THEORY OF ANGULAR MOMENTUM

$$pr\sin\alpha = \vec{r}\times\vec{p} = \vec{l}$$

$$\bar{p} = \vec{i}p_x + \vec{j}p_y + \vec{k}p_z$$

$$\vec{l} = \vec{i}(yp_z - zp_y) + \vec{j}(zp_x - xp_z) + \vec{k}(xp_y - yp_x)$$

$$\Downarrow$$

$$\hat{\vec{l}} = -i\hbar\left\{\vec{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) + \vec{j}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) + \vec{k}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right\}$$

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

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

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

$$\Downarrow$$

$$\left.\begin{aligned} \langle lm|\hat{L}_z|l'm'\rangle &= m\hbar\,\delta(mm') \\ \langle lm|\hat{L}^2|lm\rangle &= l(l+1)\hbar^2 \end{aligned}\right\} \text{EIGENVALUES}$$

$$\langle lm|\hat{L}_+|l\,m-1\rangle = \hbar\left(l(l+1) - m(m-1)\right)^{1/2}$$

$$\langle lm|\hat{L}_-|l\,m+1\rangle = \hbar\left((l(l+1) - m(m+1)\right)^{1/2}$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

ANGULAR MEMENTUM OPERATORS =
GENERATORS OF ALL ROTATIONS IN O(3) (≡ R_3)
(ISOTROPY OF SPACE)

$$\Downarrow$$

$$\left.\begin{matrix}[\hat{H}, L^2]=0 \\ [\hat{H}, \hat{L}_z]=0\end{matrix}\right\}$$ $\hat{H}, \hat{L}^2, \hat{L}_z$:
- COMMON EIGENFUNCTIONS
- SIMULTANEOUSLY MEASURED EIGENVALUES

ROTATIONS ARE SYMMETRY OPERATIONS

$H\Psi_E = E\Psi_E$; Ψ_E – STATIONARY STATE WITH WELL DEFINED ENERGY

$\hat{L}_1$ $[\hat{H}, \hat{L}_1]=0$

$$\hat{L}_1\hat{H}\Psi_E = \hat{L}_1 E\Psi_E, \quad \hat{H}\underbrace{\hat{L}_1\Psi_E}_{a_1\Psi_E} = E\underbrace{\hat{L}_1\Psi_E}_{a_1\Psi_E} :$$

$\hat{L}_1\Psi_E = a_1\Psi_E$ EIGENVALUE PROBLEM

$$\Psi_E \Rightarrow \Psi_{E,a_1}$$

$$\Psi_E \Rightarrow \Psi_{E,l,m}$$

QUANTUM NUMBERS!

IDENTIFICATION OF ENERGY STATES

ONE-PARTICLE (ELECTRON) STATES

$|nlsm_lm_s\rangle$:

$n = 1, 2, 3, \ldots$

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

$m_l = -l, \ldots l \quad (2l+1)$

$s = \frac{1}{2}$

$m_s = -\frac{1}{2}, \frac{1}{2}$

$$\langle \bar{r}\sigma | \overset{\hat{H}}{n} \overset{\hat{L}^2}{l} \overset{\hat{S}^2}{s} \overset{\hat{L}_z}{m_l} \overset{\hat{S}_z}{m_s}\rangle = \langle r|nl\rangle\langle\vartheta\varphi|lm_l\rangle\langle\sigma|sm_s\rangle$$

$$\langle r|nl\rangle = -\frac{(2Z)^{l+1}}{n^{l+2}}\left[\frac{Z(n-l-1)!}{(n+l)!^3}\right]^{1/2} e^{-Zr/n}\, L^{2l+1}_{n+l}\left(\frac{2Zr}{n}\right)$$

ASSOCIATED LAGUERRE POLYNOMIALS

$\langle\vartheta\varphi|lm_l\rangle$ – SPHERICAL HARMONICS

II 3.

Table 5.6. *Properties of the Spherical Harmonics and of Angular Momentum*

DEFINITION

$$Y_l^m(\theta, \phi) = (-1)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{\frac{1}{2}} P_l^m(\cos\theta)e^{im\phi}$$

DIFFERENTIAL EQUATION

$$\mathsf{L}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$$

Other differential relations involving angular momentum [see Eqs. (5.38), (5.44), and (5.50) for the definitions of L_z, L_+, L_-, L_x, and L_y]:

$$\mathsf{L}_z Y_l^m = m\hbar Y_l^m$$

$$\mathsf{L}_+ Y_l^m = \hbar[(l-m)(l+m+1)]^{\frac{1}{2}} Y_l^{m+1}$$

$$\mathsf{L}_- Y_l^m = \hbar[(l+m)(l-m+1)]^{\frac{1}{2}} Y_l^{m-1}$$

$$\mathsf{L}_x Y_l^m = \tfrac{1}{2}\hbar[(l-m)(l+m+1)]^{\frac{1}{2}} Y_l^{m+1} + \tfrac{1}{2}\hbar[(l+m)(l-m+1)]^{\frac{1}{2}} Y_l^{m-1}$$

$$\mathsf{L}_y Y_l^m = -\tfrac{1}{2}i\hbar[(l-m)(l+m+1)]^{\frac{1}{2}} Y_l^{m+1} + \tfrac{1}{2}i\hbar[(l+m)(l-m+1)]^{\frac{1}{2}} Y_l^{m-1}$$

THE FIRST FEW SPHERICAL HARMONICS

Eigenfunctions of L_z **Noneigenfunctions of L_z**

$$Y_0^0 = \frac{1}{2(\pi)^{\frac{1}{2}}}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\theta \ (\cong P_0) \qquad = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\frac{z}{r}$$

$$Y_1^1 = -\left(\frac{3}{8\pi}\right)^{\frac{1}{2}}\sin\theta e^{i\phi} \ (P_1) \qquad Y_1^{1,c} = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\sin\theta\cos\phi \ (P_x) \qquad = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\frac{x}{r}$$

or) $\pm$

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{\frac{1}{2}}\sin\theta e^{-i\phi} \ (P_{-1}) \qquad Y_1^{1,s} = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\sin\theta\sin\phi \ (P_y) \qquad = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\frac{y}{r}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}}(3\cos^2\theta - 1) \qquad = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}}\frac{(3z^2-1)}{r^2}$$

$$Y_2^1 = -\left(\frac{15}{8\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta e^{i\phi} \qquad Y_2^{1,c} = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta\cos\phi = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}}\frac{xz}{r^2}$$

or

$$Y_2^{-1} = \left(\frac{15}{8\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta e^{-i\phi} \qquad Y_2^{1,s} = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}}\sin\theta\cos\theta\sin\phi = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}}\frac{yz}{r^2}$$

$$Y_2^2 = \left(\frac{15}{32\pi}\right)^{\frac{1}{2}}\sin^2\theta e^{2i\phi} \qquad Y_2^{2,c} = \left(\frac{15}{16\pi}\right)^{\frac{1}{2}}\sin^2\theta\cos 2\phi \qquad = \left(\frac{15}{16\pi}\right)^{\frac{1}{2}}\frac{(x^2-y^2)}{r^2}$$

or

$$Y_2^{-2} = \left(\frac{15}{32\pi}\right)^{\frac{1}{2}}\sin^2\theta\, e^{-2i\phi} \qquad Y_2^{2,s} = \left(\frac{15}{16\pi}\right)^{\frac{1}{2}}\sin^2\theta\sin 2\phi \qquad = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}}\frac{xy}{r^2}$$

Table 5.8. *Hydrogen Atom Wavefunctions* (ORBITALS)

$\psi_{n,l,m} = R_{nl}(r)Y_l^m(\theta, \phi)$; Y_l^m can be put in one of the alternate forms given in Table 5.6; $a = a_0/Z = \hbar^2/Z\mu e^2$, a unit of length.

l=0 1 2 3 4 5...
s p d f g h...

FROM SPECTRAL LINES:
sharp
principal
diffuse
fine...

$$\psi_{1,0,0} = \psi_{1s} = \left(\frac{1}{\pi a^3}\right)^{\frac{1}{2}} e^{-r/a}$$

$$\psi_{2,0,0} = \psi_{2s} = \left(\frac{1}{32\pi a^3}\right)^{\frac{1}{2}} \left(2 - \frac{r}{a}\right) e^{-r/2a}$$

$$\psi_{2,1,0} = \psi_{2p_z} = \left(\frac{1}{32\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a} e^{-r/2a} \cos\theta$$

$$\psi_{2,1,1,c} = \psi_{2p_x} = \left(\frac{1}{32\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a} e^{-r/2a} \sin\theta\cos\phi$$

$$\psi_{2,1,1,s} = \psi_{2p_y} = \left(\frac{1}{32\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a} e^{-r/2a} \sin\theta\sin\phi$$

$$\psi_{3,0,0} = \psi_{3s} = \frac{1}{81}\left(\frac{1}{3\pi a^3}\right)^{\frac{1}{2}} \left[27 - 18\frac{r}{a} + 2\left(\frac{r}{a}\right)^2\right] e^{-r/3a}$$

$$\psi_{3,1,0} = \psi_{3p_z} = \frac{1}{81}\left(\frac{2}{\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a}\left(6 - \frac{r}{a}\right) e^{-r/3a} \cos\theta$$

$$\psi_{3,1,1,c} = \psi_{3p_x} = \frac{1}{81}\left(\frac{2}{\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a}\left(6 - \frac{r}{a}\right) e^{-r/3a} \sin\theta\cos\phi$$

$$\psi_{3,1,1,s} = \psi_{3p_y} = \frac{1}{81}\left(\frac{2}{\pi a^3}\right)^{\frac{1}{2}} \frac{r}{a}\left(6 - \frac{r}{a}\right) e^{-r/3a} \sin\theta\sin\phi$$

$$\psi_{3,2,0} = \psi_{3d_{z^2}} = \frac{1}{81}\left(\frac{1}{6\pi a^3}\right)^{\frac{1}{2}} \left(\frac{r}{a}\right)^2 e^{-r/3a} (3\cos^2\theta - 1)$$

$$\psi_{3,2,1,c} = \psi_{3d_{xz}} = \frac{1}{81}\left(\frac{2}{\pi a^3}\right)^{\frac{1}{2}} \left(\frac{r}{a}\right)^2 e^{-r/3a} \sin\theta\cos\theta\cos\phi$$

$$\psi_{3,2,1,s} = \psi_{3d_{yz}} = \frac{1}{81}\left(\frac{2}{\pi a^3}\right)^{\frac{1}{2}} \left(\frac{r}{a}\right)^2 e^{-r/3a} \sin\theta\cos\theta \,\mathrm{cin}\,\phi$$

$$\psi_{3,2,2,c} = \psi_{3d_{x^2-y^2}} = \frac{1}{81}\left(\frac{1}{2\pi a^3}\right)^{\frac{1}{2}} \left(\frac{r}{a}\right)^2 e^{-r/3a} \sin^2\theta\cos^2\phi$$

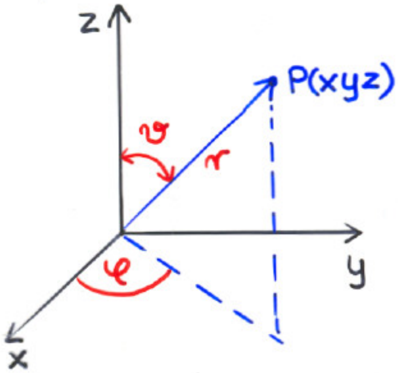
$$\psi_{3,2,2,s} = \psi_{3d_{xy}} = \frac{1}{81}\left(\frac{1}{2\pi a^3}\right)^{\frac{1}{2}} \left(\frac{r}{a}\right)^2 e^{-r/3a} \sin^2\theta\sin^2\phi$$

.
.
.

HYDROGEN ATOM

(SPHERICAL SYMMETRY)

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}\right)\Psi = E\Psi$$



$$\begin{cases} x = r\sin\vartheta\cos\varphi \\ y = r\sin\vartheta\sin\varphi \\ z = r\cos\varphi \end{cases}$$

$0 \leq r < \infty$

$0 \leq \vartheta \leq \pi$

$0 \leq \varphi \leq 2\pi$

$$d\tau = r^2 \sin\vartheta \, dr \, d\vartheta \, d\varphi$$

$$\Delta_{xyz} \equiv \nabla^2_{xyz} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\Delta_{r\vartheta\varphi} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + $$
$$+ \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

$$\Psi(xyz) \Rightarrow \Psi(r,\vartheta,\varphi) = R(r)Y(\vartheta,\varphi)$$

SPHERICAL HARMONICS

$$\frac{d^2R}{dx^2} + \frac{2}{x}\frac{dR}{dx} + \left[-\frac{l(l+1)}{x^2} + \frac{n}{x} + \frac{E_n^2\hbar^2}{2\mu e^4 Z^2}\right]R(r) = 0$$

$x = \frac{2Z}{na_0}r$

$a_0 = \hbar^2/\mu e^2$

$$\left.\begin{array}{l} n = \text{natural number} \\ \dfrac{E_n^2\hbar^2}{2\mu e^4 Z^2} = -\dfrac{1}{4} \end{array}\right\} Q$$

$$E_n = -\frac{\mu Z^2 e^4}{2n^2\hbar^2}$$

$n = 1, 2, \ldots$

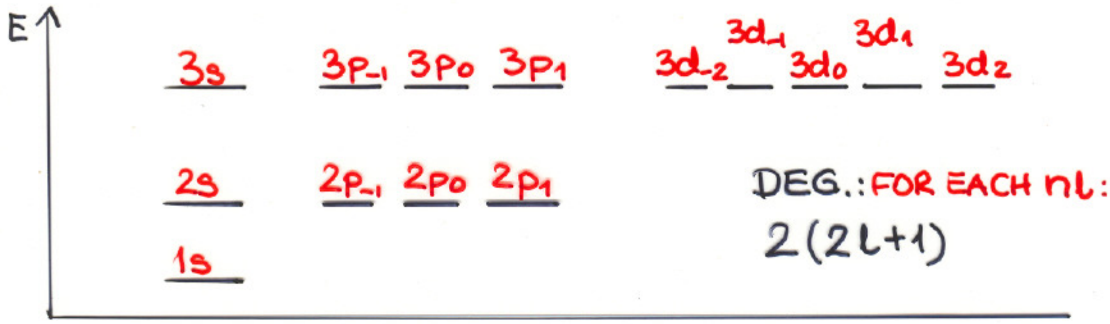
PRINCIPAL QUANTUM NUMBER

$$R(r) \equiv R_{nl}(r) \sim x^l e^{-x/2} L^{2l+1}_{n+1}(x)$$

LAGUERRE POLINOM.

ENERGY SCHEME

ONE-ELECTRON SYSTEM



$$H_H = -\frac{\hbar^2}{2\mu}\nabla^2 + V(r)$$

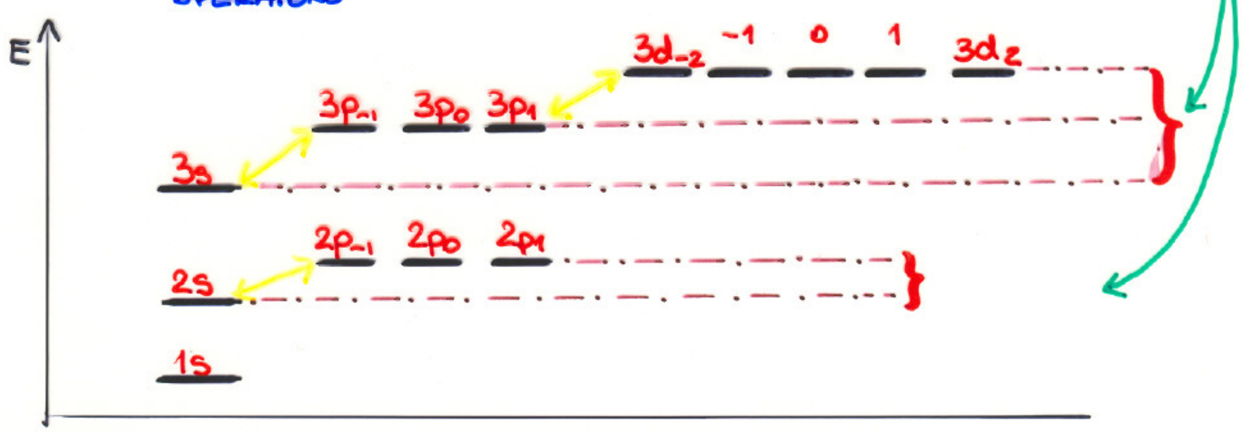
$$\Downarrow$$

MANY-ELECTRON SYSTEM

$$H = \sum H_H + \sum_{i<j} \frac{e^2}{r_{ij}}$$

COULOMB INTERACTION

SUM OF ONE-ELECTRON OPERATORS



CENTRAL-FIELD APPROXIMATION

$$H = \underbrace{\sum_i^N \left(-\frac{\hbar^2}{2\mu}\nabla_i^2 + U(r_i)\right)}_{\hat{\mathcal{H}}(i)} + \sum_{i<j}^N \frac{e^2}{r_{ij}} - \sum_i^N U(r_i)$$

NEW POTENTIAL

THEORY OF ATOMS ⇒ FUTURE

$\mathcal{H}(i) = H_H$ WITH $V(r)$ REPLACED BY $U(r)$

HOW TO CONSTRUCT N-ELECTRON WAVE FUNCTION OF GOOD SYMMETRY?

COUPLING OF ANGULAR MOMENTA

N=2

$1\bar{e}: \bar{l}_1, \bar{s}_1; \quad 2\bar{e}: \bar{l}_2, \bar{s}_2 \Rightarrow (n_1 l_1)^1 (n_2 l_2)^1$

a). $\boxed{\vec{l}_1 + \vec{l}_2 = \vec{L}, \quad \vec{s}_1 + \vec{s}_2 = \vec{S}, \quad \vec{L} + \vec{S} = \vec{J}}$ COUPLING **LS** $\quad [H, L^2] = 0$, $[H, S^2] = 0$

b). $\bar{l}_1 + \bar{l}_2 = \bar{L}, \quad \bar{L} + \vec{s}_1 = \bar{K}, \quad \bar{K} + \vec{s}_2 = \bar{J}$ LK

c). $\bar{l}_1 + s_1 = \bar{j}_1, \quad \vec{j}_1 + \bar{l}_2 = \bar{K}, \quad \bar{K} + \bar{s}_2 = \bar{J}$ jK

d). $\boxed{\vec{l}_1 + \vec{s}_1 = \vec{j}_1, \quad \bar{l}_2 + \bar{s}_2 = \bar{j}_2, \quad \vec{j}_1 + \vec{j}_2 = \vec{J}}$ COUPLING **jj** $\quad [H, J] = 0$

$$\underbrace{(2s_1+1)}_{(m_{s_1})}\underbrace{(2l_1+1)}_{(m_{l_1})}\underbrace{(2s_2+1)}_{(m_{s_2})}\underbrace{(2l_2+1)}_{(m_{l_2})} = 4(2l_1+1)(2l_2+1)$$

NUMBER OF STATES FOR THE CONFIGURATION $(n_1 l_1)^1 (n_2 l_2)^1$ $\quad \equiv 4[l_1; l_2]$ (ATOMIC SPECTROSCOPY)

LS COUPLING

$^{2S+1}L_J$

2S+1 FOR L≥S
2L+1 FOR L<S
MULTIPLICITY

OBSERVED ATOMIC TERMS

2J+1 STATES ($M_J = -J, \dots J$)

L = 0 1 2 3 4 5 6 7 8
S P D F G H I K L

EACH TERM ^{2S+1}L : $(2S+1)(2L+1)$-FOLD DEGENERATE

EXAMPLE: $np\, n'f$: $l_1 = 1 \quad l_2 = 3$

$|l_1 - l_2| \le L \le l_1 + l_2 \qquad |s_1 - s_2| \le S \le s_1 + s_2$

$2 \le L \le 4 \qquad 0 \le S \le 1$

$L = 2, 3, 4 \qquad S = 0, 1$

	^1D	^3D	^1F	^3F	^1G	^3G
TERMS:	S=0 L=2, J=2	S=1 L=2, J=1,2,3	S=0 L=3, J=3	S=1 L=3, J=2,3,4	S=0 L=4, J=4	S=1 L=4, J=3,4,5
LEVELS:	$^1D_2$	$^3D_1$, $^3D_2$, $^3D_3$	$^1F_3$	$^3F_2$, $^3F_3$, $^3F_4$	$^1G_4$	$^3G_3$, $^3G_4$, $^3G_5$

ARE ALL THESE VALUES OF TOTAL S AND L DEFINE ATOMIC TERMS? REMEMBER: SLATER DETERMINANT!

FUNCTION OF GOOD SYMMETRY: $|\gamma S M_S L M_L\rangle \Rightarrow |s m_s l m_l\rangle$

$2p^3$ – TOTAL ANGULAR MOMENTA

$$\left.\begin{array}{l} l_1 = 1 \\ l_2 = 1 \end{array}\right\} L' = 0, 1, 2$$

$$l_3 = 1 \quad (+) \quad \left\}\begin{array}{l} L = 1 \\ L = 0, 1, 2 \\ L = 1, 2, 3 \end{array}\right. \Rightarrow L = \overset{S}{0}, \overset{P}{1}, \overset{D}{2}, \overset{F}{3}$$

$L=0$: $M_L = 0$

$L=1$: $M_L = -1, 0, 1$

$L=2$: $M_L = -2, -1, 0, 1, 2$

$L=3$: $M_L = -3, -2, -1, 0, 1, 2, 3$

$$\left.\begin{array}{l} s_1 = 1/2 \\ s_2 = 1/2 \end{array}\right\} S' = 0, 1$$

$$s_3 = 1/2 \quad (+) \quad \left\}\begin{array}{l} S = \frac{1}{2} \\ S = \frac{1}{2}, \frac{3}{2} \end{array}\right. \Rightarrow S = \frac{1}{2}, \frac{3}{2}$$

WHICH FROM THE FOLLOWING ARE SPECTROSCOPIC TERMS?

$$^2S \quad ^2P \quad ^2D \quad ^2F$$

$$^4S \quad ^4P \quad ^4D \quad ^4F$$

FOR EXAMPLE:

$L = 3$ (MAX): $M_L = -3, -2, -1, 0, 1, 2, 3$

p^3: $\cancel{\underset{p_1}{\underline{\bullet\bullet\bullet}} \quad \underset{p_0}{\underline{\quad\quad}} \quad \underset{p_{-1}}{\underline{\quad\quad}}}$ $\quad M_L = 3$

PHYSICALLY IMPOSSIBLE

CONCLUSION:

THERE IS NO TERM F FOR p^3

EXAMPLE: $1s^2\,2s^2\,2p^3$

$1s^2 \equiv$ ↑↓ $1s$ (PAULI PRINCIPLE)

$l=0 \; (l_1=0,\, l_2=0)$; $s_1=\frac{1}{2}$ $s_2=\frac{1}{2}$

$S=0, 1$ BUT $m_{s_1}=\frac{1}{2}$ $m_{s_2}=-\frac{1}{2}$

$M_S=0$ ONLY

$L=0$ $S=0$

NO CONTRIBUTION TO THE TOTAL L AND S FROM THE CLOSED SHELLS:

$2(2l+1)$ ELECTRONS

FOR $ns: 2$; $np: 6$; $nd: 10$; $nf: 14$ ...

$2p^3$ – OPEN SHELL $\Rightarrow$ 3 EQUIVALENT ELECTRONS IN THE STATE $2p$

$2p$: $2p_{+1}$, $2p_0$, $2p_{-1}$

↑ ↑ ↑ DEGENERATE

$M_L=0$ $M_S=3/2$

$|\overset{+}{p}_1\,\overset{+}{p}_0\,\overset{+}{p}_{-1}|$

↑↓ ↑ —

$M_L=2$ $M_S=\frac{1}{2}$

$|\overset{+}{p}_1\,\bar{p}_1\,\overset{+}{p}_0|$

~~↑↑ ↑ —~~ ! PAULI PRINCIPLE

↑↓ — ↑

$M_L=1$ $M_S=\frac{1}{2}$

$|\overset{+}{p}_1\,\bar{p}_1\,\overset{+}{p}_{-1}|$

POSSIBLE FUNCTIONS (DETERMINANTS)

M_S \ M_L	2	1	0
3/2	–	–	$\vert\overset{+}{p}_1\,\overset{+}{p}_0\,\overset{+}{p}_{-1}\vert$ (1)
1/2	$\vert\overset{+}{p}_1\,\bar{p}_1\,\overset{+}{p}_0\vert$ (1)	$\vert\overset{+}{p}_1\,\bar{p}_1\,\overset{+}{p}_{-1}\vert$ $\vert\overset{+}{p}_1\,\overset{+}{p}_0\,\bar{p}_0\vert$ (2)	$\vert\overset{+}{p}_1\,\overset{+}{p}_{-1}\,\bar{p}_0\vert$ $\vert\overset{+}{p}_1\,\bar{p}_{-1}\,\overset{+}{p}_0\vert$ $\vert\bar{p}_1\,\overset{+}{p}_{-1}\,\overset{+}{p}_0\vert$ (3)

STATISTICS:

M_S \ M_L	2	1	0
3/2	0	0	1
1/2	1	2	3

^2D

M_S \ M_L	2	1	0
3/2	0	0	1
1/2	0	1	2

^2P

M_S \ M_L	2	1	0
3/2	0	0	1
1/2	0	0	1

^4S (GROUND STATE)

$L=2$: $M_L=-2,-1,0,1,2$

THERE ARE NO OTHER TERMS FOR p^3!

9.
l=1

CLOSED SHELL: $\underbrace{2(2l+1)}$ $m_l = -l, \dots l$

$m_s = -\frac{1}{2}\ \frac{1}{2}$

$l=1$	p	: 6
2	d	: 10
3	f	: 14

SYMMETRY

O(3) TRANSFORMATION PROPERTIES UNDER ROTATIONS

p^n	$p^1, p^5 : {}^2P$; $p^2, p^4 : {}^3P, {}^1D, {}^1S$; $p^3 : {}^4S, {}^2D, {}^2P$
d^1, d^9	${}^2D$
d^2, d^8	${}^3F, {}^3P, {}^1G, {}^1D, {}^1S$
d^3, d^7	${}^4F, {}^4P, {}^2H, {}^2G, {}^2F, {}^2D(2), {}^2P$
d^4, d^6	${}^5D, {}^3H, {}^3G, {}^3F(2), {}^3D, {}^3P(2), {}^1I, {}^1G(2), {}^1F, {}^1D(2), {}^1S(2)$
d^5	${}^6S, {}^4G, {}^4F, {}^4D, {}^4P, {}^2I, {}^2H, {}^2G(2), {}^2F(2), {}^2D(3), {}^2P, {}^2S$
f^1, f^{13}	${}^2F$
f^2, f^{12}	${}^3H, {}^3F, {}^3P, {}^1I, {}^1G, {}^1D, {}^1S$
f^3, f^{11}	${}^4I, {}^4G, {}^4F, {}^4D, {}^4S, {}^2L, {}^2K, {}^2I, {}^2H(2), {}^2G(2), {}^2F(2), {}^2D(2), {}^2P$
f^4, f^{10}	${}^5S, {}^5D, {}^5F, {}^5G, {}^5I, {}^3P(3), {}^3D(2), {}^3F(4), {}^3G(3), {}^3H(4), {}^3I(2),$ ${}^3K(2), {}^3L, {}^3M, {}^1S(2), {}^1D(4), {}^1F, {}^1G(4), {}^1H(2), {}^1I(3), {}^1K, {}^1L(2), {}^1N$
f^5, f^9	${}^6P, F, H; {}^4S, P(2), D(3), F(4), G(4), H(3), I(3), K(2), L, M;$ ${}^2P(4), D(5), F(7), G(6), H(7), I(5), K(5), L(3), M(2), N, O;$
f^6, f^8	${}^7F, {}^5S, P, D(3), F(2), G(3), H(2), I(2), K, L,$ ${}^3P(6), D(5), F(9), G(7), H(9), I(6), K(6), L(3), M(3), N, O,$ ${}^1S(4), P, D(6), F(4), G(8), H(4), I(7), K(3), L(4), M(2), N(2), Q;$
f^7	${}^8S, {}^6P, D, F, G, H, I, {}^4S(2), P(2), D(6), F(5), G(7), H(5), I(5),$ $K(3), {}^4L(3), M, N, {}^2S(2), P(5), D(7), F(10), G(10), H(9),$ $I(9), K(7), L(5), M(4)\ {}^2N(2), O, Q.$

Table 1 „NEW QUANTUM NUMBERS?"
(Continued.)

^{2S+1}L	v	Q	W	U	w	^{2S+1}L	v	Q	W	U	w	^{2S+1}L	v	Q	W	U	w
^1G	4	3/2	(220)	(21)	3	^4F	5	1	(211)	(30)	4	^2F	7	0	(222)	(40)	10
^1G	4	3/2	(220)	(22)	4	^4F	7	0	(220)	(21)	5	^2G	3	2	(210)	(20)	1
^1G	6	1/2	(222)	(20)	5	^4G	3	2	(111)	(20)	1	^2G	3	2	(210)	(21)	2
^1G	6	1/2	(222)	(30)	6	^4G	5	1	(211)	(20)	2	^2G	5	1	(221)	(20)	3
f^6 ^1G	6	1/2	(222)	(40)	7	^4G	5	1	(211)	(21)	3	^2G	5	1	(221)	(21)	4
^1G	6	1/2	(222)	(40)	8	^4G	5	1	(211)	(30)	4	^2G	5	1	(221)	(30)	5
^1H	4	3/2	(220)	(21)	1	^4G	7	0	(220)	(20)	5	^2G	5	1	(221)	(31)	6
^1H	4	3/2	(220)	(22)	2	^4G	7	0	(220)	(21)	6	^2G	7	0	(222)	(20)	7
^1H	6	1/2	(222)	(30)	3	^4G	7	0	(220)	(22)	7	^2G	7	0	(222)	(30)	8
^1H	6	1/2	(222)	(40)	4	^4H	5	1	(211)	(11)	1	^2G	7	0	(222)	(40)	9
^1I	2	5/2	(200)	(20)	1	^4H	5	1	(221)	(21)	2	^2G	7	0	(222)	(40)	10
^1I	4	3/2	(220)	(20)	2	^4H	5	1	(221)	(30)	3	^2H	3	2	(210)	(11)	1
7 ^1I	4	3/2	(220)	(22)	3	^4H	7	0	(220)	(21)	4	^2H	3	2	(210)	(21)	2
^1I	6	1/2	(222)	(20)	4	^4H	7	0	(220)	(22)	5	^2H	5	1	(221)	(11)	3
^1I	6	1/2	(222)	(30)	5	^4I	3	2	(111)	(20)	1	^2H	5	1	(221)	(21)	4
^1I	6	1/2	(222)	(40)	6	^4I	5	1	(211)	(20)	2	^2H 9	5	1	(211)	(30)	5
^1I	6	1/2	(222)	(40)	7	^4I	5	1	(211)	(30)	3	^2H	5	1	(221)	(31)	6
^1K	4	3/2	(220)	(21)	1	^4I	7	0	(220)	(20)	4	^2H	5	1	(221)	(31)	7
^1K	6	1/2	(222)	(30)	2	^4I	7	0	(220)	(22)	5	^2H	7	0	(222)	(30)	8
^1K	6	1/2	(222)	(40)	3	^4K	5	1	(211)	(21)	1	^2H	7	0	(222)	(40)	9
^1L	4	3/2	(220)	(21)	1	^4K	5	1	(211)	(30)	2	^2I	3	2	(210)	(20)	1
^1L	4	3/2	(220)	(22)	2	^4K	7	0	(220)	(21)	3	^2I	5	1	(221)	(20)	2
^1L	6	1/2	(222)	(40)	3	^4L	5	1	(211)	(21)	1	^2I	5	1	(221)	(30)	3
^1L	6	1/2	(222)	(40)	4	^4L	7	0	(220)	(21)	2	^2I	5	1	(221)	(31)	4
^1M	6	1/2	(222)	(30)	1	^4L	7	0	(220)	(22)	3	^2I	5	1	(221)	(31)	5
^1M	6	1/2	(222)	(40)	2	^4M	5	1	(211)	(30)	0	^2I	7	0	(222)	(20)	6
^1N	4	3/2	(220)	(22)	1	^4N	7	0	(220)	(22)	0	^2I	7	0	(222)	(30)	7
^1N	6	1/2	(222)	(40)	2	^2S	7	0	(222)	(00)	1	^2I	7	0	(222)	(40)	8
^1Q	6	1/2	(222)	(40)	0	^2S	7	0	(222)	(40)	2	^2I	7	0	(222)	(40)	9
f^7 subshell f^7						^2P	3	2	(210)	(11)	1	^2K	3	2	(210)	(21)	1
^8S	7	0	(000)	(00)	0	^2P	5	1	(221)	(11)	2	^2K	5	1	(221)	(21)	2
^8S ^6P	5	1	(110)	(11)	0	^2P	5	1	(221)	(30)	3	^2K	5	1	(221)	(30)	3
^6D	7	0	(200)	(20)	0	^2P	5	1	(221)	(31)	4	^2K	5	1	(221)	(31)	4
^6F	5	1	(110)	(10)	0	^2P	7	0	(222)	(30)	5	^2K	5	1	(221)	(31)	5
^6G	7	0	(200)	(20)	0	^2D	3	2	(210)	(20)	1	^2K	7	0	(222)	(30)	6
^6H	5	1	(110)	(11)	0	^2D	3	2	(210)	(21)	2	^2K	7	0	(222)	(40)	7
^6I	7	0	(200)	(20)	0	^2D	5	1	(221)	(20)	3	^2L	3	2	(210)	(21)	1
^4S	3	2	(111)	(00)	1	^2D	5	1	(221)	(21)	4	^2L	5	1	(221)	(21)	2
^4S	7	0	(220)	(22)	2	^2D	5	1	(221)	(31)	5	^2L	5	1	(221)	(31)	3
^4P	5	1	(211)	(11)	1	^2D	7	0	(222)	(20)	6	^2L	7	0	(222)	(40)	4
^4P	5	1	(211)	(30)	2	^2D	7	0	(222)	(40)	7	^2L	7	0	(222)	(40)	5
^4D	3	2	(111)	(20)	1	^2F	1	3	(100)	(10)	1	^2M	5	1	(221)	(30)	1
^4D	5	1	(211)	(20)	2	^2F	3	2	(210)	(21)	2	^2M	5	1	(221)	(31)	2
6 ^4D	5	1	(211)	(21)	3	^2F	5	1	(221)	(10)	3	^2M	7	0	(222)	(30)	3
^4D	7	0	(220)	(20)	4	^2F	5	1	(221)	(21)	4	^2M	7	0	(222)	(40)	4
^4D	7	0	(220)	(21)	5	^2F	5	1	(221)	(30)	5	^2N	5	1	(221)	(31)	1
^4D	7	0	(220)	(22)	6	^2F	5	1	(221)	(31)	6	^2N	7	0	(222)	(40)	2
^4F	3	2	(111)	(10)	1	^2F	5	1	(221)	(31)	7	^2O	5	1	(221)	(31)	0
^4F	5	1	(211)	(10)	2	^2F	7	0	(222)	(10)	8	^2Q	7	0	(222)	(40)	0
^4F	5	1	(221)	(21)	3	^2F	7	0	(222)	(30)	9						

f^7: $l=3$ $m_l=-3,-2,\dots 2,3$: $2l+1=7$

↑	↑	↑	↑	↑	↑	↑
−3	−2	−1	0	1	2	3

$$\left.\begin{array}{l} M_S = 7/2 \Rightarrow S = 7/2 \\ M_L = 0 \Rightarrow L = 0 \end{array}\right\} {}^8S$$

j-j COUPLING

EXAMPLE: $npn'p$

$l_1 = 1 \quad s_1 = \frac{1}{2} \qquad j_1 = 1/2,\ 3/2$

$l_2 = 1 \quad s_2 = \frac{1}{2} \qquad j_2 = 1/2,\ 3/2$

$$\left.\begin{matrix} j_1 = 1/2,\ 3/2 \\ j_2 = 1/2,\ 3/2 \end{matrix}\right\} \quad |j_1 - j_2| \le J \le j_1 + j_2$$

$npn'p$		jj': 3/2 3/2	3/2 1/2	1/2 3/2	1/2 1/2
M	3	(3/2 3/2)	—	—	—
	2	(3/2 1/2)(1/2 3/2)	(3/2 1/2)	(1/2 3/2)	—
	1	(3/2 −1/2)(−1/2 3/2)(1/2 1/2)	(1/2 1/2)(3/2 −1/2)	(1/2 1/2)(−1/2 3/2)	(1/2 1/2)
	0	(3/2 −3/2)(−3/2 3/2)(1/2 −1/2)(−1/2 1/2)	(1/2 −1/2)(−1/2 1/2)	(1/2 −1/2)(−1/2 1/2)	(1/2 −1/2)(−1/2 1/2)
	−1	(1/2 −3/2)(−3/2 1/2)(−1/2 −1/2)	(−1/2 −1/2)(−3/2 1/2)	(−1/2 −1/2)(1/2 −3/2)	(−1/2 −1/2)
	−2	(−3/2 −1/2)(−1/2 −3/2)	(−3/2 −1/2)	(−1/2 −3/2)	—
	−3	(−3/2 −3/2)	—	—	—
J:		3, 2, 1, 0	2, 1	2, 1	1, 0

$m_{j_1} = 3/2$

$np_1 \quad np_0 \quad np_{-1}$

$n'p_1 \quad n'p_0 \quad n'p_{-1}$

$m_{j_2} = 3/2$

$J_{MAX} = 3$, $M = -3, -2, -1, 0, 1, 2, 3$; $M = m_{j_1} + m_{j_2}$

$j = 3/2$, $m_j = -3/2, -1/2, 1/2, 3/2$

EXAMPLE: np^2 (EQUIVALENT ELECTRONS)

$\cancel{np_1 \quad np_0}$ $\quad np_{-1}$ $\quad (3/2\ 3/2): M = 3$

PAULI PRINCIPLE!

$\Rightarrow$ $\cancel{J = 3}$!

np^2		jj': 3/2 3/2	3/2 1/2	1/2 1/2
M	2	(3/2 1/2)	(3/2 1/2)	
	1	(3/2 −1/2)	(3/2 −1/2)(1/2 1/2)	
	0	(3/2 −3/2)(1/2 −1/2)	(1/2 −1/2)(−1/2 1/2)	(1/2 −1/2)
	−1	(−3/2 1/2)	(−3/2 1/2)(−1/2 −1/2)	
	−2	(−3/2 −1/2)	(−3/2 −1/2)	
J:		2, 0	2, 1	0

$|j_1 m_1 j_2 m_2; j m\rangle$

$(3/2\ 1/2) \equiv |\underset{1.}{3/2\ 3/2}\ \underset{2.}{3/2\ 1/2}; 2\ 2\rangle$

$(1/2\ 1/2) \equiv |\underset{1.}{3/2\ 1/2}\ \underset{2.}{1/2\ 1/2}; 2\ 2\rangle$

$(1/2\ -1/2) \equiv |3/2\ 1/2\ 3/2\ -1/2; 0\ 0\rangle$

$(1/2\ -1/2) \equiv |\underset{1.}{1/2\ 1/2}\ \underset{2.}{1/2\ -1/2}; 0\ 0\rangle$

$(j, j') = (3/2\ 3/2)$

$$\left.\begin{matrix} m_{j_1} = -3/2 & -1/2 & 1/2 & 3/2 \\ m_{j_2} = -3/2 & -1/2 & 1/2 & 3/2 \end{matrix}\right\} \text{DIFFERENT VALUES OF } m_{j_1} \text{ e } m_{j_2}$$