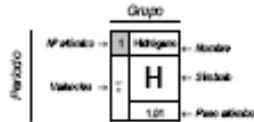


Tabla Periódica de los elementos

IA																												VIIIA (01)		
1	Hidrógeno																1	Helio												
1	H																2	He												
2	IIA																VIIA		VIIIA (02)											
2	3	4															5	6	7	8	9	10								
2	Li		Be																B		C		N		O		F		Ne	
2	Li		Be																B		C		N		O		F		Ne	
3	11	12															13	14	15	16	17	18								
3	Na		Mg																Al		Si		P		S		Cl		Ar	
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36												
4	K		Ca		Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr										
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54												
5	Rb		Sr		Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe										
6	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80				
6	Cs		Ba		La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn										
7	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112				
7	Fr		Ra		Ac	Unq	Unp	Unh	Uns	Unc	Uue																			



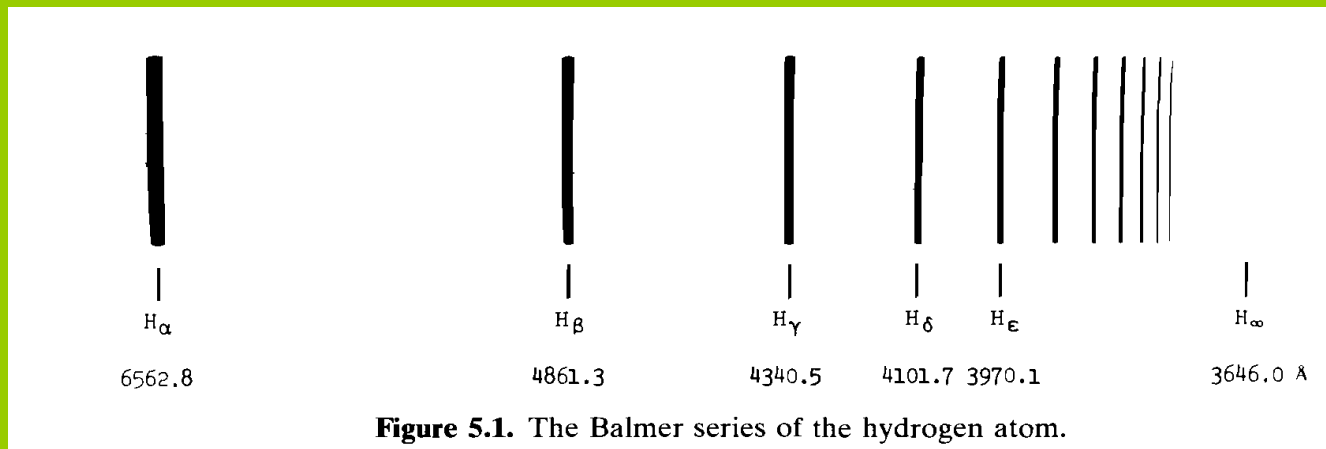
Tierras Raras Ligeras (TRLA)														
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

* Número atómico del átomo más ligero.
Peso atómico basado en ¹²C



ESPECTROS ATOMICOS

SERIE DE BALMER



$$\tilde{\nu} = 109,678 \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \text{ cm}^{-1}, \quad n = 3, 4, \dots$$

$$= R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right),$$

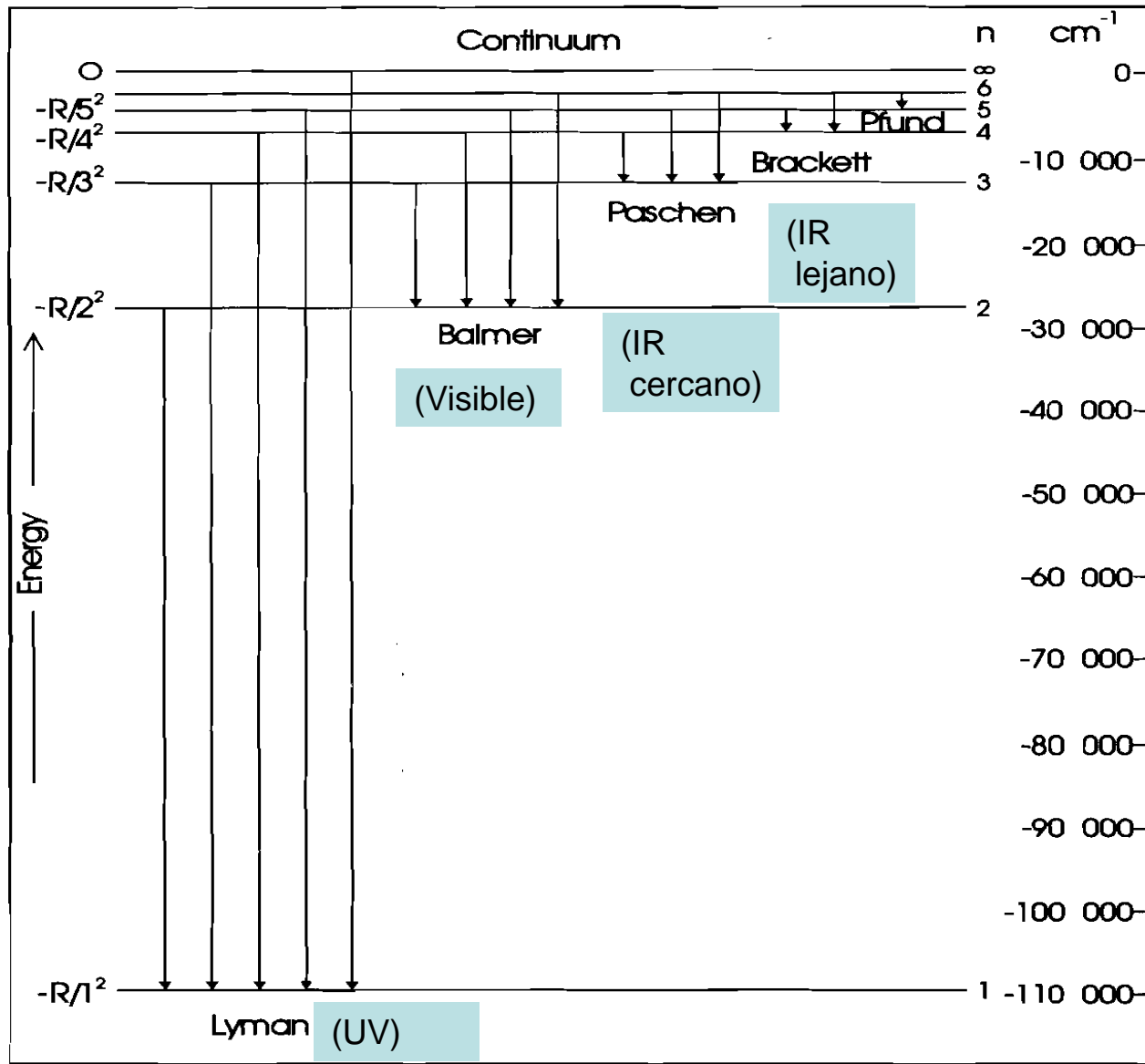


Figure 5.2. Energy levels of the hydrogen atom.

S=momento de spin electrónico

Matrices de Pauli

ATOMO DE HIDRÓGENO-espectro de un electrón

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi - \frac{Ze^2 \psi}{4\pi\epsilon_0 r} = E\psi.$$

$$\frac{-\hbar^2}{2mr^2} \frac{\partial}{\partial r} r^2 \frac{\partial \psi}{\partial r} + \frac{1}{2mr^2} \hat{L}^2 \psi - \frac{Ze^2 \psi}{4\pi\epsilon_0 r} = E\psi.$$

$$\psi = R_{nl}(r) Y_{lm}(\theta, \phi),$$

$$n = 1, 2, 3, \dots, \infty,$$

$$l = 0, 1, \dots, n - 1,$$

$$m = 0, \pm 1, \dots, \pm l.$$

$$E_n = \frac{-\mu Z^2 (e^2 / 4\pi\epsilon_0)^2}{2n^2 \hbar^2} = \frac{-R}{n^2}, \quad n = 1, 2, 3, \dots,$$

$$l = 0, 1, 2, 3, \dots \rightarrow s, p, d, f, \dots$$

$$R = R_H = 109,677,4212 \text{ cm}^{-1}$$

$$R_H = \frac{R_\infty}{1 + m_e/m_p},$$

=

Momento angular

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y,$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0,$$

$$\hat{L}^2 Y_{LM}(\theta, \phi) = \hbar^2 L(L+1) Y_{LM}(\theta, \phi),$$

$$\hat{L}_z Y_{LM}(\theta, \phi) = M\hbar Y_{LM}(\theta, \phi).$$

$$L_{\pm} = L_x \pm iL_y$$

$$L_{\pm} Y_{LM} = \hbar L(L+1)[L(L+1) - M(M \pm 1)]^{1/2} Y_{L, M \pm 1}$$

Funciones de spin:

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left| \frac{1}{2}; +\frac{1}{2} \right\rangle$$

$$|\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left| \frac{1}{2}; -\frac{1}{2} \right\rangle$$

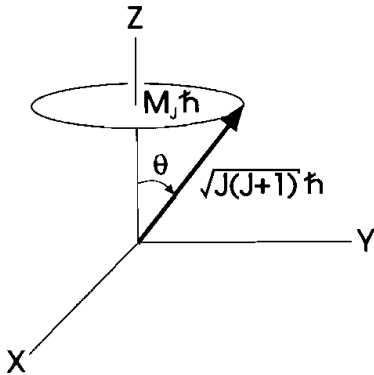
$$[\hat{H}, \hat{l}_z] = [\hat{H}, \hat{l}^2] = 0,$$

$$\hat{H}\psi_{nlm} = E_n\psi_{nlm},$$

$$\hat{l}^2\psi_{nlm} = l(l+1)\hbar^2\psi_{nlm},$$

$$\hat{l}_z\psi_{nlm} = m\hbar\psi_{nlm}.$$

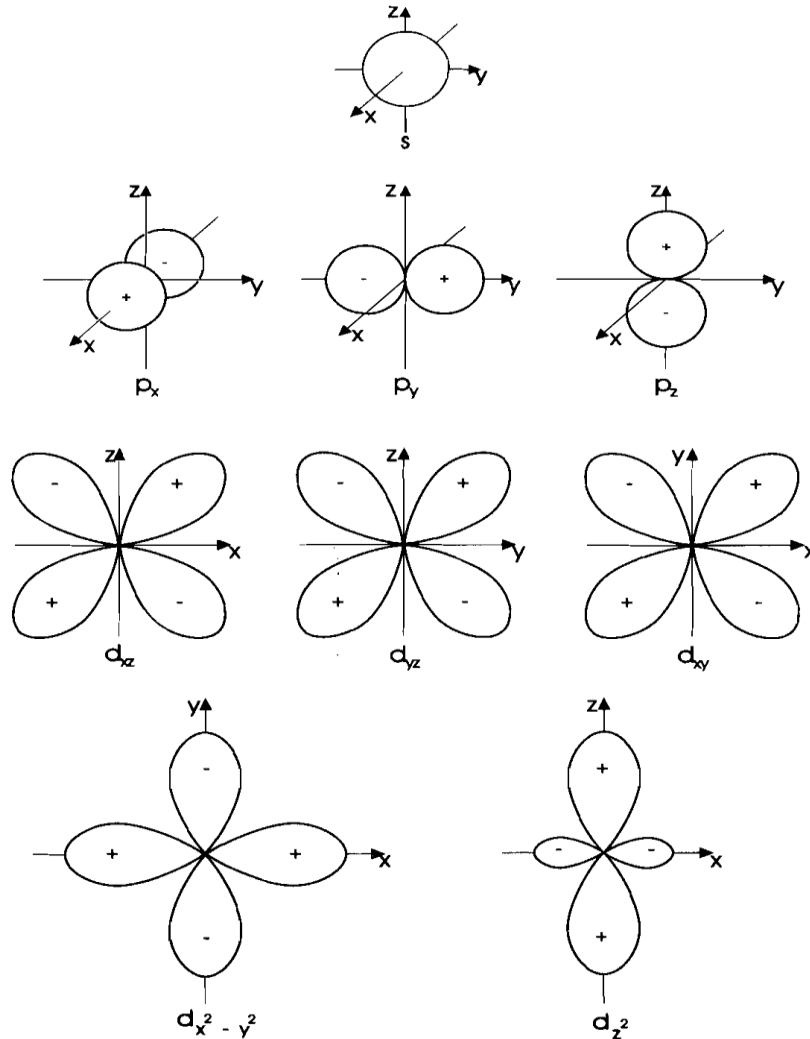
Para un momento angular J



M_J : Diferentes orientaciones Espaciales de J

Degeneración $(2J+1)$, para un espacio isótropo (ausencia de campos externos)

PARTE ANGULAR DE LOS ORBITALES 1s, 2p, 3d



$$\psi = R_{nl}(r)Y_{lm}(\theta, \phi),$$

Acoplamiento spin órbita

(estructura fina)

e^- (partícula cargada)



El movimiento orbital=corriente

$$\boldsymbol{\mu}_s = -g_e \mu_B \mathbf{S}$$

$$E = -\boldsymbol{\mu} \cdot \mathbf{B}$$

Campo en el e^- proporcional al
momento angular \mathbf{l}

$$\hat{H}_{so} = \xi(r) \hat{\mathbf{l}} \cdot \hat{\mathbf{s}}$$

$$\xi(r) = \frac{1}{2\mu^2 c^2} \frac{1}{r} \frac{\partial V}{\partial r} = \frac{1}{2\mu^2 c^2} \left(\frac{Ze^2}{4\pi\epsilon_0 r^3} \right)$$

$$V = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

Atracción COULOMBIANA
entre electrón y núcleos

$$[\hat{H}^{(0)} + \xi(r)\hat{\mathbf{l}} \cdot \hat{\mathbf{s}}]\psi = E\psi,$$

(derivación adecuada: EQR
(electrodinámica cuántica relativista))

l_z y s_z ya no conmutan con \mathbf{H}

\mathbf{j} conmuta con \mathbf{H}

(cte de movimiento)

$$\mathbf{j} = \mathbf{l} + \mathbf{s}$$

j^2 y j_z **SI** conmutan con \mathbf{H}

Ejemplo:
electrones p

$$|l = 1, m_l = 1\rangle |s = \frac{1}{2}, m_s = \pm \frac{1}{2}\rangle,$$
$$|l = 1, m_l = 0\rangle |s = \frac{1}{2}, m_s = \pm \frac{1}{2}\rangle,$$

(Representación desacoplada:
Producto de funciones angular
y spin de un electrón: 6 funciones)

$$|l = 1, m_l = -1\rangle |s = \frac{1}{2}, m_s = \pm \frac{1}{2}\rangle.$$

Representación en estados acoplados y desacoplados

$$\hat{H} = \hat{H}^{(0)} + \xi(r)\hat{\mathbf{l}} \cdot \hat{\mathbf{s}} = (\hat{H}^{(0)} + \xi(r)\hat{l}_z\hat{s}_z) + \frac{\xi(r)(\hat{l}_+\hat{s}_- + \hat{l}_-\hat{s}_+)}{2}$$

$$\begin{aligned} \langle l = 1, m_l | \langle s = \frac{1}{2}, m_s | \hat{H} | s = \frac{1}{2}, m_s \rangle | l = 1, m_l \rangle \\ = E_{2p}^{(0)} + \zeta_{2p} m_l m_s \end{aligned}$$

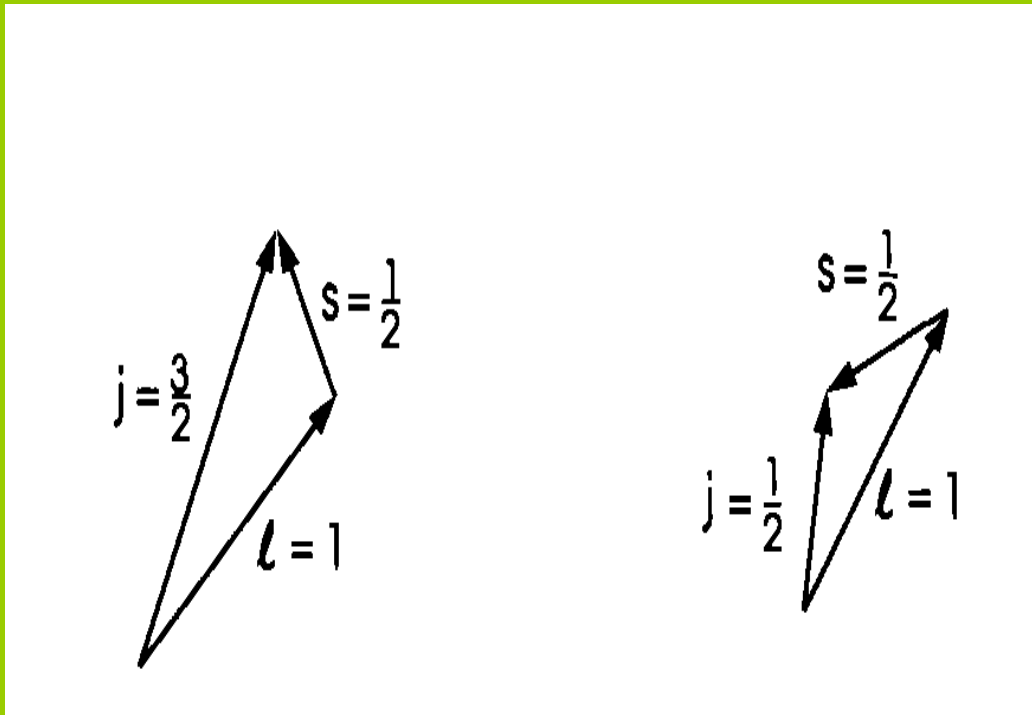
$$E_{2p}^{(0)} = -R_H/4$$

$$\zeta_{2p} = \hbar^2 \int R_{2p}^*(r) \xi(r) R_{2p}(r) r^2 dr.$$

$$\xi \hat{\mathbf{l}} \cdot \hat{\mathbf{s}} = \frac{\xi(\hat{j}^2 - \hat{l}^2 - \hat{s}^2)}{2}.$$

$$\hat{j}^2 = (\hat{\mathbf{l}} + \hat{\mathbf{s}}) \cdot (\hat{\mathbf{l}} + \hat{\mathbf{s}}) = \hat{l}^2 + \hat{s}^2 + 2\hat{\mathbf{l}} \cdot \hat{\mathbf{s}}$$

J^2 conmuta con H



$$|2p, j = \frac{3}{2}, m_j = \frac{3}{2}\rangle,$$

$$|2p, j = \frac{3}{2}, m_j = \frac{1}{2}\rangle,$$

$$|2p, j = \frac{3}{2}, m_j = -\frac{1}{2}\rangle,$$

$$|2p, j = \frac{3}{2}, m_j = -\frac{3}{2}\rangle,$$

$$|2p, j = \frac{1}{2}, m_j = \frac{1}{2}\rangle,$$

$$|2p, j = \frac{1}{2}, m_j = -\frac{1}{2}\rangle.$$

Los estados acoplados $|J M_J\rangle$ están relacionados con los no acoplados $|j_1 m_1\rangle |j_2 m_2\rangle$ por

$$|j_1, j_2 J, M_J\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle j_1, j_2; m_1, m_2 | JM_J\rangle |j_1 m_1\rangle |j_2 m_2\rangle,$$

Aparecen los coeficientes de Glebsh Gordan

SISTEMA DE MUCHOS ELECTRONES

$$\left(\frac{-\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 - \sum_{i=1}^N \frac{Ze^2}{4\pi\epsilon_0 r_i} + \sum_{i,j>i}^N \frac{e^2}{4\pi\epsilon_0 r_{ij}} \right) \psi = E\psi.$$

$$\hat{\mathbf{L}} = \hat{\mathbf{l}}_1 + \hat{\mathbf{l}}_2 + \dots + \hat{\mathbf{l}}_N = \sum_{i=1}^N \hat{\mathbf{l}}_i.$$

$$\hat{\mathbf{S}} = \sum_{i=1}^N \hat{\mathbf{s}}_i$$

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}.$$

$$\hat{L}_z = \hat{l}_{z1} + \hat{l}_{z2} + \cdots + \hat{l}_{zN},$$

$$\hat{S}_z = \hat{s}_{z1} + \hat{s}_{z2} + \cdots + \hat{s}_{zN},$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2,$$

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2.$$

$$\hat{L}^2 \psi \approx L(L + 1)\hbar^2 \psi$$

$$[\hat{l}_{zi}, \hat{H}] \neq 0,$$

$$\hat{l}_{zi} \psi \neq m_{li} \hbar \psi,$$

$$\hat{L}_z \psi = M_L \hbar \psi,$$

$$M_L = m_{l1} + m_{l2} + \cdots + m_{lN}.$$

$$[\hat{L}_z, \hat{H}] = 0,$$

$$[\hat{L}_x, \hat{H}] = 0 \quad \text{and} \quad [\hat{L}_y, \hat{H}] = 0.$$

$$[\hat{L}_z^2, \hat{H}] = 0, \quad [\hat{L}_x^2, \hat{H}] = 0, \quad \text{and} \quad [\hat{L}_y^2, \hat{H}] = 0,$$

$$[\hat{L}^2, \hat{H}] = 0$$

Table 5.4. One-electron and Multi-electron Atoms

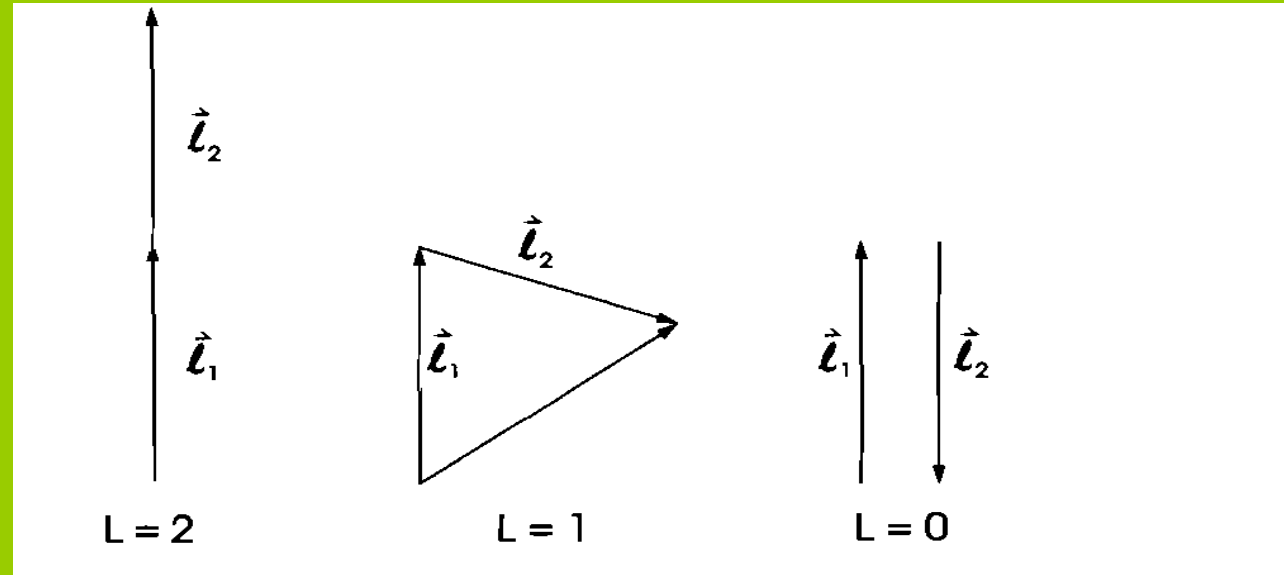
Multi-electron Atoms	One-electron Atoms
$\hat{L}^2 \psi = L(L + 1)\hbar^2 \psi$	$\hat{l}^2 \psi = l(l + 1)\hbar^2 \psi$
$\hat{L}_z \psi = M_L \hbar \psi$	$\hat{l}_z \psi = m_l \hbar \psi$
$\hat{S}^2 \psi = S(S + 1)\hbar^2 \psi$	$\hat{s}^2 \psi = s(s + 1)\hbar^2 \psi$
$\hat{S}_z \psi = M_S \hbar \psi$	$\hat{s}_z \psi = m_s \hbar \psi$
$L = 0, 1, 2, 3, 4, 5$	$l = 0, 1, 2, 3, 4, 5$
$S \quad P \quad D \quad F \quad G \quad H$	$s \quad p \quad d \quad f \quad g \quad h$

$$2S+1 L,$$

Degeneración
→

$$g = (2L + 1)(2S + 1).$$

Ejemplo $l_1=1, l_2=1$



Configuración $2p^2$ del
Átomo de carbono

2 electrones y
6 spin orbitales

$$\begin{aligned} \chi_1 &= p_1\alpha \\ \chi_2 &= p_0\alpha; \\ \chi_3 &= p_{-1}\alpha; \\ \chi_4 &= p_1\beta; \\ \chi_5 &= p_0\beta; \\ \chi_6 &= p_{-1}\beta \end{aligned}$$

15
determinantes
=
15
configuraciones

	$M_S = 1$	0	-1
$M_L = 2$	—	$ 1, \bar{1} $	—
$M_L = 1$	$ 1, 0 $	$ 1, \bar{0} 1, 0 $	$ \bar{1}, \bar{0} $
$M_L = 0$	$ 1, -1 $	$ 1, -\bar{1} \bar{1}, -1 0, \bar{0} $	$ \bar{1}, -\bar{1} $
$M_L = -1$	$ 0, -1 $	$ -1, \bar{0} -\bar{1}, 0 $	$ \bar{0}, -\bar{1} $
$M_L = -2$	—	$ -1, -\bar{1} $	—

microestado

15 configuraciones: no todas spin adaptadas

Notación

$|1, \bar{0}|$

significa.

$$m_{l1} = 1, m_{s1} = \frac{1}{2}, m_{l2} = 0, m_{s2} = -\frac{1}{2}$$

Acoplamiento Spin órbita

$$\hat{H}_{so} = \zeta \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}.$$

Valores permitidos

$$J=L+S, L+S-1, \dots, |L-S|$$

$$\hat{J}^2 = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = \hat{L}^2 + \hat{S}^2 + 2\mathbf{L} \cdot \mathbf{S}.$$

$$\mathbf{L} \cdot \mathbf{S} = \frac{\hat{J}^2 - \hat{L}^2 - \hat{S}^2}{2}$$

Las **componentes** de **L** y **S** no conmutan con H

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

J, **L**² y **S**² conmutan con H

$$\begin{aligned} \langle H_{so} \rangle &= \zeta \langle \mathbf{L} \cdot \mathbf{S} \rangle = \zeta \langle nJM_JLS | \mathbf{L} \cdot \mathbf{S} | nJM_JLS \rangle \\ &= \frac{\zeta [J(J+1) - L(L+1) - S(S+1)]}{2}. \end{aligned}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{ee}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{ee} + \zeta \mathbf{L} \cdot \mathbf{S}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{ee} + \sum \xi(r_i) \mathbf{l}_i \cdot \mathbf{s}_i$$

$$\hat{H}\psi = E\psi$$

$$\hat{L}^2\psi = L(L+1)\hbar^2\psi$$

$$\hat{L}_z\psi = M_L\hbar\psi$$

$$\hat{S}^2\psi = S(S+1)\hbar^2\psi$$

$$\hat{S}_z\psi = M_S\hbar\psi$$

$$\hat{H}\psi = E\psi$$

$$\hat{L}^2\psi = L(L+1)\hbar^2\psi$$

$$\hat{S}^2\psi = S(S+1)\hbar^2\psi$$

$$\hat{J}^2\psi = J(J+1)\hbar^2\psi$$

$$\hat{J}_z\psi = M_J\hbar\psi$$

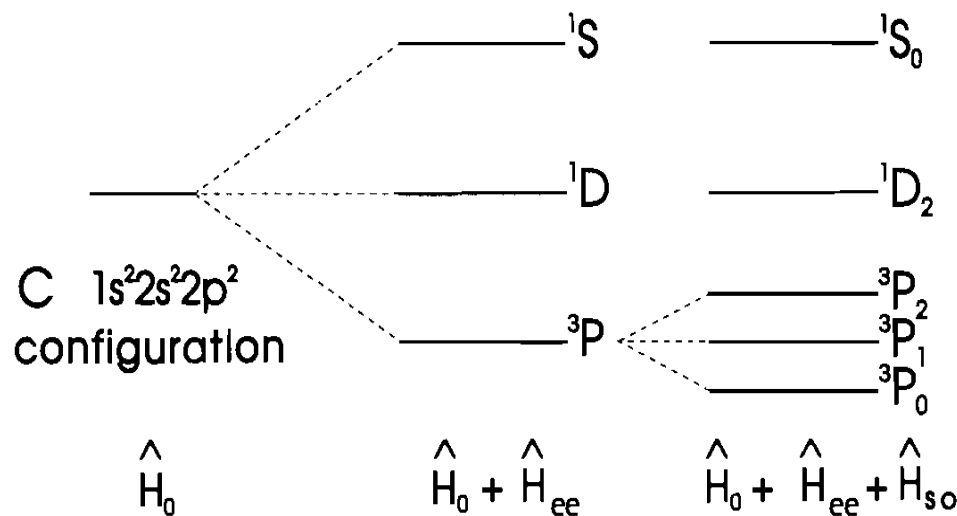
$$\hat{H}\psi = E\psi$$

$$\hat{L}^2\psi \approx L(L+1)\hbar^2\psi$$

$$\hat{S}^2\psi \approx S(S+1)\hbar^2\psi$$

$$\hat{J}^2\psi = J(J+1)\hbar^2\psi$$

$$\hat{J}_z\psi = M_J\hbar\psi$$



Reglas de selección

Regla de Hund

- Al llenar orbitales de igual energía, los electrones prefieren acomodarse con spin paralelo

Ejemplo: **3 electrones en el orbital 2p;**

$p_x^1 p_y^1 p_z^1$ (vs) $p_x^2 p_y^1 p_z^0$

$(p_x^2 p_y^1 p_z^0 = p_x^0 p_y^1 p_z^2 = p_x^1 p_y^0 p_z^2 = p_x^2 p_y^0$

$p_z^1 = \dots)$

1era. Regla: mayor proyección de spin ($2S+1$).

2da. Regla mayor Momento angular (L).

3era. Regla Acoplamiento spin órbita.

Cuando varios electrones están descritos por orbitales degenerados, la mayor estabilidad energética es aquella en donde los espines electrónicos están desapareados (correlación de espines):

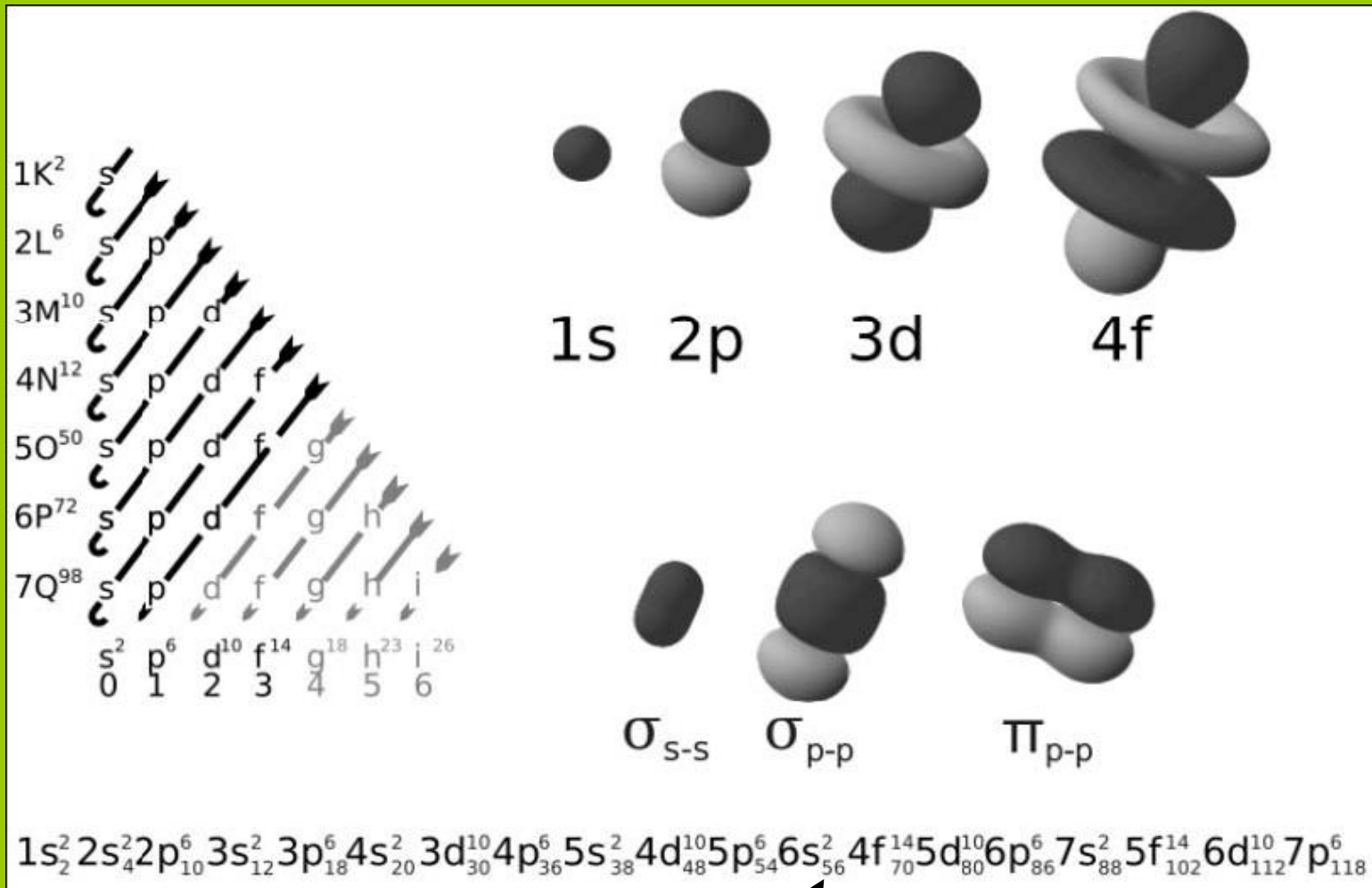
principio de Aufbau

subcapa 2p tres niveles energéticos, 2p_x, 2p_y, 2p_z.

orbital **2p** hasta seis electrones,

un electrón en cada uno antes que alguno llegue a tener dos.





Columna de gases nobles

REGLA DEL SERRUCHO: $1s \rightarrow 2s \rightarrow 2p \rightarrow 3s \rightarrow 3p \rightarrow 4s \rightarrow 3d \rightarrow 4p \rightarrow 5s \dots$

Configuraciones atómicas p^n y d^n

p^1 : 2P

p^2 : $^1S, ^1D, ^3P$

p^3 : $^2P, ^2D, ^4S$

p^4 : $^1S, ^1D, ^3P$

p^5 : 2P

d^1, d^9 : 2D

d^2, d^8 : $^1S, ^1D, ^1G, ^3P, ^3F$

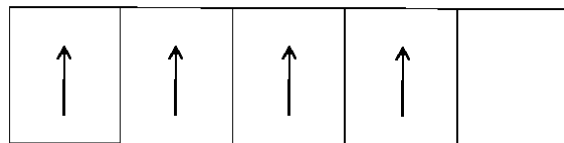
d^3, d^7 : $^2P, ^2D$ (twice), $^2F, ^2G, ^2H, ^4P, ^4F$

d^4, d^6 : 1S (twice), 1D (twice), $^1F, ^1G$ (twice), $^1I, ^3P$ (twice)

$^3D, ^3F$ (twice), $^3G, ^3H, ^5D$

d^5 : $^2S, ^2P, ^2D$ (three times), 2F (twice), 2G (twice),

$^2H, ^2I, ^4P, ^4D, ^4F, ^4G, ^6S$



m_l

2

1

0

-1

-2

Microestado d^4 ; $M_l=2$,
 $M_s=2$

 $2S + 1$

Name

 $2S + 1$ Name

1

Singlet

6

Sextet

2

Doublet

7

Septet

3

Triplet

8

Octet

4

Quartet

9

Nonet

5

Quintet

10

Decet

$$\begin{aligned} \langle H_{\text{so}} \rangle &= \zeta \langle \mathbf{L} \cdot \mathbf{S} \rangle = \zeta \langle nJM_JLS | \mathbf{L} \cdot \mathbf{S} | nJM_JLS \rangle \\ &= \frac{\zeta [J(J+1) - L(L+1) - S(S+1)]}{2}. \end{aligned}$$

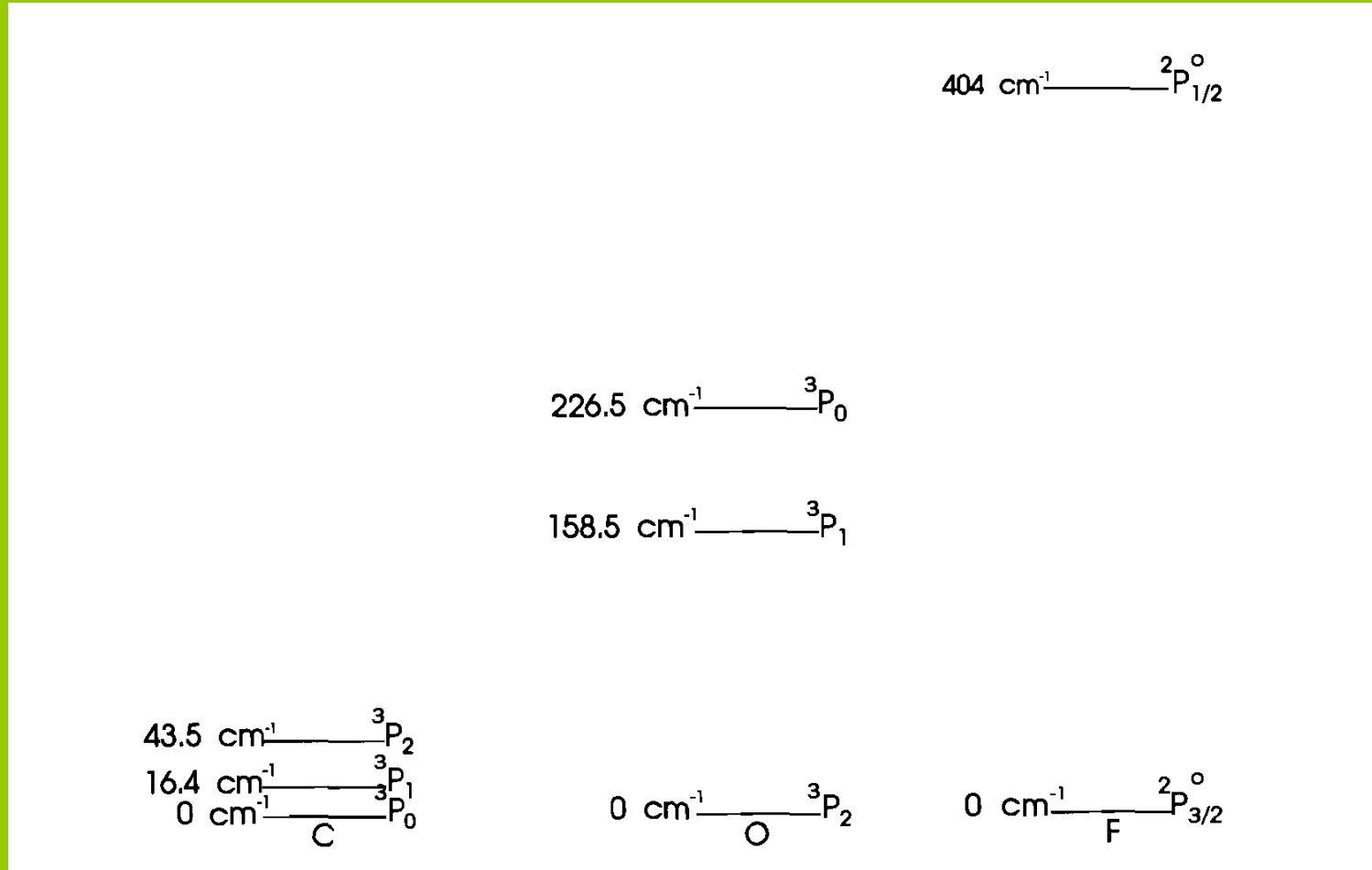
$$E_{J+1} - E_J = \frac{\zeta [(J+1)(J+2) - J(J+1)]}{2} = \zeta(J+1).$$

Intervalo de Landé



Valores permitidos de J: L+S, L+S-1, | L-S|

Splitting de los multipletes mas bajos de C, O, F (Landé)



C: $1s^2, 2s^2, 2p^2$

O: $1s^2, 2s^2, 2p^4$

F: $1s^2, 2s^2, 2p^5$

$2S+1L_J$

Efecto Zeeman

$$\boldsymbol{\mu}_L = \gamma \mathbf{L}.$$

$$|\mathbf{L}| = [L(L + 1)]^{1/2} \hbar$$

$$|\boldsymbol{\mu}_L| = -\left(\frac{e\hbar}{2m_e}\right) \sqrt{L(L + 1)} = -\mu_B \sqrt{L(L + 1)},$$

$$\boldsymbol{\mu}_S = g_e \gamma \mathbf{S} = g_e \left(\frac{-\mu_B}{\hbar}\right) \mathbf{S},$$

$$g_e = 2.0023$$

Campo \mathbf{B} externo

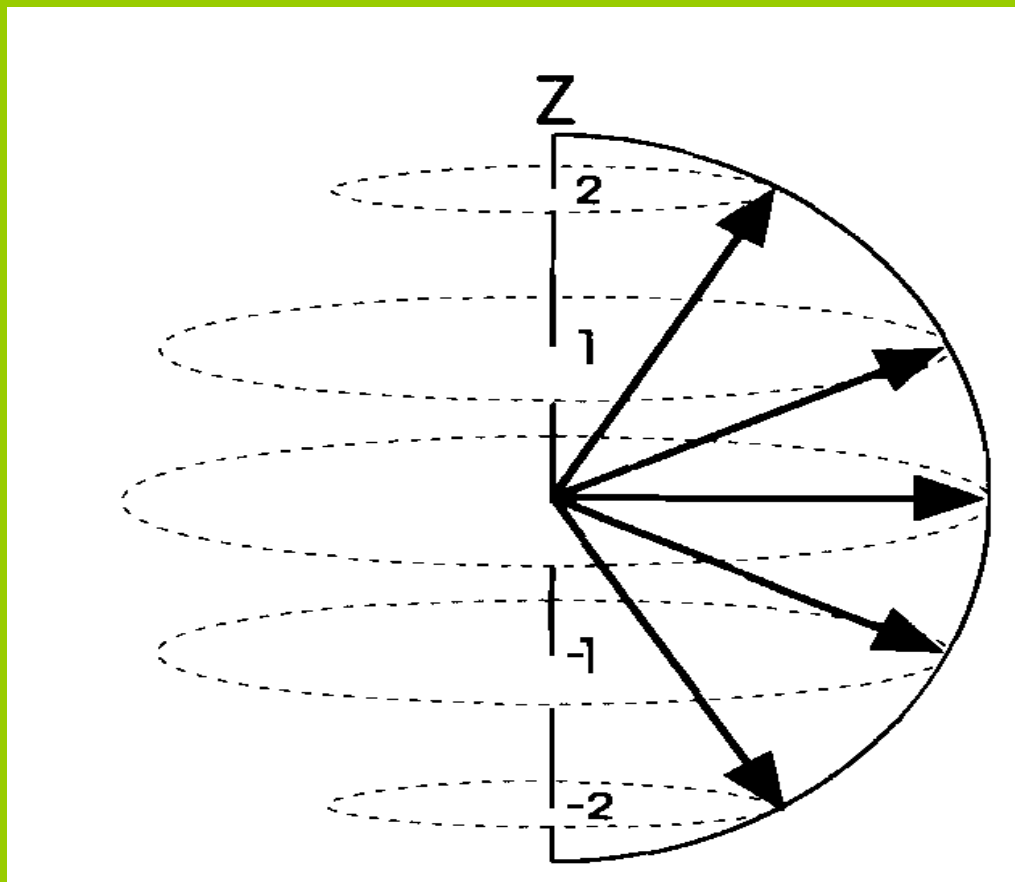
$$\hat{H}' = -\boldsymbol{\mu} \cdot \mathbf{B}$$

Momento magnético nuclear:

$$\boldsymbol{\mu}_I = \gamma_I \mathbf{I} = g_I \frac{\mu_N}{\hbar} \mathbf{I}$$

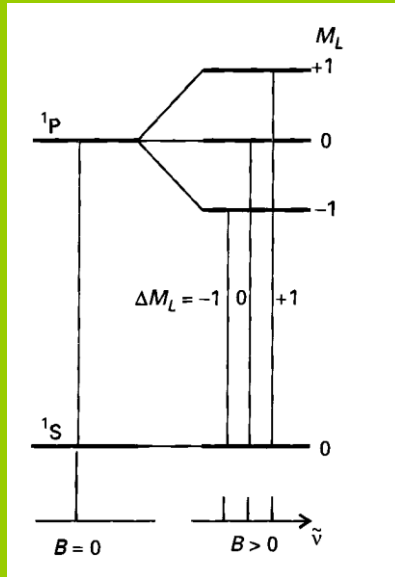
$$\mu_N = \frac{e\hbar}{2m_p}$$

$$\nu = \frac{\Delta(\boldsymbol{\mu} \cdot \mathbf{B})}{\hbar}$$



ZEEMAN normal (**singletes**)
para sistema de muchos electrones

$$H^{(1)} = -m_z \mathcal{B} = -\gamma_e (l_{z1} + l_{z2} + \dots) \mathcal{B} = -\gamma_e L_z \mathcal{B}$$



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

Intervalo: $\mu_L B$
Independiente de L

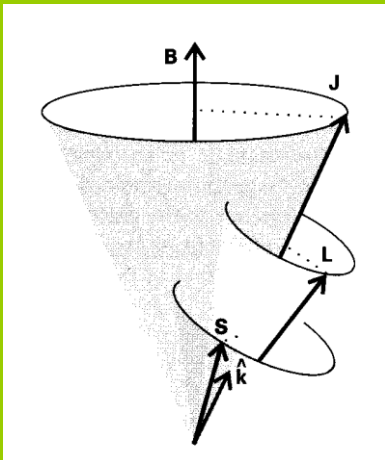
$$\Delta M_L = \pm 1$$

Luz polarizada perpend a **B**

$$\Delta M_L = 0$$

Luz polarizada paralela a **B**

EFEECTO ZEEMAN ANOMALO



$$H^{(1)} = -\mathbf{m}_{\text{orbital}} \cdot \mathbf{B} - \mathbf{m}_{\text{spin}} \cdot \mathbf{B} = -\gamma_e (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B}$$

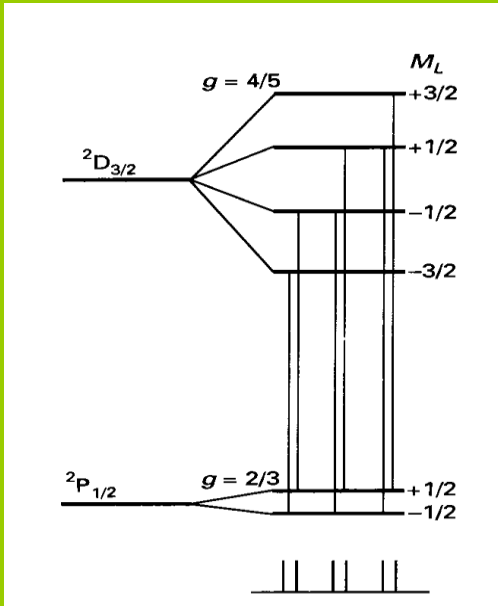
(el momento de **spin** es no nulo)

$$\begin{aligned}\boldsymbol{\mu}_J &= \left[\boldsymbol{\mu}_S \cdot \frac{\mathbf{J}}{|\mathbf{J}|^2} + \frac{\boldsymbol{\mu}_L \cdot \mathbf{J}}{|\mathbf{J}|^2} \right] \mathbf{J} \\ &= \left[\gamma(g_s \mathbf{S} + \mathbf{L}) \cdot \frac{\mathbf{J}}{|\mathbf{J}|^2} \right] \mathbf{J},\end{aligned}$$

$$H^{(1)} = -g_J \gamma_e \mathbf{J} \cdot \mathbf{B}$$

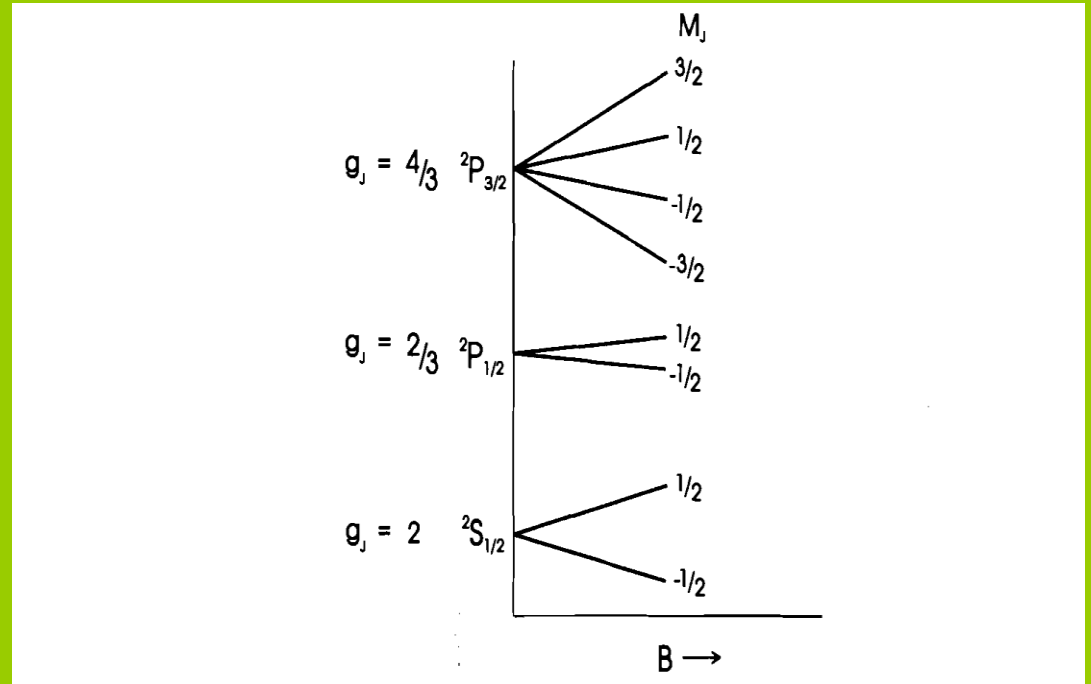
$$\begin{aligned}H^{(1)} &= -\gamma_e (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B} \\ &= -\gamma_e \left\{ 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right\} \mathbf{J} \cdot \mathbf{B}\end{aligned}$$

Zeeman normal



$$\nu_L = \frac{\mu_B B}{h}$$

Zeeman (anómalo) para los primeros 3 estados de un alcalino



$$E_{M_J} = \langle \hat{H}' \rangle = -\langle \mu_J \cdot \mathbf{B} \rangle = g_J \frac{\mu_B}{\hbar} \langle \mathbf{J} \cdot \mathbf{B} \rangle = g_J \frac{\mu_B B}{\hbar} \langle J_z B_z \rangle = g_J \mu_B M_J B,$$

Poca utilidad en espectroscopía atómica pq depende de J