Lecture 5 January 2019

Electrons in Atoms: Energy, Magnetism;

Term Symbols, Z_{eff} as Determinant of Ionization Energies, and Other Properties

Electrons have Energy; and they have spins.

Gouy Balance for Magnetic Susceptibility

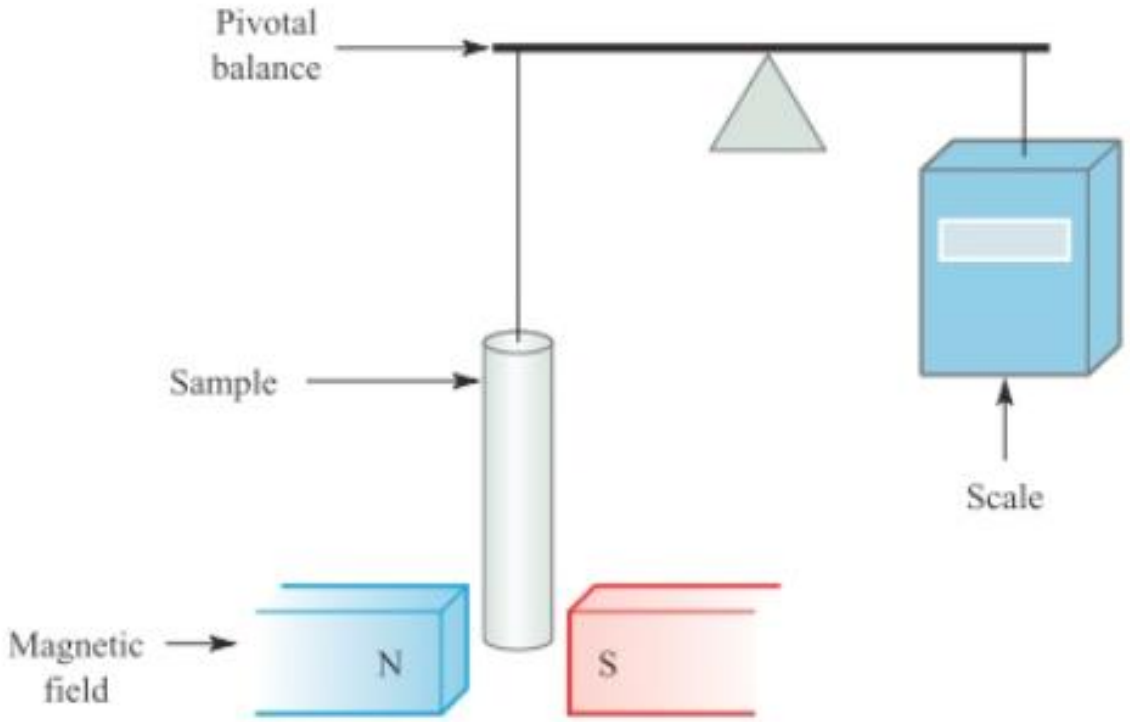


Fig. 20.21 Schematic representation of a Gouy balance.

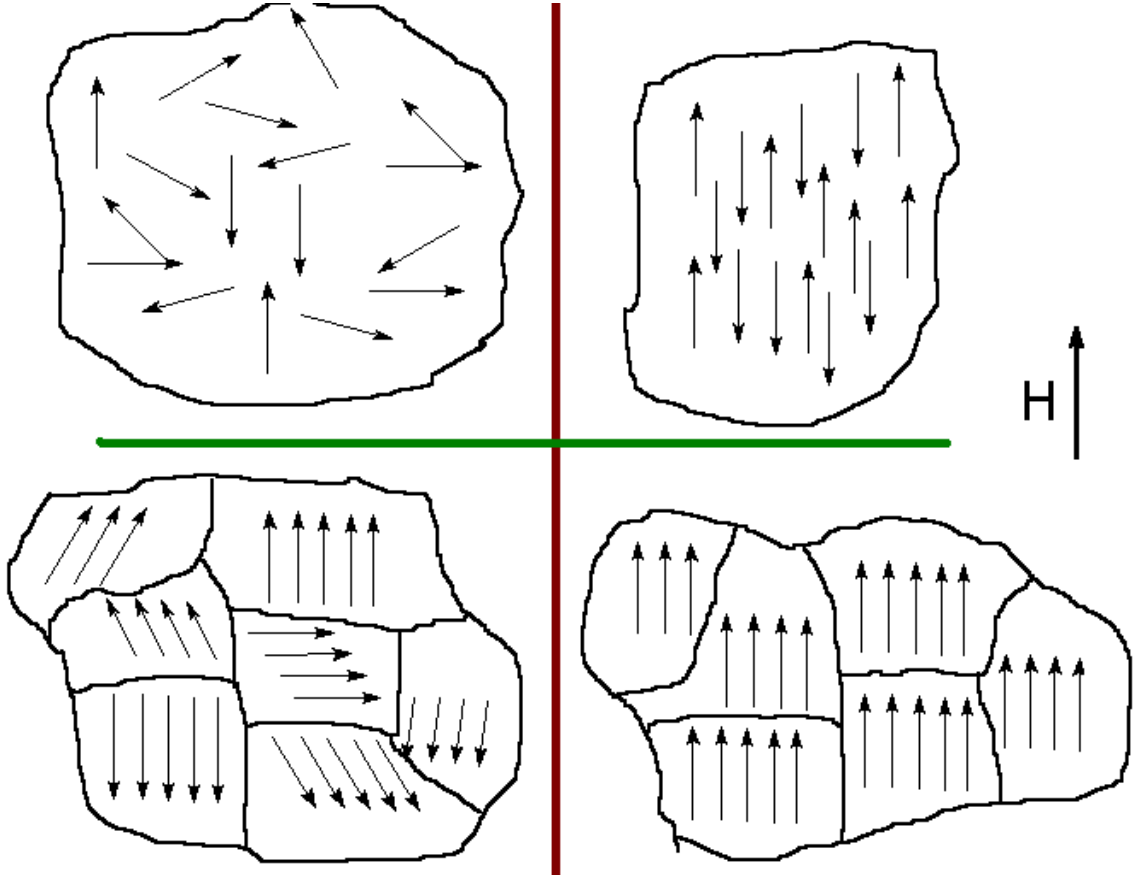
Three types of Magnetic Behavior

Paramagnetism: atoms, molecules, and solids with unpaired electrons are attracted in a magnetic field

Diamagnetic: substances with no unpaired electrons which are weakly repelled in a magnetic field

Ferro-magnetism: the unpaired electons are aligned with their neighbors even in the absence of a magnetic field

Magnetic domains: the groups of mutually aligned spins in a ferromagnetic substance



Ferro-magnet
In the absence of a magnetic field

Ferro-magnet
In the presence of a magnetic field

First approach to both energy and magnetism?

Electron Assignments:
Identify each and every quantum number for each and every electron:

n l m_ℓ m_s

Electrons Characterized by

a) Principal energy level, **n**

b) Orbital or angular momentum, l = # of angular nodes

c) Z_{eff}

In the presence of a magnetic field of ℓ is oriented and composed of m_ℓ components.

d) Spin-spin and spin-orbital coupling

*n*d vs. (*n* + 1)s in the Transition Metals

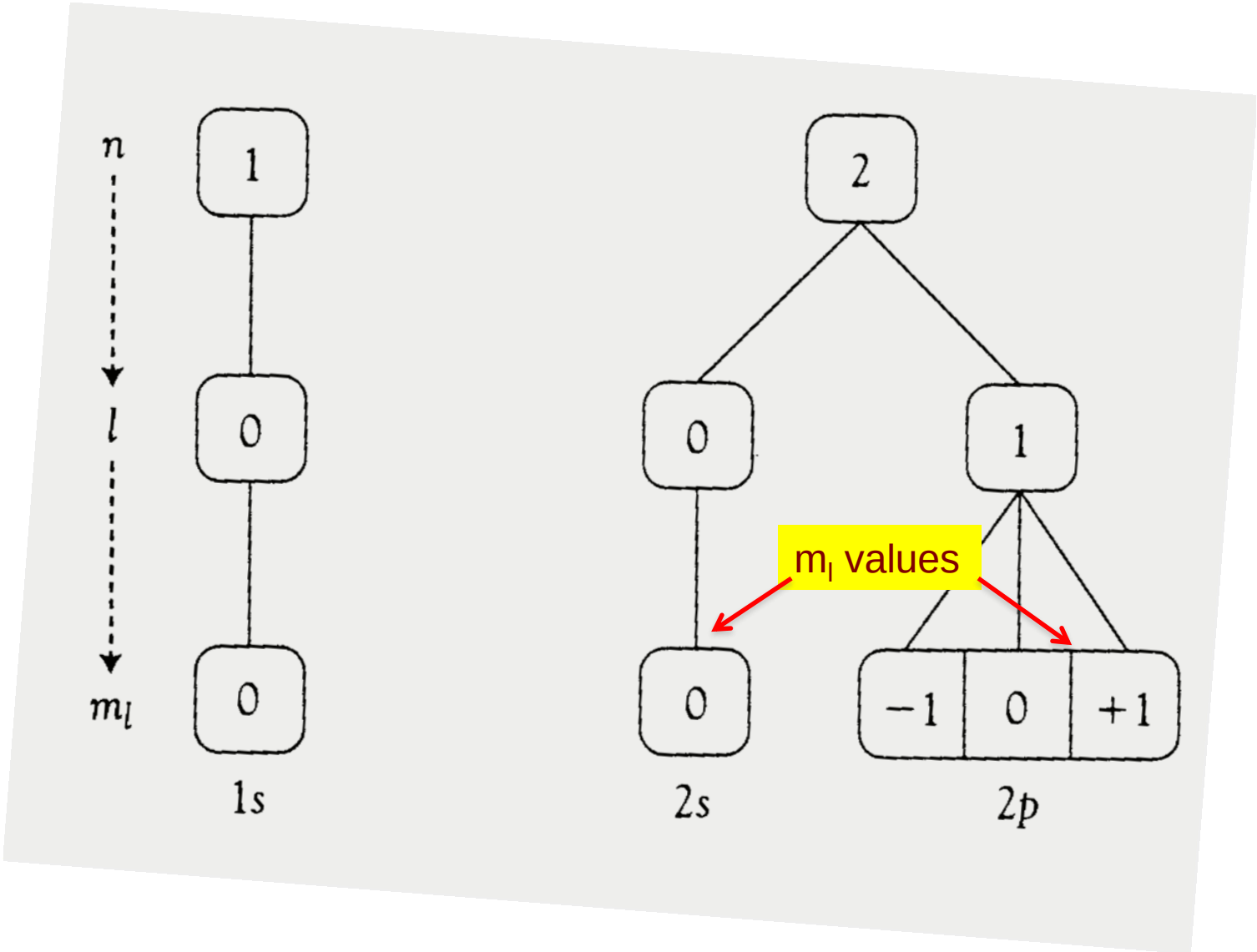
	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
4s	1	2	2	2	2	1	2	2	2	2	1	2
3d			1	2	3	5	5	6	7	8	10	10

	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
5s	1	2	2	2	1	1	1	1	1	0	1	2
4d			1	2	4	5	6	7	8	10	10	10

	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
6s	1	2	2	2	2	2	2	2	2	0	1	2
5d			1	2	3	4	5	6	7	10	10	10

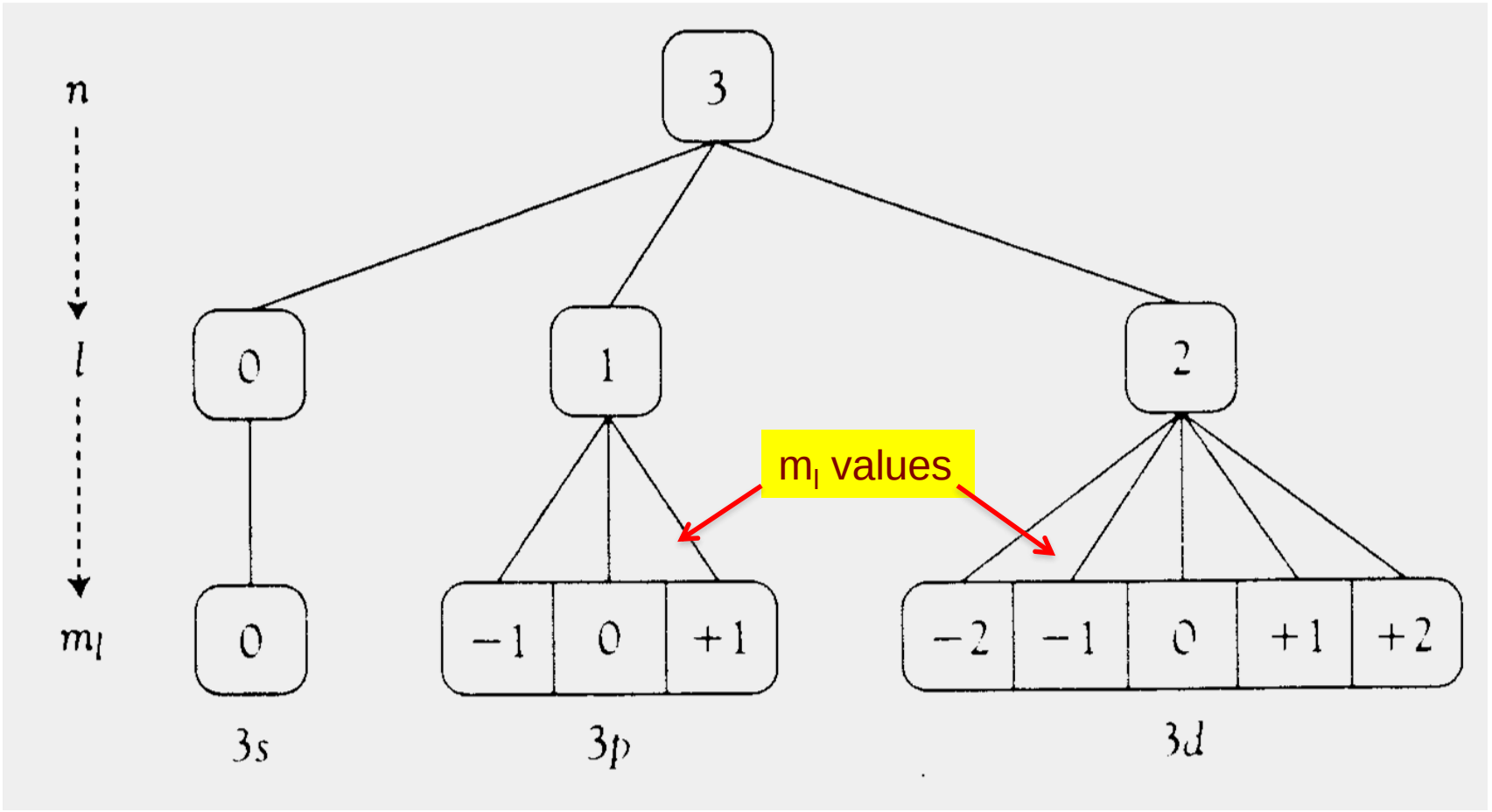
Box Diagrams—help with magnetism

Figure 1.4 The possible sets of quantum numbers for $n = 1$ and $n = 2$.



Box Diagrams

Figure 1.5 The possible sets of quantum numbers for $n = 3$.



Ground State vs. Excited State Configurations

Term Symbols: $^{2S+1}L_J$

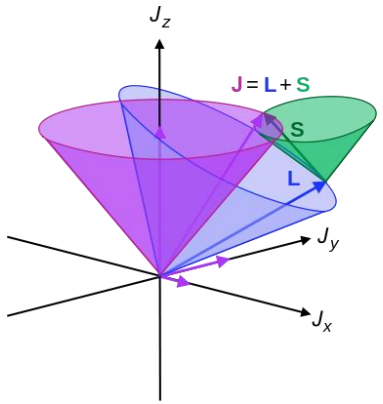
Spin: $S = \Sigma m_s$

= total spin angular momentum

2S + 1 (called spin "multiplicity")

L = total orbital angular momentum = $= \Sigma m_l$

$J = L + S$



Term Symbols for Ground State Electronic Configurations

- Pauli Exclusion Principle => Assignments to n and to l quantum numbers. But there are other possibilities within assignment

- Hund's Rule: Describes ground state only.

- Ground states will have

1st * Maximum value of S

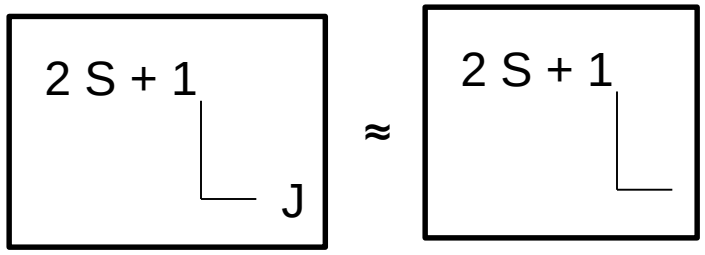
2nd * Maximum value of L within that S

Russell Saunders Coupling (L-S Coupling) for Ground States

Configuration => Term Symbol

Σm_L = max. M_L or L

Σm_S = M_S or S



Spin Multiplicity

# unpaired e⁻	S	2 S + 1		L	State
1	1/2	2	⇒ doublet	0	⇒ S
2	1	3	⇒ triplet	1	⇒ P
3	3/2	4	⇒ quartet	2	⇒ D
4	2	5	⇒ pentet	3	⇒ F
				4	⇒ G
				etc.	

Russell Saunders Coupling: Spin/Orbit Coupling