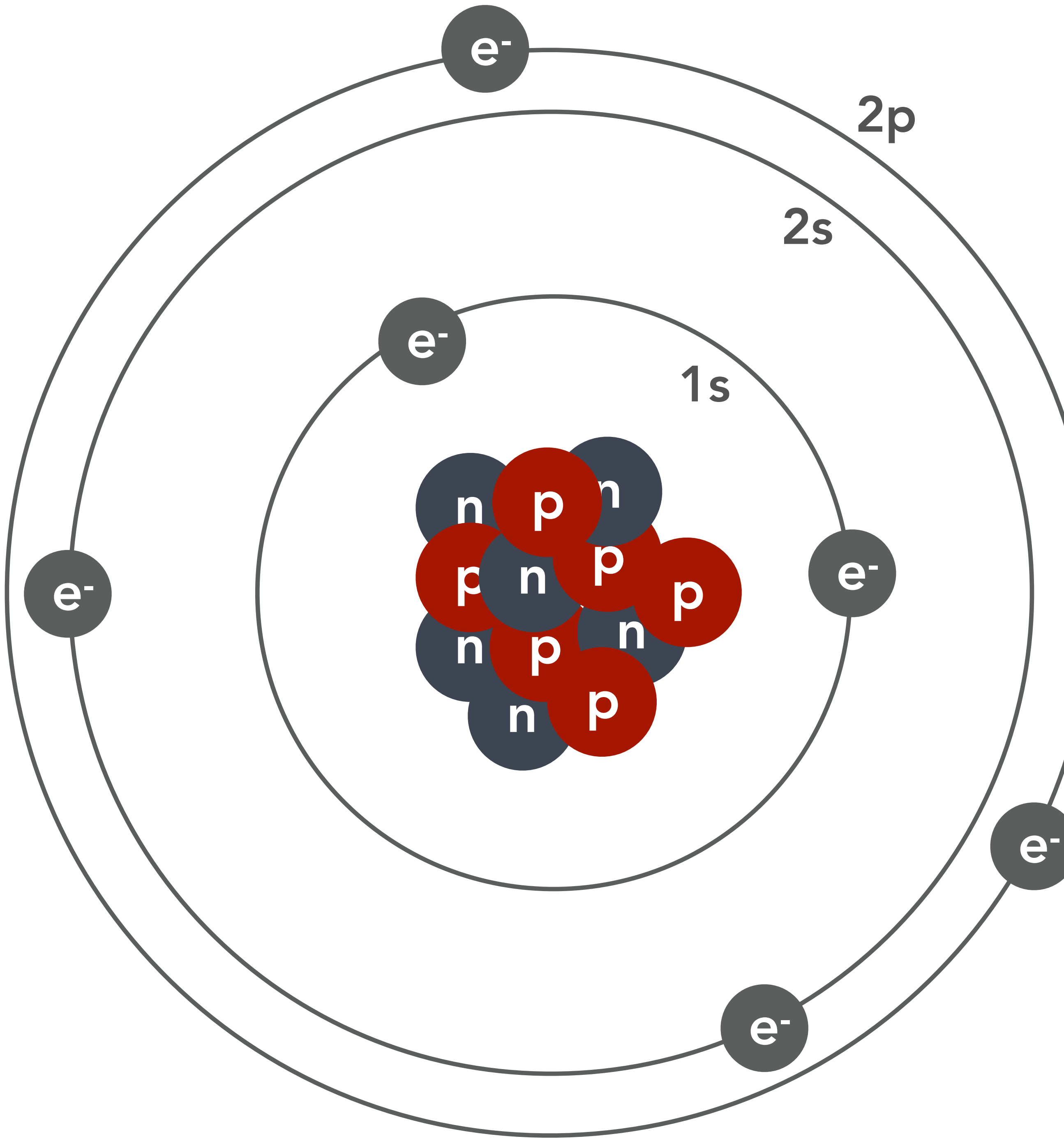
Quantum numbers

Principal quantum #
n = 1, 2, 3…

Orbital angular momentum #
l = 0, 1 … (n-1)
(0, 1, 2, 3) = ("s, p, d, f")

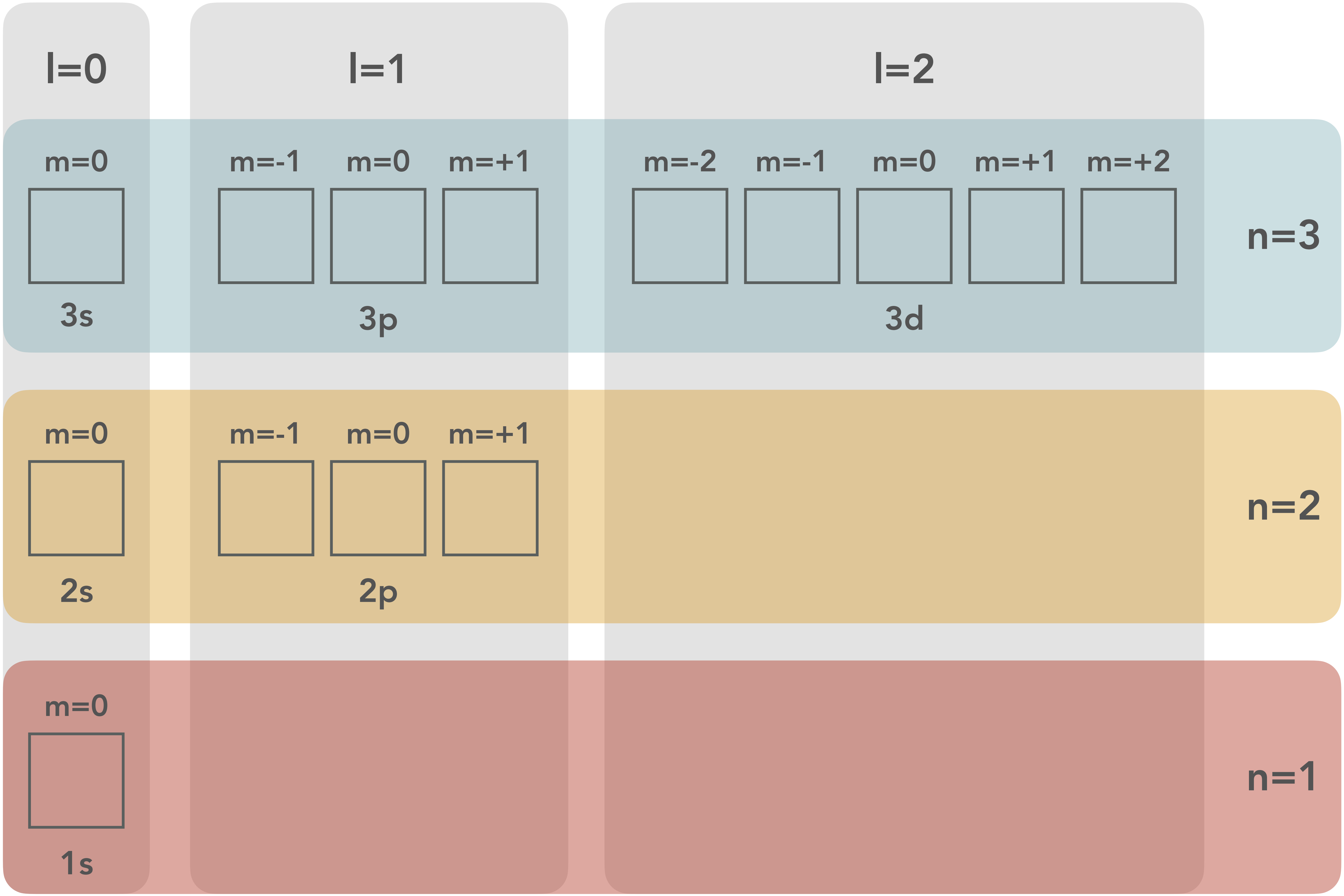
z-orbital angular momentum #
m = -l … 0 … l

Spin quantum #
s = +1/2, -1/2



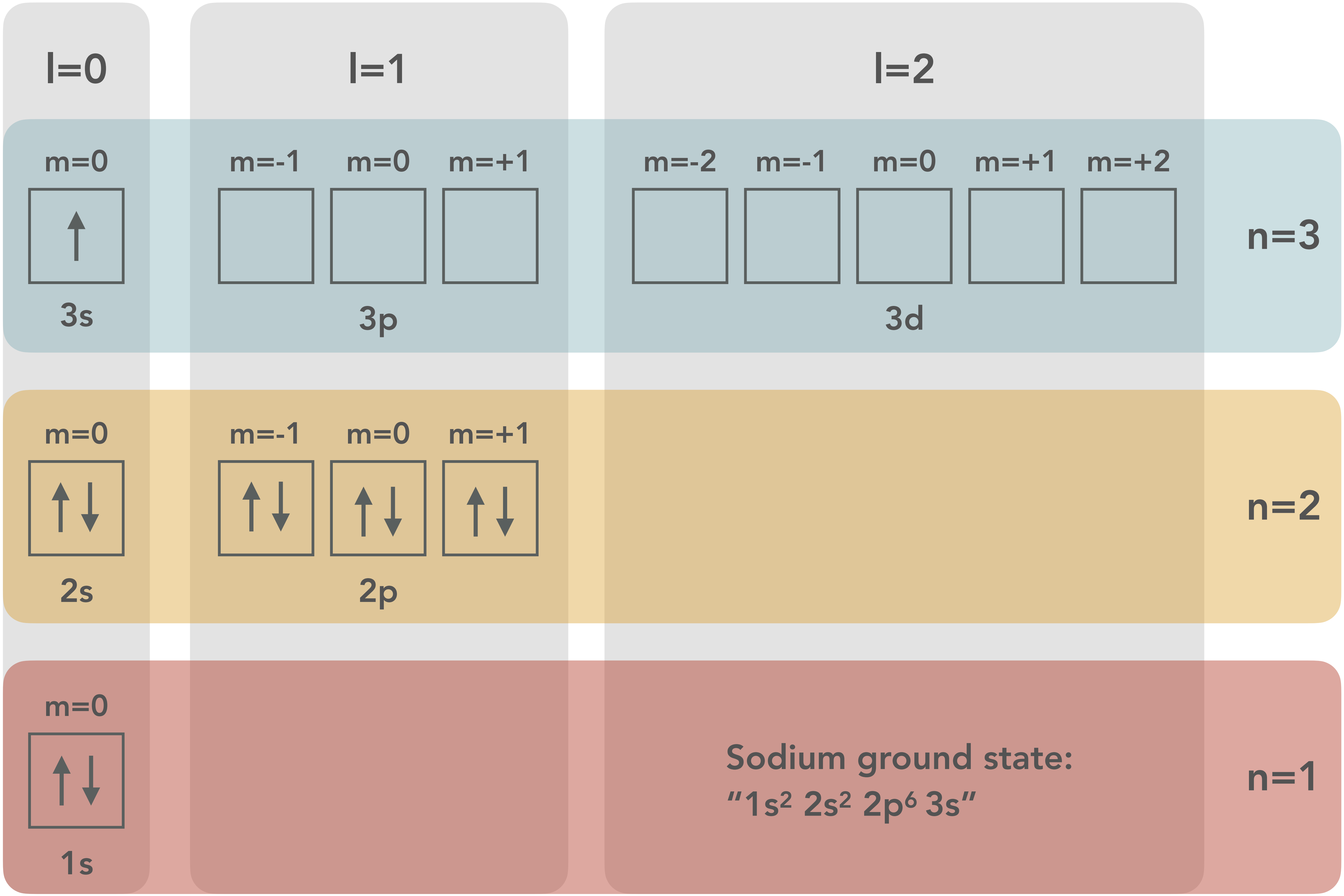
Carbon ground state:
"$1s^2$ $2s^2$ $2p^2$"

Subshells

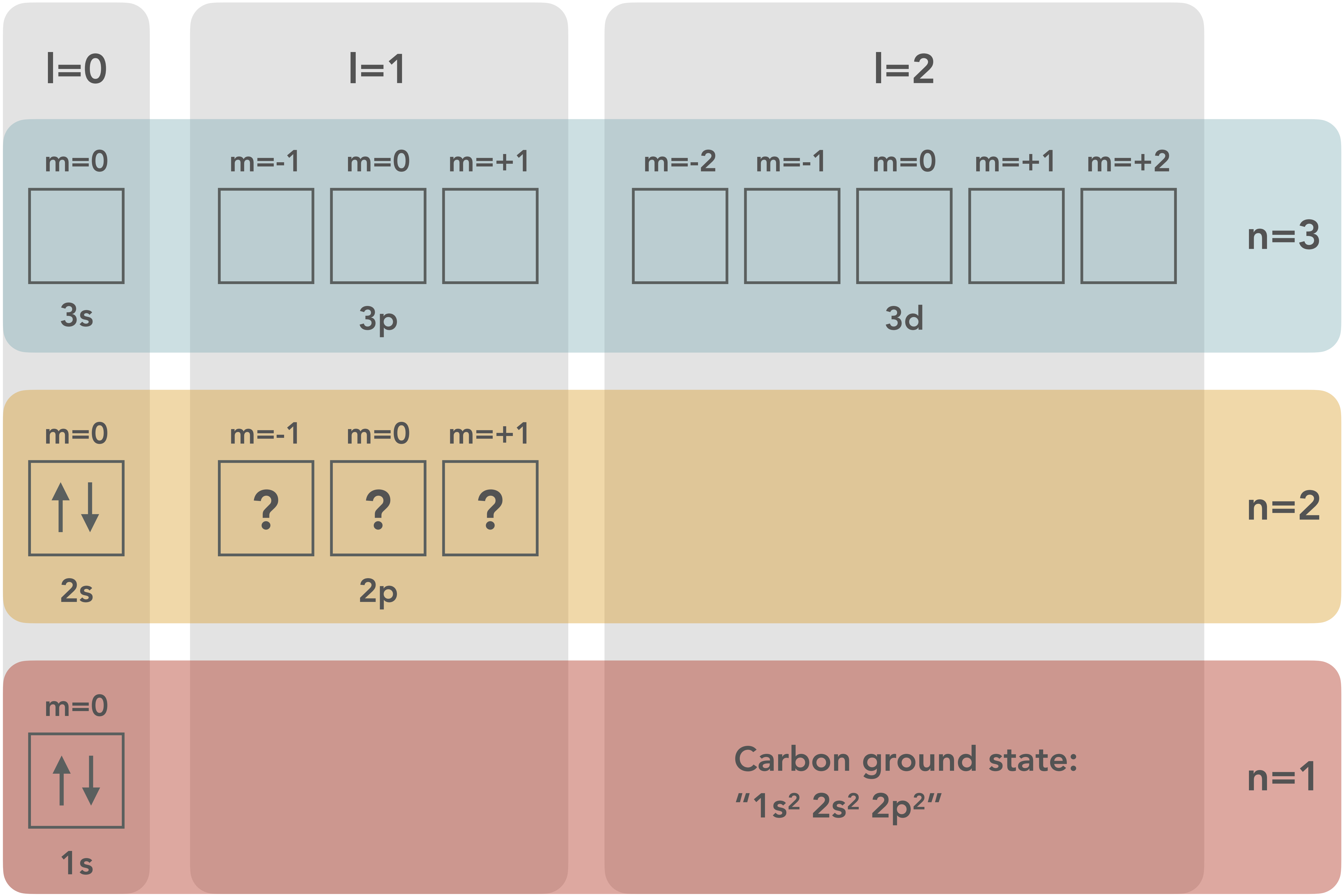


l=0
l=1
l=2
m=0
m=-1
m=0
m=+1
m=-2
m=-1
m=0
m=+1
m=+2
3s
3p
3d
n=3
m=0
m=-1
m=0
m=+1
2s
2p
n=2
m=0
1s
n=1

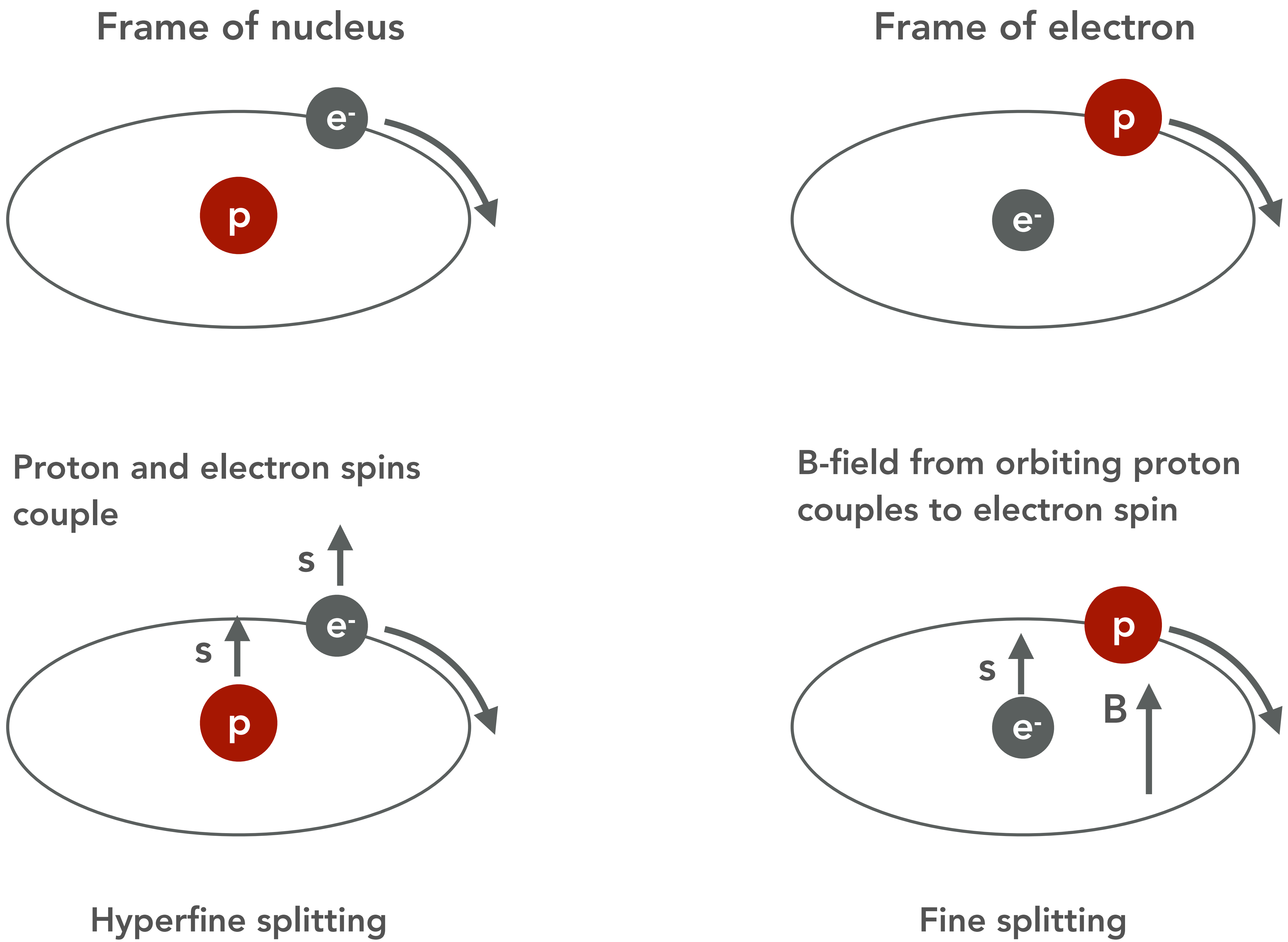
Subshells for Sodium



Subshells for Carbon



Fine and hyperfine splitting



Spectroscopic notation

Principal quantum #
n = 1, 2, 3…

Parity
p = “” (even) or “o” (odd)

Total orbital angular mom. #
$L = \Sigma l$ (vector addition)
(0, 1, 2, 3) = (“S, P, D, F”)

Total spin #
$S = \Sigma s$ (vector addition)

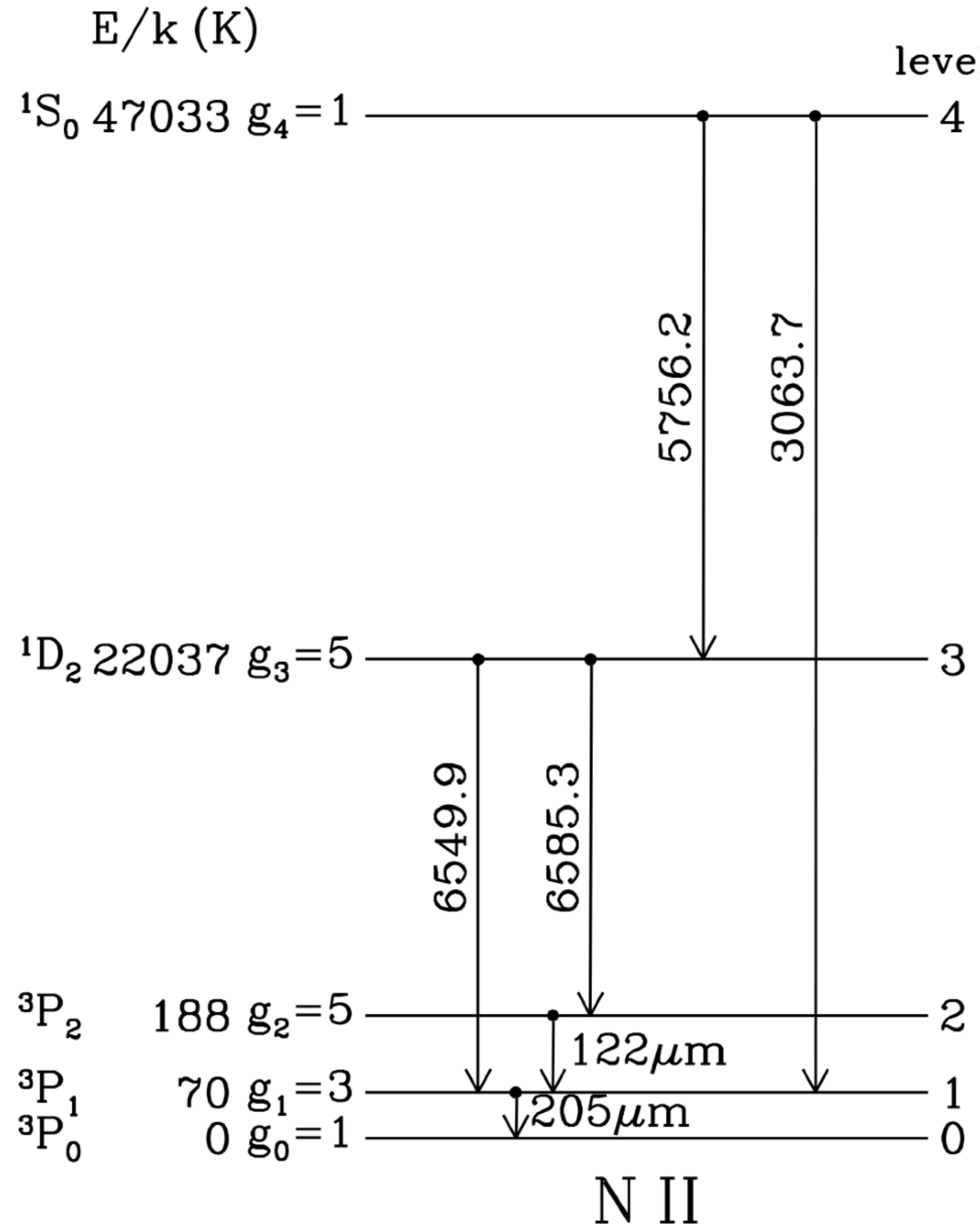
Total ang. mom. (L + S) #
J = |L - S| .. |L + S|
(vector addition)

e.g. 3^2P_1

Energy levels of ionized nitrogen

Degeneracy

$$g = 2J + 1$$



Draine §4.5

Examples of subshell configurations

Ground configuration	Terms (in order of increasing energy)	Examples
$...ns^1$	$^2S_{1/2}$	H I, He II, C IV, N V, O VI
$...ns^2$	$^1S_0$	He I, C III, N IV, O V
$...np^1$	$^2P^o_{1/2,3/2}$	C II, N III, O IV
$...np^2$	$^3P_{0,1,2}$, $^1D_2$, $^1S_0$	C I, N II, O III, Ne V, S III
$...np^3$	$^4S^o_{3/2}$, $^2D^o_{3/2,5/2}$, $^2P^o_{1/2,3/2}$	N I, O II, Ne IV, S II, Ar IV
$...np^4$	$^3P_{2,1,0}$, $^1D_2$, $^1S_0$	O I, Ne III, Mg V, Ar III
$...np^5$	$^2P^o_{3/2,1/2}$	Ne II, Na III, Mg IV, Ar IV
$...np^6$	$^1S_0$	Ne I, Na II, Mg III, Ar III

Draine §4.5

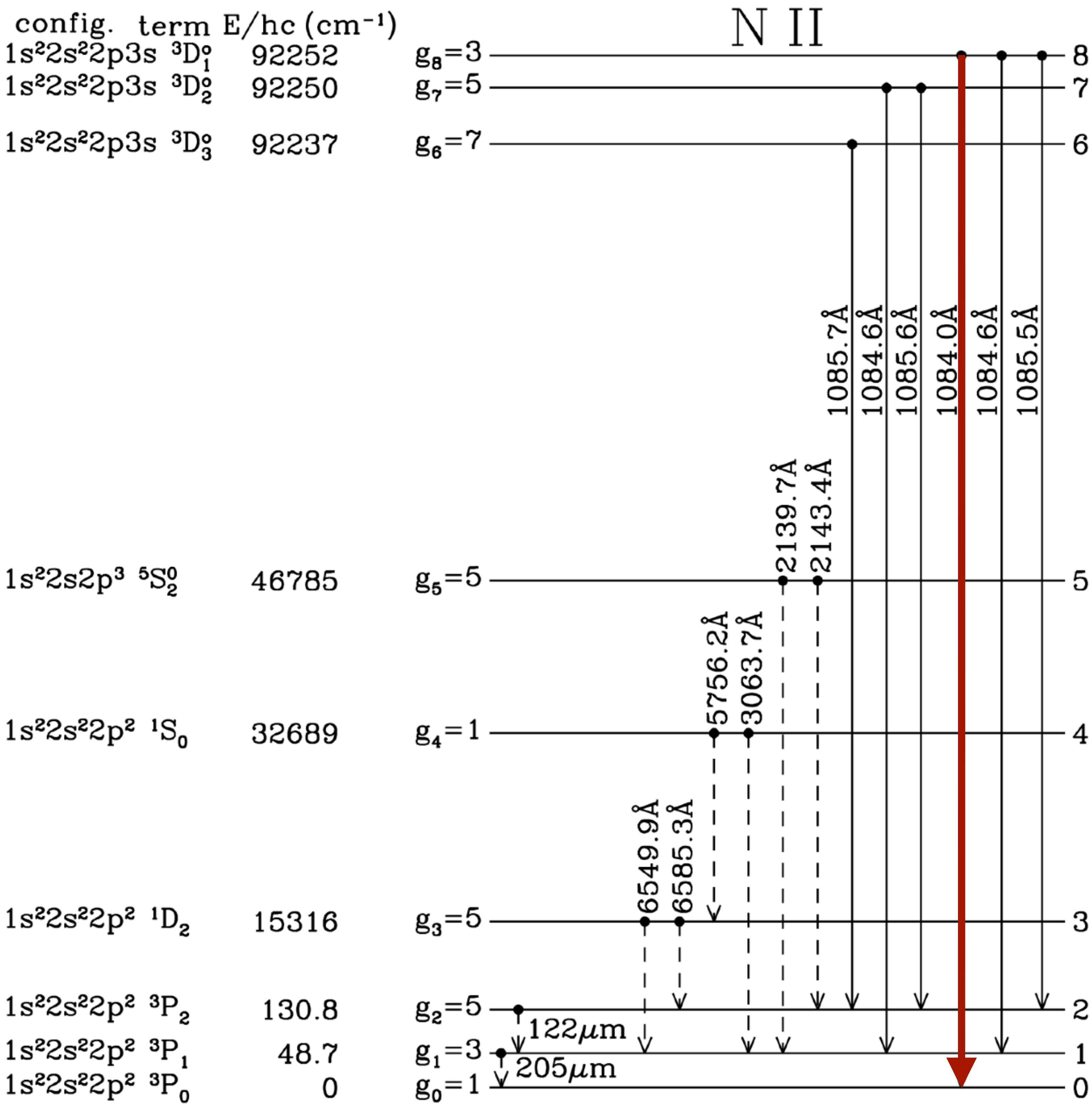
§3.2 • Transitions between levels

Rules for transitions

"Allowed transitions" = electric dipole transitions

- Parity must change
- $\Delta L = 0, \pm 1$, but $L = 0 \rightarrow 0$ is forbidden
- $\Delta J = 0, \pm 1$, but $J = 0 \rightarrow 0$ is forbidden
- $\Delta S = 0$
- If a single electron is involved, $\Delta l = \pm 1$

Allowed and (semi-)forbidden transitions



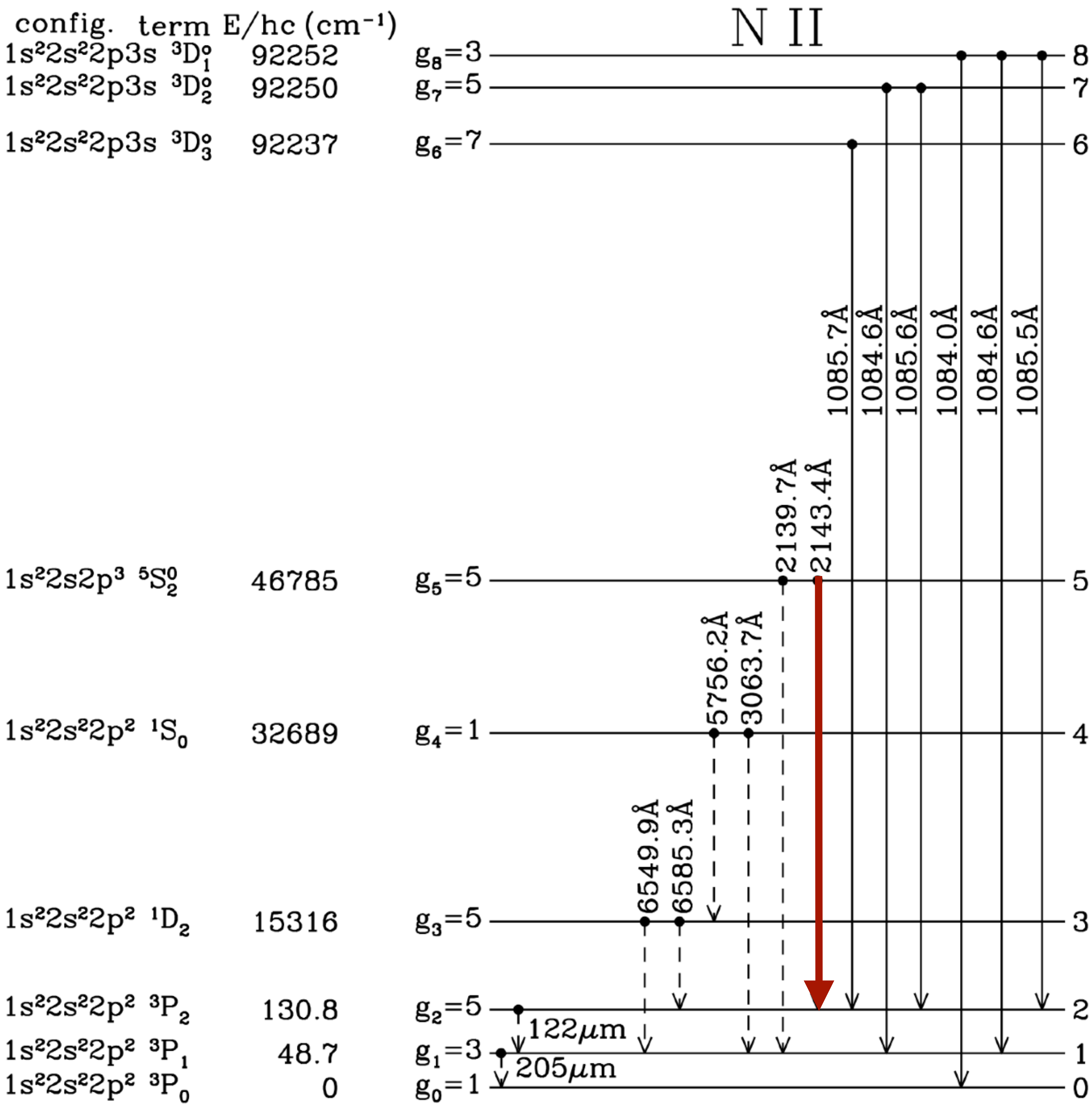
- Parity must change
- $\Delta L = 0, \pm 1$, but no $L = 0 \to 0$
- $\Delta J = 0, \pm 1$, but no $J = 0 \to 0$
- $\Delta S = 0$
- If a single electron, $\Delta l = \pm 1$

- odd changes to even
- $D \to P$ ($L = 2 \to 1$)
- $J = 1 \to 0$
- $S = 1 \to 1$

NII 1084.4Å $^3D^o_1 \to \ ^3P_0$

Draine §6.7.1

Allowed and (semi-)forbidden transitions



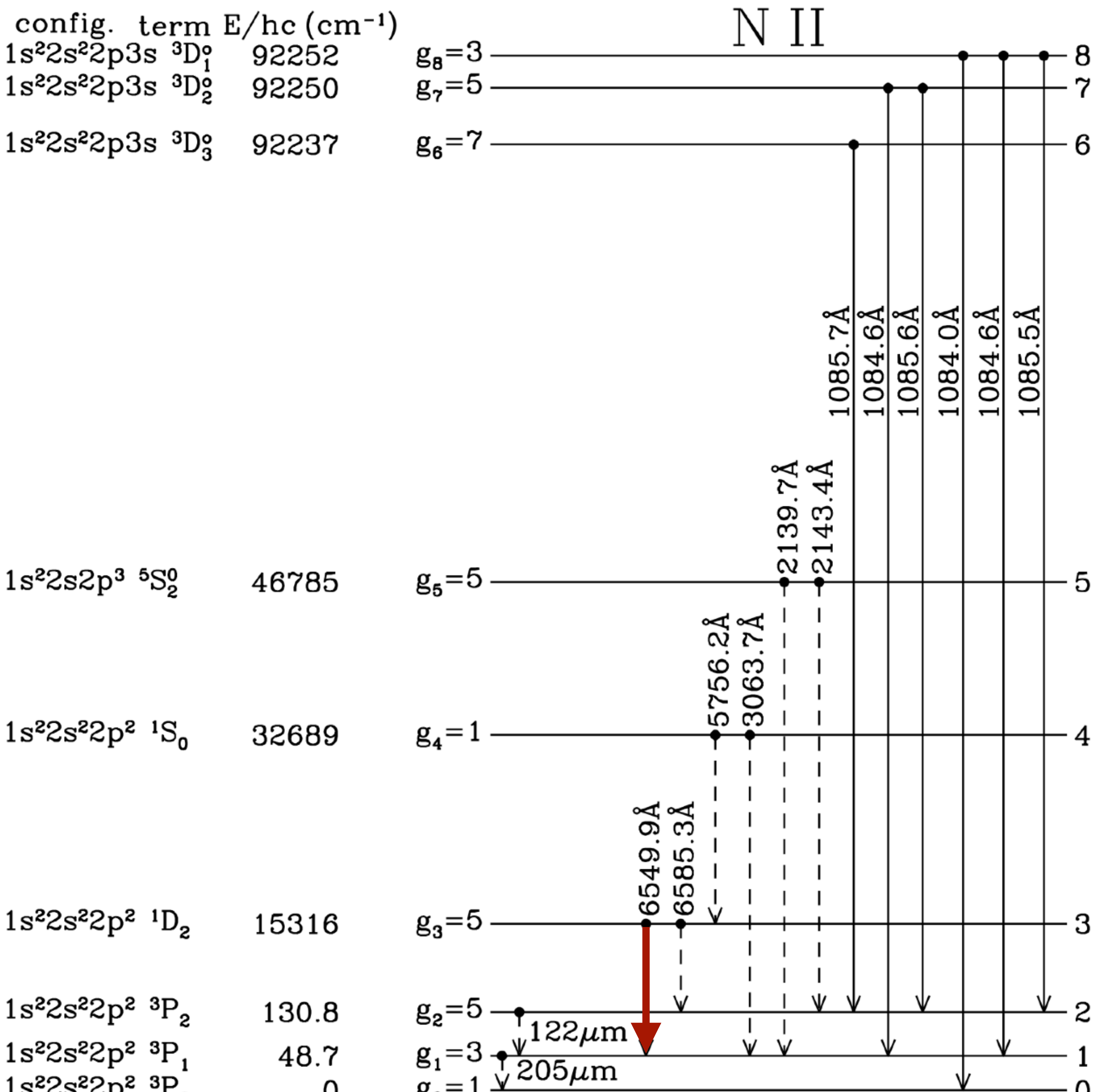
- Parity must change
- $\Delta L = 0, \pm 1$, but no $L = 0 \to 0$
- $\Delta J = 0, \pm 1$, but no $J = 0 \to 0$
- $\Delta S = 0$
- If a single electron, $\Delta l = \pm 1$

- odd changes to even
- $S \to P$ $(L = 0 \to 1)$
- $J = 2 \to 2$
- $S = 2 \to 1$ ✖

NII] 2143.4Å $^5S_2^o \to \, ^3P_2$

Draine §6.7.1

Allowed and (semi-)forbidden transitions



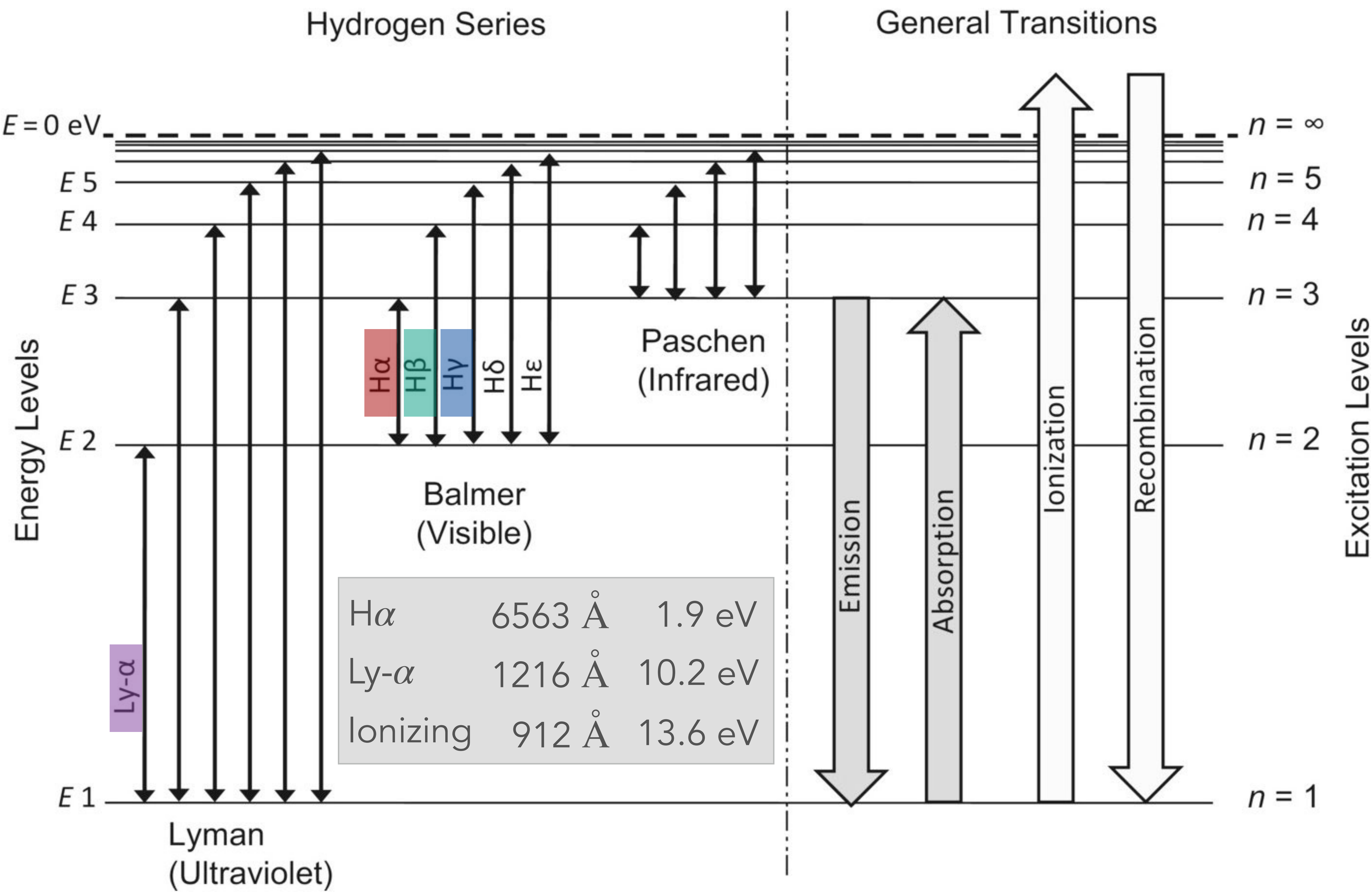
- Parity must change
- $\Delta L = 0, \pm 1$, but no $L = 0 \rightarrow 0$
- $\Delta J = 0, \pm 1$, but no $J = 0 \rightarrow 0$
- $\Delta S = 0$
- If a single electron, $\Delta l = \pm 1$

- odd changes to even ✖
- $D \rightarrow P$ ($L = 2 \rightarrow 1$)
- $J = 2 \rightarrow 1$
- $S = 0 \rightarrow 1$ ✖

[NII] 6549.9Å $^1D_2 \rightarrow \ ^3P_1$

Draine §6.7.1

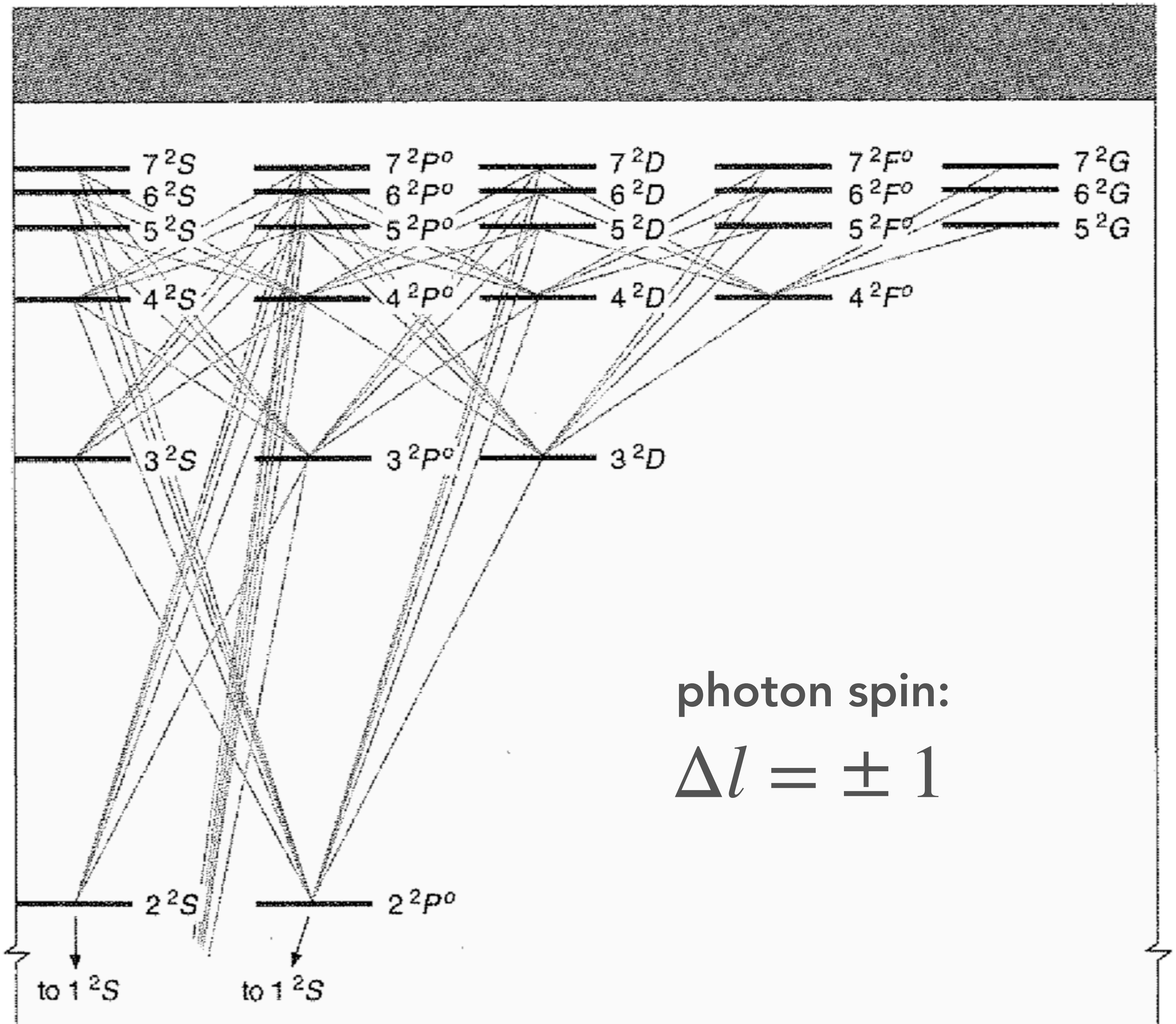
Energy level diagram of hydrogen



Hα	6563 Å	1.9 eV
Ly-α	1216 Å	10.2 eV
Ionizing	912 Å	13.6 eV

Trypsteen & Walker 2017

Energy level diagram of hydrogen



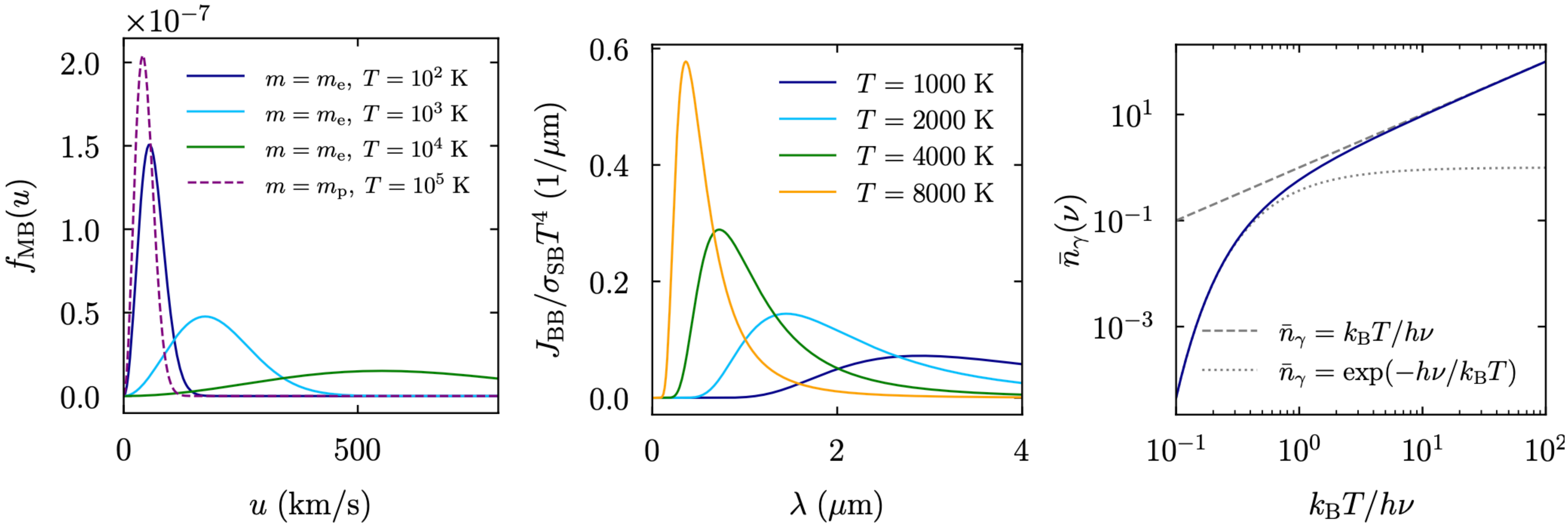
photon spin:

$$\Delta l = \pm 1$$

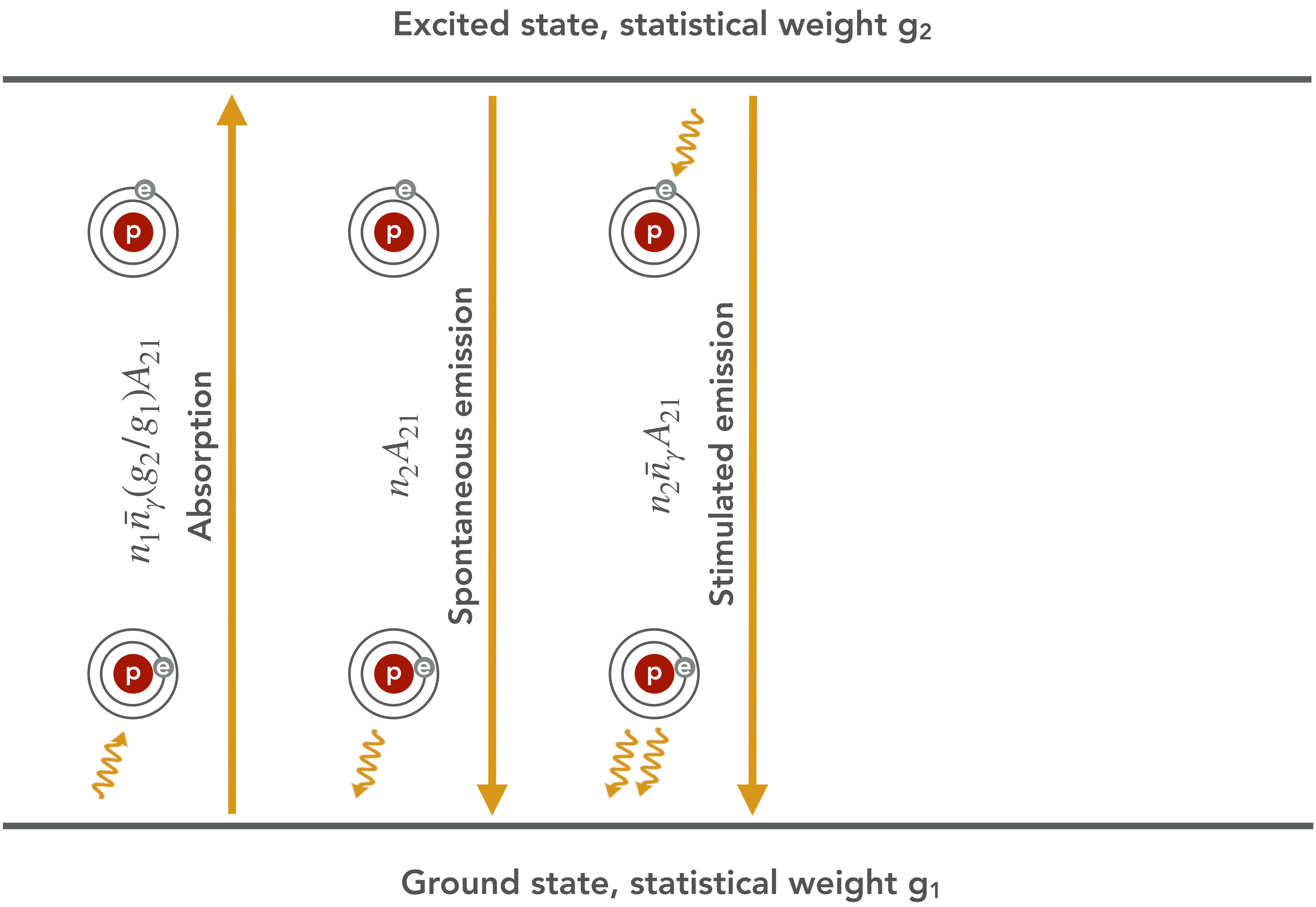
Osterbrock & Ferland §2.2

§3.3 • Thermodynamic equilibrium and blackbody radiation

Equilibrium distributions



§3.4 • Absorption and emission



Excited state, statistical weight g2
Absorption
$n_1\bar{n}_\gamma(g_2/g_1)A_{21}$
Spontaneous emission
n_2A_{21}
Stimulated emission
$n_2\bar{n}_\gamma A_{21}$
Ground state, statistical weight g1

Transition probability tables

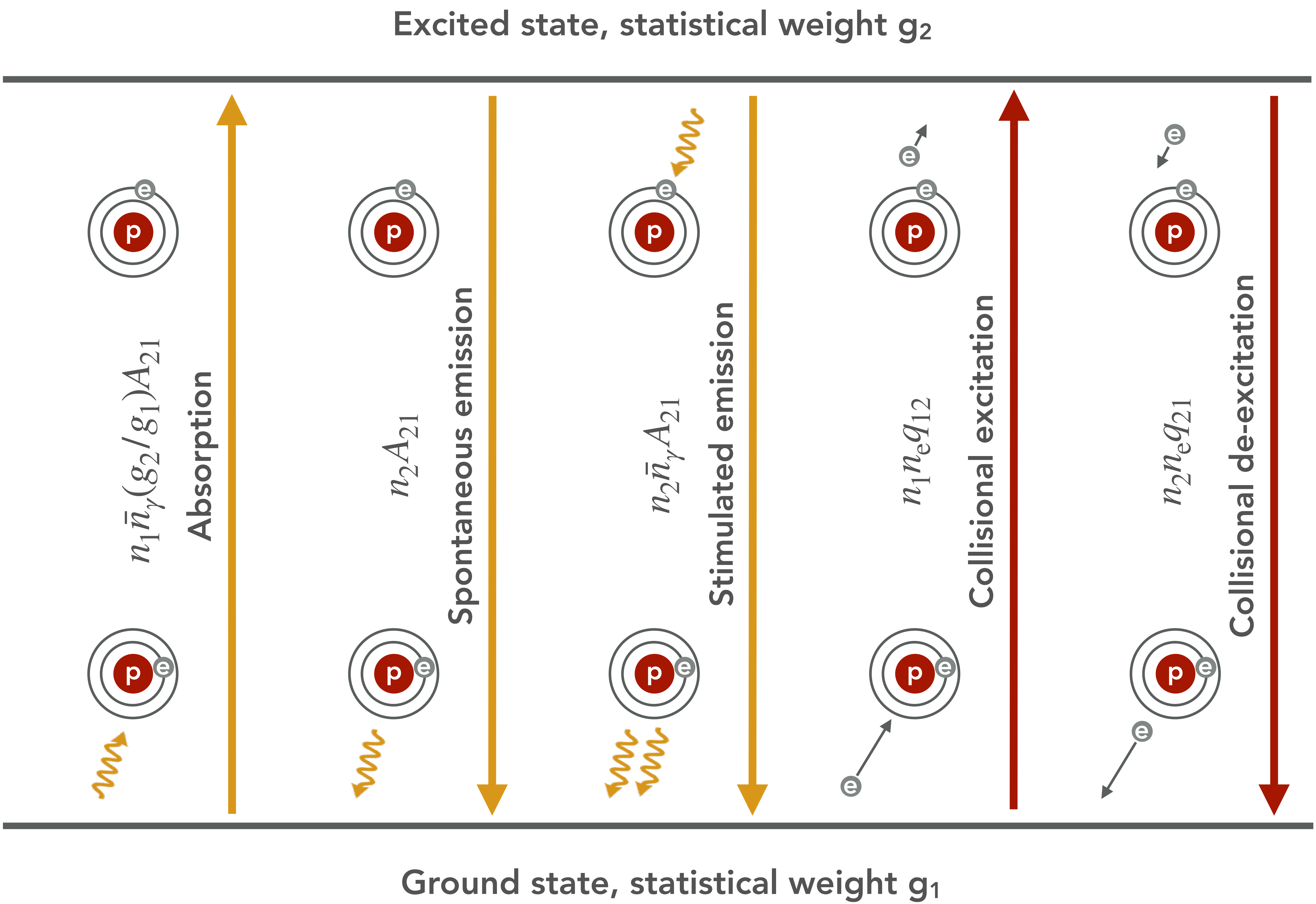
Table 3.12

Transition probabilities for C-like $2p^2$ and Si-like $3p^2$ ions

Transition	[N II]		[O III]		[Ne V]		[S III]		[Ar V]	
	A (s^{-1})	λ (Å)	A (s^{-1})	λ (Å)	A (s^{-1})	λ (Å)	A (s^{-1})	λ (Å)	A (s^{-1})	λ (Å)
$^1D_2$–$^1S_0$	1.0	5754.6	1.6	4363.2	2.8	2972.8	2.3	6312.0	3.5	4625.3
$^3P_2$–$^1S_0$	1.3×10^{-4}	3070.8	6.1×10^{-4}	2331.4	6.3×10^{-3}	1593.3	1.3×10^{-2}	3797.2	6.8×10^{-2}	2786.0
$^3P_1$–$^1S_0$	3.3×10^{-2}	3062.8	2.3×10^{-1}	2321.0	4.0	1574.6	8.4×10^{-1}	3721.7	6.7	2691.0
$^3P_2$–$^1D_2$	3.0×10^{-3}	6583.4	2.0×10^{-2}	5006.9	3.5×10^{-1}	3425.9	5.5×10^{-2}	9531.0	4.7×10^{-1}	7005.9
$^3P_1$–$^1D_2$	9.8×10^{-4}	6548.0	6.8×10^{-3}	4958.9	1.2×10^{-1}	3345.9	2.1×10^{-2}	9068.9	2.0×10^{-1}	6435.1
$^3P_0$–$^1D_2$	3.6×10^{-7}	6527.1	1.7×10^{-6}	4931.1	1.9×10^{-5}	3300.5	1.3×10^{-5}	8829.9	6.1×10^{-5}	6133.8
$^3P_1$–$^3P_2$	7.5×10^{-6}	121.89 μm	9.7×10^{-5}	51.814 μm	4.6×10^{-3}	14.32 μm	2.1×10^{-3}	18.713 μm	2.7×10^{-2}	7.9 μm
$^3P_0$–$^3P_2$	1.1×10^{-12}	76.5 μm	3.1×10^{-11}	32.661 μm	5.0×10^{-9}	9.01 μm	4.3×10^{-8}	12.00 μm	1.2×10^{-6}	4.9 μm
$^3P_0$–$^3P_1$	2.1×10^{-6}	205.5 μm	2.7×10^{-5}	88.356 μm	1.3×10^{-3}	24.28 μm	4.7×10^{-4}	33.47 μm	8.0×10^{-3}	13.1 μm
$^3P_2$–$^5S^o_2$	$1.3 \times 10^{+2}$	2142.8	$5.8 \times 10^{+2}$	1666.2	$6.0 \times 10^{+3}$	1146.1	1.2×10^4	1728.9	—	—
$^3P_1$–$^5S^o_2$	$5.5 \times 10^{+1}$	2139.0	$2.4 \times 10^{+2}$	1660.8	2.4×10^3	1137.0	4.4×10^3	1713.1		

Osterbrock & Ferland §3.5

§3.5 • Collisional excitation



Excited state, statistical weight g_2
$n_1 \bar{n}_\gamma (g_2/g_1) A_{21}$
Absorption
$n_2 A_{21}$
Spontaneous emission
$n_2 \bar{n}_\gamma A_{21}$
Stimulated emission
$n_1 n_e q_{12}$
Collisional excitation
$n_2 n_e q_{21}$
Collisional de-excitation
p
e
Ground state, statistical weight g_1

Collision strength tables

Table 3.6

Collision strengths Υ for C-like $2p^2$, O-like $2p^4$, Si-like $3p^2$ and S-like $3p^4$ ions

Ion	$^3P,\ ^1D$	$^3P,\ ^1S$	$^1D,\ ^1S$	$^3P_0,\ ^3P_1$	$^3P_0,\ ^3P_2$	$^3P_1,\ ^3P_2$	$^3P,\ ^5S^o$
N^+	2.64	0.29	0.83	0.41	0.27	1.12	1.27
O^{+2}	2.29	0.29	0.58	0.55	0.27	1.29	0.18
Ne^{+4}	2.09	0.25	0.58	1.41	1.81	5.83	1.51
Ne^{+2}	1.36	0.15	0.27	0.24	0.21	0.77	—
S^{+2}	6.95	1.18	1.38	3.98	1.31	7.87	2.85
Ar^{+4}	3.21	0.56	1.65	2.94	1.84	7.81	—
Ar^{+2}	4.83	0.84	1.22	1.26	0.67	3.09	—

Osterbrock & Ferland §3.5

Collision strength tables

RATE COEFFICIENTS FOR THE EXCITATION OF INFRARED AND ULTRAVIOLET LINES IN C II, N III, AND O IV

ROBERT D. BLUM AND ANIL K. PRADHAN
Department of Astronomy, Ohio State University, Columbus, OH 43210
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ABSTRACT

Electron impact excitation of boron-like C, N, and O is the primary mechanism for the formation of a number of IR and UV emission lines that are useful density and temperature diagnostics for a variety of astrophysical sources. New and improved collision strengths and Maxwellian-averaged rate coefficients for temperatures between 1000 and 40,000 K are presented for all the prominent transitions in the spectra of C II, N III, and O IV. The collision strengths show extensive autoionization structures that are delineated in detail and which enhance the rate coefficients for several transitions by a considerable amount. Particular attention is directed toward the fine-structure IR transition $^2P^o_{1/2}$–$^2P^o_{3/2}$ and the dipole-allowed and intercombination UV transitions $^2P^o_{1/2,3/2}$–$^2D^2_{3/2,5/2}$, $^2S^2_{1/2}$, $^2P_{1/2,3/2}$, and $^2P^o_{1/2,3/2}$–$^4P_{1/2,3/2,5/2}$, respectively, in the three ions. Maxwellian-averaged collision strengths are calculated for all possible fine-structure transitions among the states included in the eigenfunction expansion of the target ion. All calculations are carried out in the close-coupling approximation using the *R*-matrix method as adapted for the Opacity Project.

Collision strength tables

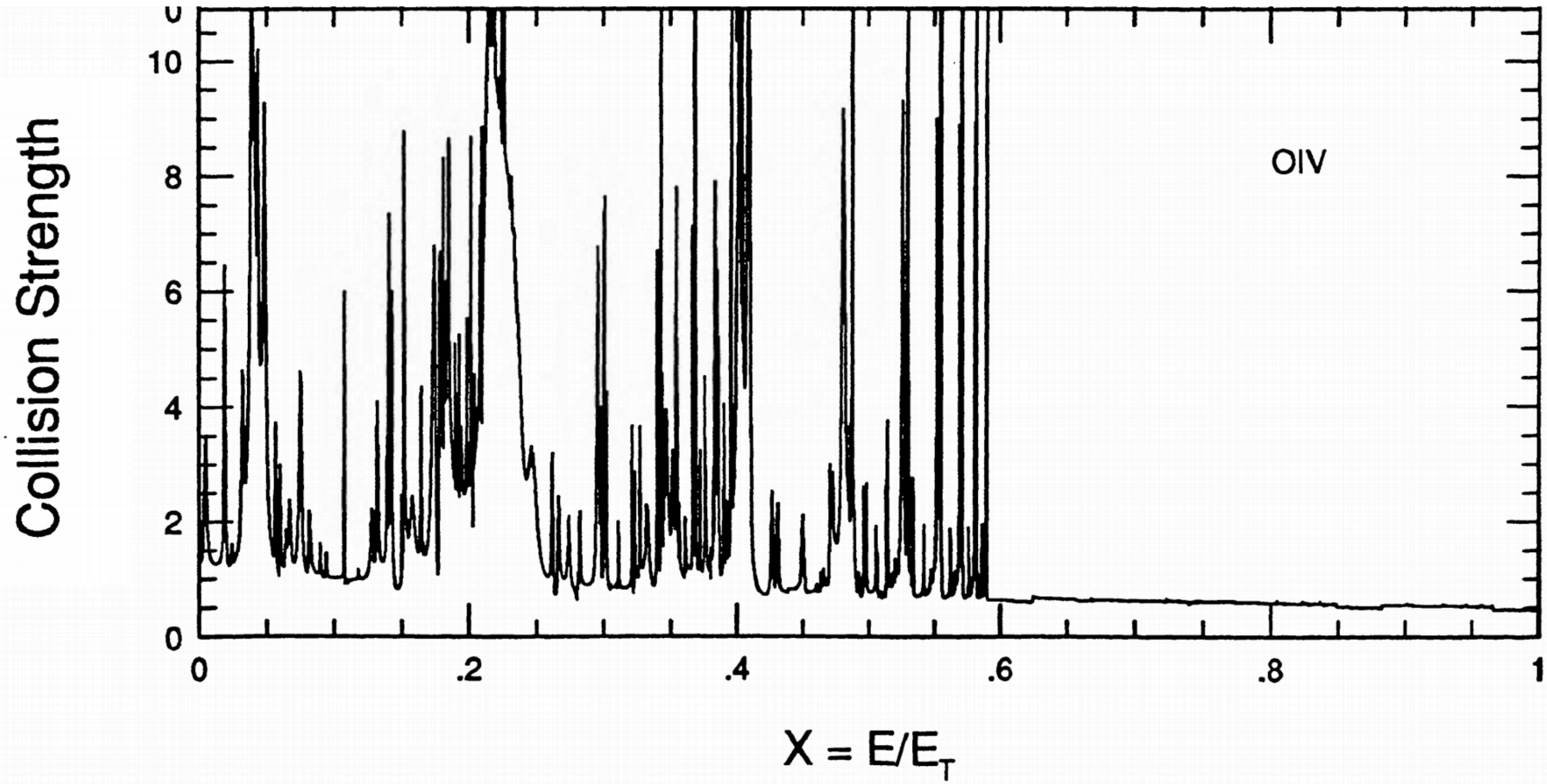

FIG. 1.—The collision strengths for the ground state fine-structure transition $^2P^o_{1/2}$–$^2P^o_{3/2}$ in C II, N III, and O IV. The *X* units are excitation energies divided by the threshold energy for the transition.

Blum & Pradhan 1992

Collision strength tables

TABLE 2

MAXWELLIAN-AVERAGED COLLISION STRENGTHS FOR C II

Temp (K)	TRANSITION KEY								
	1 2	1 3	1 4	1 5	1 6	1 7	1 8	1 9	1 10
	1 11	1 12	1 13	1 14	1 15	1 16	1 17	1 18	2 3
	2 4	2 5	2 6	2 7	2 8	2 9	2 10	2 11	2 12
	2 13	2 14	2 15	2 16	2 17	2 18	3 4	3 5	3 6
	3 7	3 8	3 9	3 10	3 11	3 12	3 13	3 14	3 15
	3 16	3 17	3 18	4 5	4 6	4 7	4 8	4 9	4 10
	4 11	4 12	4 13	4 14	4 15	4 16	4 17	4 18	5 6
	5 7	5 8	5 9	5 10	5 11	5 12	5 13	5 14	5 15
	5 16	5 17	5 18	6 7	6 8	6 9	6 10	6 11	6 12
	6 13	6 14	6 15	6 16	6 17	6 18	7 8	7 9	7 10
	7 11	7 12	7 13	7 14	7 15	7 16	7 17	7 18	8 9
	8 10	8 11	8 12	8 13	8 14	8 15	8 16	8 17	8 18
	9 10	9 11	9 12	9 13	9 14	9 15	9 16	9 17	9 18
	10 11	10 12	10 13	10 14	10 15	10 16	10 17	10 18	11 12
	11 13	11 14	11 15	11 16	11 17	11 18	12 13	12 14	12 15
	12 16	12 17	12 18	13 14	13 15	13 16	13 17	13 18	14 15
	14 16	14 17	14 18	15 16	15 17	15 18	16 17	16 18	17 18
1000.	1.5763	0.2653	0.3925	0.2435	1.2826	0.5206	0.7915	1.1607	0.6689
	0.2056	0.2114	0.1175	0.0050	0.1153	0.0837	0.1811	0.1066	0.1853
	0.5088	1.1084	0.8812	2.7251	1.5831	0.6689	2.9904	0.4113	0.1175
	0.5403	0.0101	0.1235	0.2746	0.1066	0.4687	0.6119	0.6588	0.4189
	0.2302	0.0642	0.0742	0.0798	0.0238	0.0075	0.0080	0.8802	0.2660
	0.1275	0.1234	0.1937	1.5041	0.6467	0.6516	0.1284	0.1209	0.1871
	0.0476	0.0122	0.0187	1.7604	0.4017	0.3854	0.2256	0.4087	0.4923
	1.4552	0.1926	0.1129	0.3491	0.0714	0.0112	0.0352	2.6406	0.2768
	0.9038	0.2853	0.6661	2.1560	0.5786	0.2364	0.6387	0.2486	0.1628
	0.1724	0.1156	2.2686	0.7841	1.2182	0.5284	0.8679	0.4929	0.8198
	0.3729	0.1165	0.3863	0.1734	0.7841	3.7946	0.2373	2.3823	0.0917
	0.1834	3.4386	0.6610	1.3220	0.0000	0.0268	0.0402	0.5244	1.0490
	0.7652	0.0257	0.0281	0.0400	0.2958	2.6477	0.1387	1.6166	0.8818
	0.0514	0.0400	0.0962	0.5916	0.6960	4.8767	0.8818	4.1154	9.5962
	19.1924	0.0000	0.0299	0.0448	0.1545	0.3090	8.7134	0.0062	0.0407
	0.0474	0.2226	0.5301	0.0124	0.0651	0.1113	0.5301	0.9752	0.9026
	1.3538	0.1657	0.3314	1.4527	0.5521	0.7312	0.5173	1.4078	0.9318
2000.	1.6361	0.2577	0.3821	0.2397	1.2879	0.5136	0.7146	1.1782	0.6800
	0.2227	0.2145	0.1184	0.0065	0.1222	0.0911	0.1784	0.1067	0.1820

Blum & Pradhan 1992

Reading

Draine

- §3.1-6
- §4.1-6
- §6.1-2, §6.7