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4.09.18 class 22: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Atomic shell models using intertwining $(S_n)^*(U(m))$ matrix operators

Single particle p^1-orbitals: U(3) triplet
- Elementary U(N) commutation
- Elementary state definitions by Boson operators
  - Summary of multi particle commutation relations

Symmetric p^2-orbitals: U(3) sextet
- Sample matrix elements
  - Combining elementary "1-jump" E_{12}, E_{23}, to get "2-jump" operator E_{13}
    - Review:Representation of *Diagonalizing Transform* (DTran T)

Relating elementary $\mathbf{E}_{jk}$ matrices to Tensor operator $\mathbf{V}^k{}_q$ *(ℓ=1 atomic p-shell)*
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Tableau calculation of 3-electron ℓ=1 orbital p^3-states and $\mathbf{V}^k{}_q$ matrices
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Level diagrams for pure atomic shells $p^{n=1-6}$, $d^{n=1-5}$, $f^{n=1-7}$
- Classical Lie Groups used to label f-shell structure (a rough sketch)

AMOP reference links (Updated list given on 2nd page of each class presentation)

Web Resources - front page
UAF Physics UTube channel

Quantum Theory for the Computer Age
Principles of Symmetry, Dynamics, and Spectroscopy
Classical Mechanics with a Bang!
Modern Physics and its Classical Foundations

2014 AMOP
2017 Group Theory for QM
2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - ajp-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.
- I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
- II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Rotation–vibration spectra of icosahedral molecules.
- I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989
- II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989
- III) Half-integral angular momentum - harter-reimer-jcp-1991

QTCA Unit 10 Ch 30 - 2013
Molecular Symmetry and Dynamics - Ch32-Springer Handbooks of Atomic, Molecular, and Optical Physics - Harter-2006
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS
- I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) OSU knowledge Bank
- II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
- III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)
Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996
Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013
Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001
Representaions Of Multidimensional Symmetries In Networks - harter-jmp-1973

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on* Apache-SOLR *Index and search for* nuanced, whole-site content/metadata level *searching. This bad boy will be a sure force multiplier.*

Intro spin ½ coupling
Unit 8 Ch. 24 p3.

H atom hyperfine-B-level crossing
Unit 8 Ch. 24 p15.

Hyperf. theory Ch. 24 p48.

Hyperf. theory Ch. 24 p48.
Deeper theory ends p53

Intro 2p3p coupling
Unit 8 Ch. 24 p17.

Intro LS-jj coupling
Unit 8 Ch. 24 p22.

CG coupling derived (start)
Unit 8 Ch. 24 p39.
CG coupling derived (formula)
Unit 8 Ch. 24 p44.

Lande' g-factor
Unit 8 Ch. 24 p26.

Irrep Tensor building
Unit 8 Ch. 25 p5.

Irrep Tensor Tables
Unit 8 Ch. 25 p12.

Wigner-Eckart tensor Theorem.
Unit 8 Ch. 25 p17.

Tensors Applied to d,f-levels.
Unit 8 Ch. 25 p21.

Tensors Applied to high J levels.
Unit 8 Ch. 25 p63.

Intro 3-particle coupling.
Unit 8 Ch. 25 p28.

Intro 3,4-particle Young Tableaus
GrpThLect29 p42.

Young Tableau Magic Formulae
GrpThLect29 p46-48.

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 7 Ch. 23-26)
(PSDS - Ch. 5, 7)

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$$e_{11}=\begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{12}=\begin{pmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{13}=\begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, e_{21}=\begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, \ldots e_{33}=\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix}.$$

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$$\left[\mathbf{a}_j,\mathbf{a}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \left[\mathbf{a}_j,\mathbf{a}_k\right]=0,\ \left[\mathbf{a}_j,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j^\dagger,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j,\mathbf{b}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \ldots$$ (Standard notation)

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Elementary state definitions by Boson operators:

$|1\rangle=\mathbf{a}_1^\dagger|0\rangle,\ |2\rangle=\mathbf{a}_2^\dagger|0\rangle,\ |3\rangle=\mathbf{a}_3^\dagger|0\rangle,$ implies conjugate bras: $\langle 1|=\langle 0|\mathbf{a}_1,\ \langle 2|=\langle 0|\mathbf{a}_2,\ \langle 3|=\langle 0|\mathbf{a}_3,$

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that form a unit matrix with kets

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Single particle p^1-orbitals: U(3) triplet $\left|p^1 \square\right\rangle$

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Following commutation relation $[\mathbf{a}_j,\mathbf{a}_k^\dagger]=\mathbf{1}\cdot\delta_{jk}=[a_j,\bar{a}_k]$:

$$\langle j|k\rangle=\langle 0|\mathbf{a}_j\mathbf{a}_k^\dagger|0\rangle=\langle 0|\left[\mathbf{a}_j,\mathbf{a}_k^\dagger\right]|0\rangle+\langle 0|\mathbf{a}_k^\dagger\mathbf{a}_j|0\rangle$$

$$= \langle 0|\mathbf{1}\delta_{jk}|0\rangle \quad + \quad 0 \ \text{ (since: } \mathbf{a}_j|0\rangle=0)$$

$$= \delta_{jk} \qquad \text{(assuming: } \langle 0|0\rangle=1)$$

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proof: $[e_{jk}, e_{pq}]= e_{jk}\, e_{pq}-e_{pq}\, e_{jk} = \delta_{kp}e_{jq} - \delta_{qj}e_{pk}$

Relating elementary $e_{jk}=|j\rangle\langle k|$ operators to Boson creation-destruction $\mathbf{a}^\dagger_j\mathbf{a}_k$ operators

$$\left[\mathbf{a}_j,\mathbf{a}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \left[\mathbf{a}_j,\mathbf{a}_k\right]=0,\ \left[\mathbf{a}_j,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j^\dagger,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j,\mathbf{b}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \ldots \text{ (Standard notation)}$$

$$\left[\bar{a}_j,a_k\right]=\delta_{jk}\mathbf{1},\ \left[\bar{a}_j,\bar{a}_k\right]=0,\ \left[\bar{a}_j,b_k\right]=0,\ \left[b_j,b_k\right]=0,\ \left[\bar{b}_j,b_k\right]=\delta_{jk}\mathbf{1},\ \ldots \text{ (Shorthand notation)}$$

Elementary state definitions by Boson operators:

$\left|1\right\rangle=\mathbf{a}_1^\dagger\left|0\right\rangle,\ \left|2\right\rangle=\mathbf{a}_2^\dagger\left|0\right\rangle,\ \left|3\right\rangle=\mathbf{a}_3^\dagger\left|0\right\rangle,$ implies conjugate bras: $\left\langle 1\right|=\left\langle 0\right|\mathbf{a}_1,\ \left\langle 2\right|=\left\langle 0\right|\mathbf{a}_2,\ \left\langle 3\right|=\left\langle 0\right|\mathbf{a}_3,$

that form a unit matrix with kets

Following commutation relation $[\mathbf{a}_j,\mathbf{a}_k^\dagger]=\mathbf{1}\cdot\delta_{jk}=[\mathrm{a}_j,\bar{\mathrm{a}}_k]$:

$$\begin{pmatrix}\langle 1|1\rangle&\langle 1|2\rangle&\langle 1|3\rangle\\ \langle 2|1\rangle&\langle 2|2\rangle&\langle 2|3\rangle\\ \langle 3|1\rangle&\langle 3|2\rangle&\langle 3|1\rangle\end{pmatrix}=\begin{pmatrix}1&\cdot&\cdot\\ \cdot&1&\cdot\\ \cdot&\cdot&1\end{pmatrix}$$

$$\begin{aligned}\left\langle j\middle|k\right\rangle=\left\langle 0\right|\mathbf{a}_j\mathbf{a}_k^\dagger\left|0\right\rangle&=\left\langle 0\right|\left[\mathbf{a}_j,\mathbf{a}_k^\dagger\right]\left|0\right\rangle+\left\langle 0\right|\mathbf{a}_k^\dagger\mathbf{a}_j\left|0\right\rangle\\ &=\left\langle 0\right|\mathbf{1}\delta_{jk}\left|0\right\rangle\quad+\quad 0\ \ (\text{since: } \mathbf{a}_j\left|0\right\rangle=0)\\ &=\delta_{jk}\qquad(\text{assuming: } \left\langle 0\middle|0\right\rangle=1)\end{aligned}$$

Relating n-particle $E_{jk}=e_{jk}(a)+e_{jk}(b)+\ldots$ operators to n-particle Boson $\mathbf{a}^\dagger_j\mathbf{a}_k$, $\mathbf{b}^\dagger_j\mathbf{b}_k$,… operator sets

n-particle operator commutation $[E_{jk}, E_{pq}]= \delta_{kp}E_{jq} - \delta_{qj}E_{pk}$ is just like $[e_{jk}, e_{pq}]= \delta_{kp}e_{jq} - \delta_{qj}e_{pk}$
as long as different types always commute.

$$0=\left[\mathbf{a}_j,\mathbf{b}_k^\dagger\right]=\left[\mathbf{a}_j,\mathbf{c}_k^\dagger\right]=\left[\mathbf{b}_j,\mathbf{c}_k^\dagger\right]\ldots,$$

$$0=\left[\bar{a}_j,b_k\right]=\left[\bar{a}_j,c_k\right]=\left[\bar{b}_j,c_k\right]\ldots,$$

AMOP reference links on page 2

4.09.18 class 22: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Atomic shell models using intertwining $(S_n)^*(U(m))$ matrix operators

Single particle p^1-orbitals: U(3) triplet
- Elementary U(N) commutation
- Elementary state definitions by Boson operators
  - Summary of multi particle commutation relations

Symmetric p^2-orbitals: U(3) sextet
- Sample matrix elements
  - Combining elementary "1-jump" E_{12}, E_{23}, to get "2-jump" operator E_{13}
    - Review:Representation of *Diagonalizing Transform* (DTran T)

Relating elementary $\mathbf{E}_{jk}$ matrices to Tensor operator $\mathbf{V}^k_q$ *(ℓ=1 atomic p-shell)*
- Condensed form tensor tables for orbital shells *p: ℓ=1, d: ℓ=2, f: ℓ=3, g: ℓ=4.*

Tableau calculation of 3-electron ℓ=1 orbital p^3-states and $\mathbf{V}^k_q$ matrices
- Tableau "Jawbone" formula
  - Calculate 2^n-pole moments
- Comparison calculation of p^3-$\mathbf{V}^k_q$ vs. calculation by cfp (fractional parentage)
  - Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

Level diagrams for pure atomic shells $p^{n=1-6}$, $d^{n=1-5}$, $f^{n=1-7}$
- Classical Lie Groups used to label f-shell structure (a rough sketch)

Summary of multi particle commutation relations

Boson ($\mathbf{a}^\dagger$,$\mathbf{a}$) operators and Elementary E_{jk} operators for multiple particles a, b, c,…:

1-particle e_{jk} — N-particle sums that make $E_{jk}= e_{jk}(a)+ e_{jk}(b)+ e_{jk}(c)+\ldots$

$$\mathbf{a}_j^\dagger \mathbf{a}_k = e_{jk} = a_j \bar{a}_k \qquad \mathbf{a}_j^\dagger \mathbf{a}_k + \mathbf{b}_j^\dagger \mathbf{b}_k + \ldots = E_{jk} = a_j \bar{a}_k + b_j \bar{b}_k + \ldots$$

Each creation ($\mathbf{a}^\dagger_j=a_j$) or destruction ($\mathbf{a}_j=\bar{a}_j$) operator has a 1-term commutation relation

$$\left[\mathbf{a}_j,\mathbf{a}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \left[\mathbf{a}_j,\mathbf{a}_k\right]=0,\ \left[\mathbf{a}_j,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j^\dagger,\mathbf{b}_k^\dagger\right]=0,\ \left[\mathbf{b}_j,\mathbf{b}_k^\dagger\right]=\delta_{jk}\mathbf{1},\ \ldots \quad \textit{(Standard notation)}$$

$$\left[\bar{a}_j,a_k\right]=\delta_{jk}\mathbf{1},\ \left[\bar{a}_j,\bar{a}_k\right]=0,\ \left[\bar{a}_j,b_k\right]=0,\ \left[b_j,b_k\right]=0,\ \left[\bar{b}_j,b_k\right]=\delta_{jk}\mathbf{1},\ \ldots \quad \textit{(Shorthand notation)}$$

Each elementary operator has a 2-term commutation relation

$$\left[e_{jk},e_{pq}\right]=e_{jk}e_{pq}-e_{pq}e_{jk} = \delta_{pk}e_{jq}-\delta_{qj}e_{pk} \qquad \left[E_{jk},E_{pq}\right]=\delta_{pk}E_{jq}-\delta_{qj}E_{pk}$$

1-particle e_{jk} relations apply to N-particle E_{jk} since all a's commute with all *other* b's, c's,….etc.

$$\begin{aligned}\left[e_{jk},e_{pq}\right] &= a_j\bar{a}_k a_p\bar{a}_q - a_p\bar{a}_q a_j\bar{a}_k \\ &= a_j\left(\delta_{pk}+a_p\bar{a}_k\right)\bar{a}_q - a_p\left(\delta_{qj}+a_j\bar{a}_q\right)\bar{a}_k \\ &= \delta_{pk}a_j\bar{a}_q + a_j a_p\bar{a}_k\bar{a}_q - \delta_{qj}a_p\bar{a}_k - a_p a_j\bar{a}_q\bar{a}_k = \delta_{kp}e_{jq}-\delta_{jq}e_{pk}\end{aligned}$$

AMOP reference links on page 2

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Atomic shell models using intertwining (S_n)*(U(m)) matrix operators

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Classical Lie Groups used to label f-shell structure (a rough sketch)

Symmetric p^2-orbitals: U(3) sextet $\left| p^2 \square\square \right\rangle$

Sample matrix elements for the [2,0]=$|\square\square\rangle$ sextet states:

$$E_{11}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{11}(a)+e_{11}(b)\right)\left|1_a,1_b\right\rangle = \left(a_1\bar{a}_1 + b_1\bar{b}_1\right)\left|1_a,1_b\right\rangle = 2\left|\boxed{1}\boxed{1}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$E_{21} = E_{12}^{\dagger}$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^{\dagger}$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

Symmetric p²-orbitals: U(3) sextet $\left|p^2 \;\square\square\right\rangle$

Sample matrix elements for the [2,0]=$|\square\square\rangle$ sextet states:

$$E_{11}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{11}(a)+e_{11}(b)\right)\left|1_a,1_b\right\rangle = \left(a_1\bar{a}_1 + b_1\bar{b}_1\right)\left|1_a,1_b\right\rangle = 2\left|\boxed{1}\boxed{1}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$E_{21} = E_{12}^{\dagger}$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^{\dagger}$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

Symmetric p²-orbitals: U(3) sextet $\left|p^2\ \square\square\right\rangle$

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$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{2}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} = \frac{2}{\sqrt{2}}\left|2_a,2_b\right\rangle = \sqrt{2}\left|\boxed{2}\boxed{2}\right\rangle$$

$E_{21} = E_{12}^{\dagger}$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^{\dagger}$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

Symmetric p²-orbitals: U(3) sextet $\left|p^2\ \square\square\right\rangle$

Sample matrix elements for the [2,0]=$|\square\square\rangle$ sextet states:

$$E_{11}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{11}(a)+e_{11}(b)\right)\left|1_a,1_b\right\rangle = \left(a_1\bar{a}_1 + b_1\bar{b}_1\right)\left|1_a,1_b\right\rangle = 2\left|\boxed{1}\boxed{1}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{2}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} = \frac{2}{\sqrt{2}}\left|2_a,2_b\right\rangle = \sqrt{2}\left|\boxed{2}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{3}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}} = \frac{\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle}{\sqrt{2}} = \left|\boxed{2}\boxed{3}\right\rangle$$

$E_{21} = E_{12}^\dagger$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^\dagger$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

Symmetric p^2-orbitals: U(3) sextet $\left|p^2 \;\square\square\right\rangle$

Sample matrix elements for the [2,0]=$|\square\square\rangle$ sextet states:

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$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{2}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} = \frac{2}{\sqrt{2}}\left|2_a,2_b\right\rangle = \sqrt{2}\left|\boxed{2}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{3}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}} = \frac{\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle}{\sqrt{2}} = \left|\boxed{2}\boxed{3}\right\rangle$$

$$E_{21}\left|\boxed{2}\boxed{3}\right\rangle = 0$$

$E_{21} = E_{12}^{\dagger}$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^{\dagger}$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

Symmetric p^2-orbitals: U(3) sextet $\left| p^2 \; \square\square \right\rangle$

Sample matrix elements for the [2,0]=$|\square\square\rangle$ sextet states:

$$E_{11}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{11}(a)+e_{11}(b)\right)\left|1_a,1_b\right\rangle = \left(a_1\bar{a}_1 + b_1\bar{b}_1\right)\left|1_a,1_b\right\rangle = 2\left|\boxed{1}\boxed{1}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{1}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\left|1_a,1_b\right\rangle = \left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle = \sqrt{2}\,\frac{\left|2_a,1_b\right\rangle + \left|1_a,2_b\right\rangle}{\sqrt{2}} = \sqrt{2}\left|\boxed{1}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{2}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} = \frac{2}{\sqrt{2}}\left|2_a,2_b\right\rangle = \sqrt{2}\left|\boxed{2}\boxed{2}\right\rangle$$

$$E_{21}\left|\boxed{1}\boxed{3}\right\rangle = \left(e_{21}(a)+e_{21}(b)\right)\frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}} = \frac{\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle}{\sqrt{2}} = \left|\boxed{2}\boxed{3}\right\rangle$$

$$E_{21}\left|\boxed{2}\boxed{3}\right\rangle = 0$$

$E_{21} = E_{12}^{\dagger}$

E_{21}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	$\sqrt{2}$	.	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	.	.	1	.

$E_{12} = E_{21}^{\dagger}$

E_{12}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	$\sqrt{2}$	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	.
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	$\sqrt{2}$	.	.	.	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	1
$\boxed{2}\boxed{3}$	.	.	.	.	.	.

$E_{23} = E_{32}^{\dagger}$

E_{23}	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	.	.	.	.	.	.
$\boxed{2}\boxed{2}$	.	.	.	.	.	$\sqrt{2}$
$\boxed{3}\boxed{3}$	.	.	.	.	.	.
$\boxed{1}\boxed{2}$	.	.	.	.	1	.
$\boxed{1}\boxed{3}$	.	.	.	.	.	.
$\boxed{2}\boxed{3}$	.	.	$\sqrt{2}$	.	.	.

AMOP reference links on page 2

4.09.18 class 22: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Atomic shell models using intertwining $(S_n)^*(U(m))$ matrix operators

Single particle p^1-orbitals: U(3) triplet
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- Elementary state definitions by Boson operators
  - Summary of multi particle commutation relations

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- Sample matrix elements
  - ➡ Combining elementary "1-jump" E_{12}, E_{23}, to get "2-jump" operator E_{13}
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Relating elementary $\mathbf{E}_{jk}$ matrices to Tensor operator $\mathbf{V}^k{}_q$ *(ℓ=1 atomic p-shell)*
- Condensed form tensor tables for orbital shells *p: ℓ=1, d: ℓ=2, f: ℓ=3, g: ℓ=4.*

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Level diagrams for pure atomic shells $p^{n=1\text{-}6}$, $d^{n=1\text{-}5}$, $f^{n=1\text{-}7}$
- Classical Lie Groups used to label f-shell structure (a rough sketch)

Combining elementary "1-jump" E_{12}, and E_{23}, … operators gives "2-jump" operator E_{13}.
$U(n)$ operators E_{24}, E_{35} …,E_{14}, E_{25}, E_{36} … include $n(n-1)/2$ operators connecting n states.

$$E_{13} = [E_{12}, E_{23}] = E_{12} \cdot E_{23} - E_{23} \cdot E_{12}$$

$$E_{13}\left|\boxed{1}\boxed{3}\right\rangle = E_{12}E_{23}\frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}} - E_{23}E_{12}\frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}}$$

$$= E_{12}\frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} \qquad - E_{23} \cdot 0$$

$$= \frac{\left|1_a,1_b\right\rangle + \left|1_a,1_b\right\rangle}{\sqrt{2}} = \frac{2}{\sqrt{2}}\left|1_a,1_b\right\rangle \qquad = \sqrt{2}\left|\boxed{1}\boxed{1}\right\rangle$$

$$E_{13}\left|\boxed{2}\boxed{3}\right\rangle = E_{12}E_{23}\frac{\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle}{\sqrt{2}} - E_{23}E_{12}\frac{\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle}{\sqrt{2}}$$

$$= E_{12}\frac{\left|2_a,2_b\right\rangle + \left|2_a,2_b\right\rangle}{\sqrt{2}} \qquad - E_{23} \cdot \frac{\left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle}{\sqrt{2}}$$

$$= \frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} - \frac{\left|1_a,2_b\right\rangle + \left|2_a,1_b\right\rangle}{\sqrt{2}} \quad = 0$$

$$E_{13}\left|\boxed{3}\boxed{3}\right\rangle = E_{12}E_{23}\left|3_a,3_b\right\rangle - E_{23}E_{12}\left|3_a,3_b\right\rangle$$

$$= E_{12}(\left|2_a,3_b\right\rangle + \left|3_a,2_b\right\rangle) \qquad - 0$$

$$= \left|1_a,3_b\right\rangle + \left|3_a,1_b\right\rangle = \sqrt{2}\left|\boxed{1}\boxed{3}\right\rangle$$

$$E_{13} = E_{31}^{\dagger} =$$

	$\boxed{1}\boxed{1}$	$\boxed{2}\boxed{2}$	$\boxed{3}\boxed{3}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{3}$	$\boxed{2}\boxed{3}$
$\boxed{1}\boxed{1}$	·	·	·	·	$\sqrt{2}$	·
$\boxed{2}\boxed{2}$	·	·	·	·	·	·
$\boxed{3}\boxed{3}$	·	·	·	·	·	·
$\boxed{1}\boxed{2}$	·	·	·	·	·	0
$\boxed{1}\boxed{3}$	·	·	$\sqrt{2}$	·	·	·
$\boxed{2}\boxed{3}$	·	·	·	·	·	·

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Review:Representation of *Diagonalizing Transform* (DTran T) made by excerpting **P**-columns

$\mathbf{P}^{□□} =$

	11	12	13	21	22	23	31	32	33
11	1	·	·	·	·	·	·	·	·
12	·	$\frac{1}{2}$	·	$\frac{1}{2}$	·	·	·	·	·
13	·	·	$\frac{1}{2}$	·	·	·	$\frac{1}{2}$	·	·
21	·	$\frac{1}{2}$	·	$\frac{1}{2}$	·	·	·	·	·
22	·	·	·	·	1	·	·	·	·
23	·	·	·	·	·	$\frac{1}{2}$	·	$\frac{1}{2}$	·
31	·	·	$\frac{1}{2}$	·	·	·	$\frac{1}{2}$	·	·
32	·	·	·	·	·	$\frac{1}{2}$	·	$\frac{1}{2}$	·
33	·	·	·	·	·	·	·	·	1

$\mathbf{P}^{□□} =$ (vertical tableau)

	11	12	13	21	22	23	31	32	33
11	0	·	·	·	·	·	·	·	·
12	·	$\frac{1}{2}$	·	$\frac{-1}{2}$	·	·	·	·	·
13	·	·	$\frac{1}{2}$	·	·	·	$\frac{-1}{2}$	·	·
21	·	$\frac{-1}{2}$	·	$\frac{1}{2}$	·	·	·	·	·
22	·	·	·	·	0	·	·	·	·
23	·	·	·	·	·	$\frac{1}{2}$	·	$\frac{-1}{2}$	·
31	·	·	$\frac{-1}{2}$	·	·	·	$\frac{1}{2}$	·	·
32	·	·	·	·	·	$\frac{-1}{2}$	·	$\frac{1}{2}$	·
33	·	·	·	·	·	·	·	·	0

$T =$

	□□ x^2	□□ y^2	□□ z^2	□□ xy	□□ xz	□□ yz	□ xp_y	□ xp_z	□ yp_z
11	1	·	·	·	·	·	·	·	·
12	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
13	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
21	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
22	·	1	·	·	·	·	·	·	·
23	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
31	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
32	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
33	·	·	1	·	·	·	·	·	·

S_2 *symmetry* of U(3):
Applying S_2 projection

DTran T Lect.21 p.13.

	11	12	13	21	22	23	31	32	33
x^2	1	·	·	·	·	·	·	·	·
y^2	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
z^2	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
xy	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
xz	·	1	·	·	·	·	·	·	·
yz	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
xp_y	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
xp_z	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
yp_z	·	·	1	·	·	·	·	·	·

E_{12}	11	12	13	21	22	23	31	32	33
11	·	1	·	1	·	·	·	·	·
12	·	·	·	·	1	·	·	·	·
13	·	·	·	·	·	1	·	·	·
21	·	·	·	·	1	·	·	·	·
22	·	·	·	·	·	·	·	·	·
23	·	·	·	·	·	·	·	·	·
31	·	·	·	·	·	·	·	1	·
32	·	·	·	·	·	·	·	·	·
33	·	·	·	·	·	·	·	·	·

$D \otimes D$

	x^2	y^2	z^2	xy	xz	yz	xp_y	xp_z	yp_z
11	1	·	·	·	·	·	·	·	·
12	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
13	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
21	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
22	·	1	·	·	·	·	·	·	·
23	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
31	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
32	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
33	·	·	1	·	·	·	·	·	·

T

D-Tran T

	11	12	13	21	22	23	31	32	33
11	·	·	·	$\sqrt{2}$	·	·	·	·	·
12	·	1	·	·	·	·	·	·	·
13	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
21	·	1	·	·	·	·	·	·	·
22	·	·	·	·	·	·	·	·	·
23	·	·	·	·	·	·	·	·	·
31	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
32	·	·	·	·	·	·	·	·	·
33	·	·	·	·	·	·	·	·	·

$D \otimes D \cdot T$
product

DTran T Lect.21 p.13.

Using *Diagonalizing Transform* (DTran T)
to derive ireps $D^{[20]}(E_{12})$ and $D^{[11]}(E_{12})$

Using *Diagonalizing Transform* (DTran T) to derive ireps $D^{[20]}(E_{12})$ and $D^{[11]}(E_{12})$

$T^{\dagger}$

	11	12	13	21	22	23	31	32	33
1 1 (x^2)	1	·	·	·	·	·	·	·	·
2 2 (y^2)	·	·	·	·	1	·	·	·	·
3 3 (z^2)	·	·	·	·	·	·	·	·	1
1 2 (xy)	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·	·	·	·	·
1 3 (xz)	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·
2 3 (yz)	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{2}}$	·
1/2	·	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$	·	·	·	·	·
1/3	·	·	$\frac{-1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·
2/3	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{-1}{\sqrt{2}}$	·

$D\otimes D$

E_{12}	11	12	13	21	22	23	31	32	33
11	·	1	·	1	·	·	·	·	·
12	·	·	·	·	1	·	·	·	·
13	·	·	·	·	·	1	·	·	·
21	·	·	·	·	1	·	·	·	·
22	·	·	·	·	·	·	·	·	·
23	·	·	·	·	·	·	·	·	·
31	·	·	·	·	·	·	·	1	·
32	·	·	·	·	·	·	·	·	·
33	·	·	·	·	·	·	·	·	·

T

	x^2	y^2	z^2	xy	xz	yz	xp_y	xp_z	yp_z
11	1	·	·	·	·	·	·	·	·
12	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
13	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
21	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
22	·	1	·	·	·	·	·	·	·
23	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
31	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
32	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
33	·	·	1	·	·	·	·	·	·

	11	12	13	21	22	23	31	32	33
x^2	1	·	·	·	·	·	·	·	·
y^2	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·	·
z^2	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·
xy	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$	·	·
xz	·	1	·	·	·	·	·	·	·
yz	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
xp_y	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$	·
xp_z	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
yp_z	·	·	1	·	·	·	·	·	·

$D\otimes D\cdot T$ product

	11	12	13	21	22	23	31	32	33
11	·	·	·	$\sqrt{2}$	·	·	·	·	·
12	·	1	·	·	·	·	·	·	·
13	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{1}{\sqrt{2}}$
21	·	1	·	·	·	·	·	·	·
22	·	·	·	·	·	·	·	·	·
23	·	·	·	·	·	·	·	·	·
31	·	·	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	$\frac{-1}{\sqrt{2}}$
32	·	·	·	·	·	·	·	·	·
33	·	·	·	·	·	·	·	·	·

$T^{\dagger}\cdot D\otimes D\cdot T$ product

E_{12}	1 1	2 2	3 3	1 2	1 3	2 3	1/2	1/3	2/3
1 1	·	·	·	$\sqrt{2}$	·	·	·	·	·
2 2	·	·	·	·	·	·	·	·	·
3 3	·	·	·	·	·	·	·	·	·
1 2	·	$\sqrt{2}$	·	·	·	·	·	·	·
1 3	·	·	·	·	·	1	·	·	·
2 3	·	·	·	·	·	·	·	·	·
1/2	·	·	·	·	·	·	·	·	·
1/3	·	·	·	·	·	·	·	·	-1
2/3	·	·	·	·	·	·	·	·	·

$D^{[20]}(E_{12})$ $D^{[11]}(E_{12})$

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Relating elementary $\mathbf{E}_{jk}$ matrices to Tensor operator $\mathbf{T}^k{}_q$ or $\mathbf{v}^k{}_q$ matrices:
ℓ=1 (atomic p-shell)

2-by-2 case: $\mathbf{H}=\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} = \frac{A+D}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + B\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + C\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{A-D}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$= \frac{A+D}{2}\,\mathbf{1} + B\,\boldsymbol{\sigma}_x + C\,\boldsymbol{\sigma}_y + \frac{A-D}{2}\,\boldsymbol{\sigma}_z$$

$$= \frac{A+D}{2}\,\mathbf{T}^0_0 + (B-iC)\,\mathbf{T}^1_1 + (B+iC)\,\mathbf{T}^1_{-1} + \frac{A-D}{2}\,\mathbf{T}^1_0$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

U(2) generators *(spin J=1/2)*

$\mathbf{u}^1_{+1}=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\mathbf{u}^1_0=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^1_{-1}=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ rank-1 (vector)

$\mathbf{u}^0_0=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{\sqrt{2}}$ rank-0 (scalar)

Relating elementary $\mathbf{E}_{jk}$ *matrices to Tensor operator* $\mathbf{T}^k_q$ *or* $\mathbf{v}^k_q$ *matrices:*
ℓ=1 (atomic p-shell)

2-by-2 case: $\mathbf{H}=\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} = \frac{A+D}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + B\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + C\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{A-D}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$= \frac{A+D}{2}\mathbf{1} + B\,\boldsymbol{\sigma}_x + C\,\boldsymbol{\sigma}_y + \frac{A-D}{2}\boldsymbol{\sigma}_z$$

$$= \frac{A+D}{2}\mathbf{T}^0_0 + (B-iC)\mathbf{T}^1_1 + (B+iC)\mathbf{T}^1_{-1} + \frac{A-D}{2}\mathbf{T}^1_0$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

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$\mathbf{u}^1_{+1}=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\mathbf{u}^1_0=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^1_{-1}=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ rank-1 (vector)

$\mathbf{u}^0_0=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{\sqrt{2}}$ rank-0 (scalar)

Generalization of U(2) spinor analysis to U(3)⊂U(4)⊂U(5)...

3-by-3 case: $\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix} = B\,\mathbf{T}^0_0 + \ldots + t_2\mathbf{T}^2_2 + \ldots$

(AMOP Lect. 11p.5)

U(3) generators *(spin J=1)*

$\mathbf{u}^2_{+2}=\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ $\mathbf{u}^2_{+1}=\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^2_0=\begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{1}{\sqrt{6}}$ $\mathbf{u}^2_{-1}=\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^2_{-2}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ rank-2 (tensor)

$\mathbf{u}^1_{+1}=\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^1_0=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}$ $\mathbf{u}^1_{-1}=\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}$ rank-1 (vector)

$\mathbf{u}^0_0=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{1}{\sqrt{3}}$ rank-0 (scalar)

Mutually commuting diagonal operators

Tensor matrices in IJMS-2013 (p9) Ch.7 p592 Tensor matrices in PSDS Ch.7 p589

Relating elementary $\mathbf{E}_{jk}$ *matrices to Tensor operator* $\mathbf{T}^k{}_q$ *or* $\mathbf{v}^k{}_q$ *matrices:*

ℓ=1 (atomic p-shell) Recall $\mathbf{v}^k{}_q$ triangular arrays:

(AMOP Lect. 11p.5)

$$\left\langle \mathbf{v}^k_q \right\rangle = \sum_{m,m'=-\ell}^{\ell} \left| \begin{smallmatrix}\ell\\ m\end{smallmatrix} \right\rangle \left\langle \begin{smallmatrix}\ell\\ m\end{smallmatrix} \right| \mathbf{v}^k_q \left| \begin{smallmatrix}\ell\\ m'\end{smallmatrix} \right\rangle \left\langle \begin{smallmatrix}\ell\\ m'\end{smallmatrix} \right|$$

$$= \sum_{m,m'=-\ell}^{\ell} \left\langle \begin{smallmatrix}\ell\\ m\end{smallmatrix} \right| \mathbf{v}^k_q \left| \begin{smallmatrix}\ell\\ m'\end{smallmatrix} \right\rangle e_{m,m'} = \sum_{m,m'=-\ell}^{\ell} \begin{pmatrix} & k & \\ m & & m' \end{pmatrix} e_{m,m'}$$

ℓ=1
tensor array
1-particle notation

$$\left\langle \mathbf{v}^2_{-2} \right\rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \end{pmatrix} \quad \left\langle \mathbf{v}^2_{-1} \right\rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{pmatrix}\tfrac{1}{\sqrt{2}} \quad \left\langle \mathbf{v}^2_{0} \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & -2 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}\tfrac{1}{\sqrt{6}} \quad \left\langle \mathbf{v}^2_{+1} \right\rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \end{pmatrix}\tfrac{1}{\sqrt{2}} \quad \left\langle \mathbf{v}^2_{+2} \right\rangle = \begin{pmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$$

$$\left\langle \mathbf{v}^1_{-1} \right\rangle = \begin{pmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{pmatrix}\tfrac{1}{\sqrt{2}} \quad \left\langle \mathbf{v}^1_{0} \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}\tfrac{1}{\sqrt{2}} \quad \left\langle \mathbf{v}^1_{+1} \right\rangle = \begin{pmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot \end{pmatrix}\tfrac{1}{\sqrt{2}}$$

note
orthonormality!

$$\left\langle \mathbf{v}^0_{0} \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}\tfrac{1}{\sqrt{3}}$$

ℓ=1
(condensed format)

$$\left\langle \mathbf{v}^2_{0} \right\rangle = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{matrix} 1 \\ \tfrac{1}{\sqrt{2}} \\ \tfrac{1}{\sqrt{6}} \end{matrix}$$

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Diagonal examples in *n-particle* notation:

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$$\left\langle \mathbf{v}^k_q \right\rangle = \sum_{m,m'=-\ell}^{\ell} \left| {\ell \atop m} \right\rangle \left\langle {\ell \atop m} \right| \mathbf{v}^k_q \left| {\ell \atop m'} \right\rangle \left\langle {\ell \atop m'} \right|$$

$$= \sum_{m,m'=-\ell}^{\ell} \left\langle {\ell \atop m} \right| \mathbf{v}^k_q \left| {\ell \atop m'} \right\rangle e_{m,m'} = \sum_{m,m'=-\ell}^{\ell} \begin{pmatrix} & k & \\ m & & m' \end{pmatrix} e_{m,m'}$$

ℓ=1
tensor array
1-particle notation

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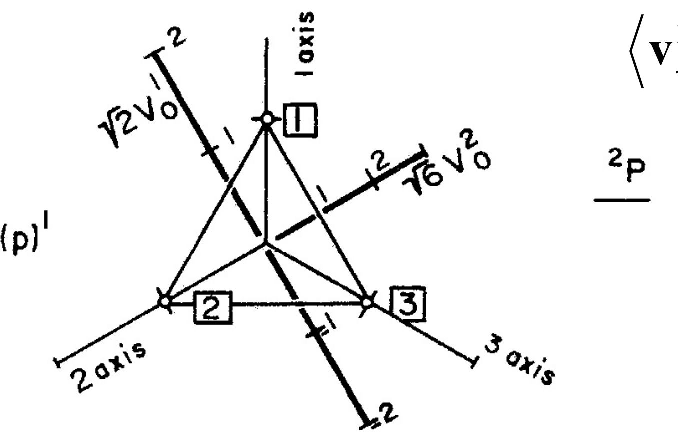

ℓ=1
(condensed format)

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$$\left\langle \mathbf{v}^0_{0} \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \tfrac{1}{\sqrt{3}}$$

Diagonal examples in *n-particle* notation:

$$\sqrt{3}\mathbf{V}^0_0 = E_{11} + E_{22} + E_{33}$$

$$\sqrt{2}\mathbf{V}^1_0 = E_{11} \qquad - E_{33} \equiv L_z$$

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ℓ=1
tensor array
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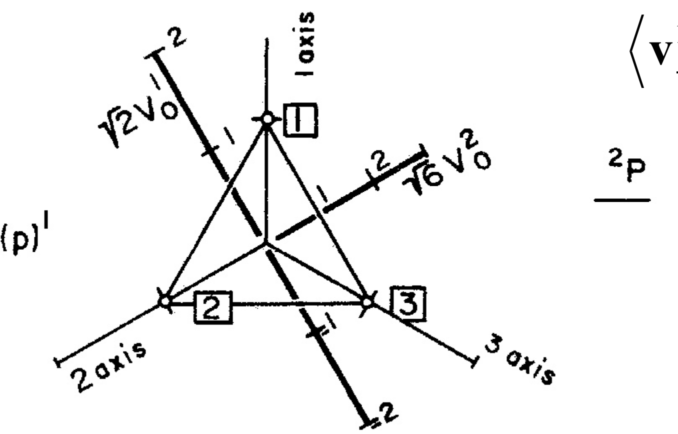
$$\left\langle \mathbf{v}^0_{0} \right\rangle = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}\tfrac{1}{\sqrt{3}}$$



ℓ=1
(condensed format)

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Off-Diagonal examples in *n-particle* notation:

$$\mathbf{V}^2_2 = E_{13}\ , \quad -2\mathbf{V}^2_1 = \sqrt{2}(E_{12} - E_{23})\ , \quad 2\mathbf{V}^2_{-1} = \sqrt{2}(E_{21} - E_{32})\ , \quad 2\mathbf{V}^2_{-2} = E_{31}\ ,$$

$$-2\mathbf{V}^1_1 = \sqrt{2}(E_{12} + E_{23}) \equiv L_+, \quad 2\mathbf{V}^1_{-1} = \sqrt{2}(E_{21} + E_{32}) \equiv L_-\ .$$

AMOP reference links on page 2

4.09.18 class 22: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Atomic shell models using intertwining $(S_n)^*(U(m))$ matrix operators

Single particle p^1-orbitals: U(3) triplet
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- ➡ Condensed form tensor tables for orbital shells *p: ℓ=1, d: ℓ=2, f: ℓ=3, g: ℓ=4.*

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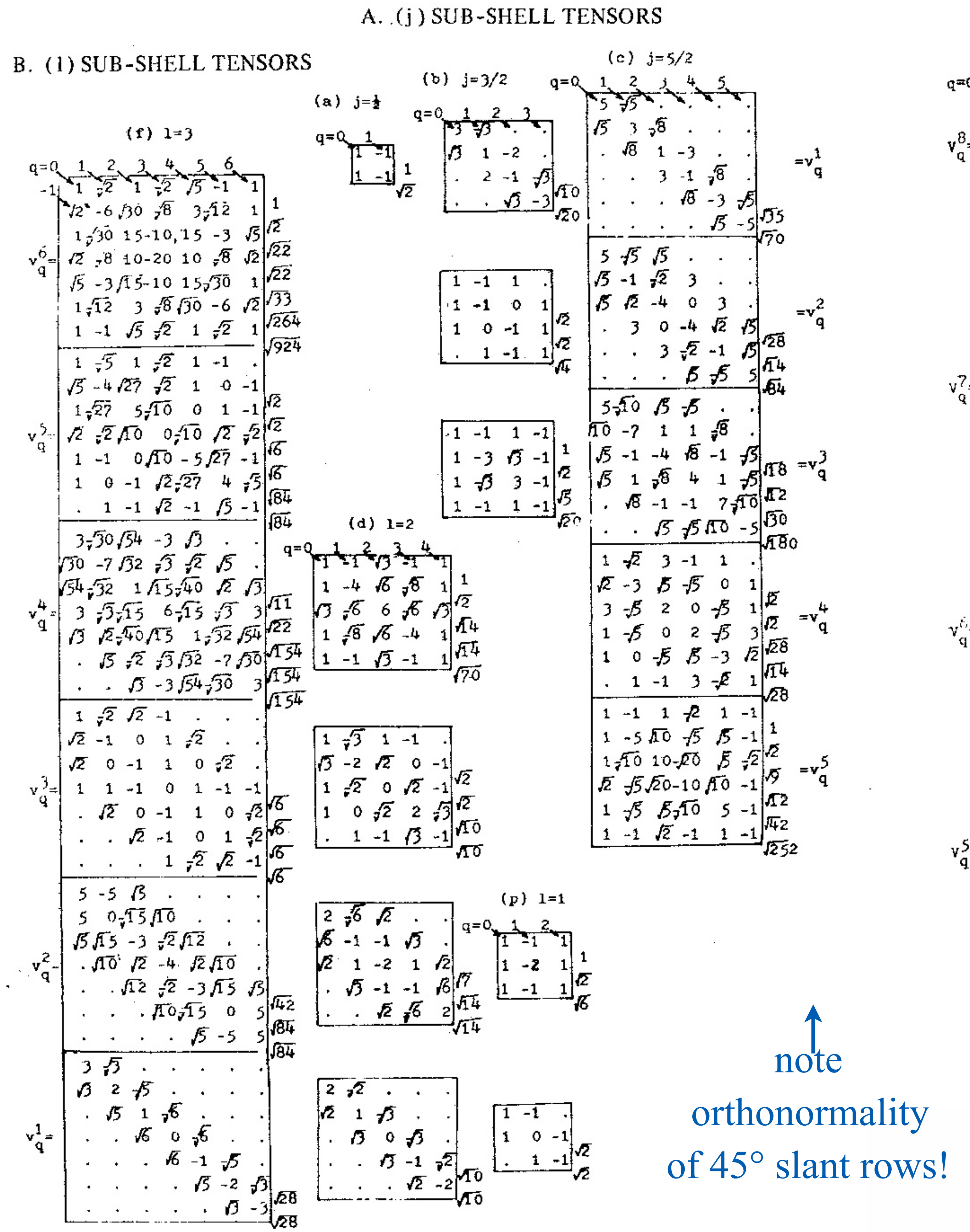

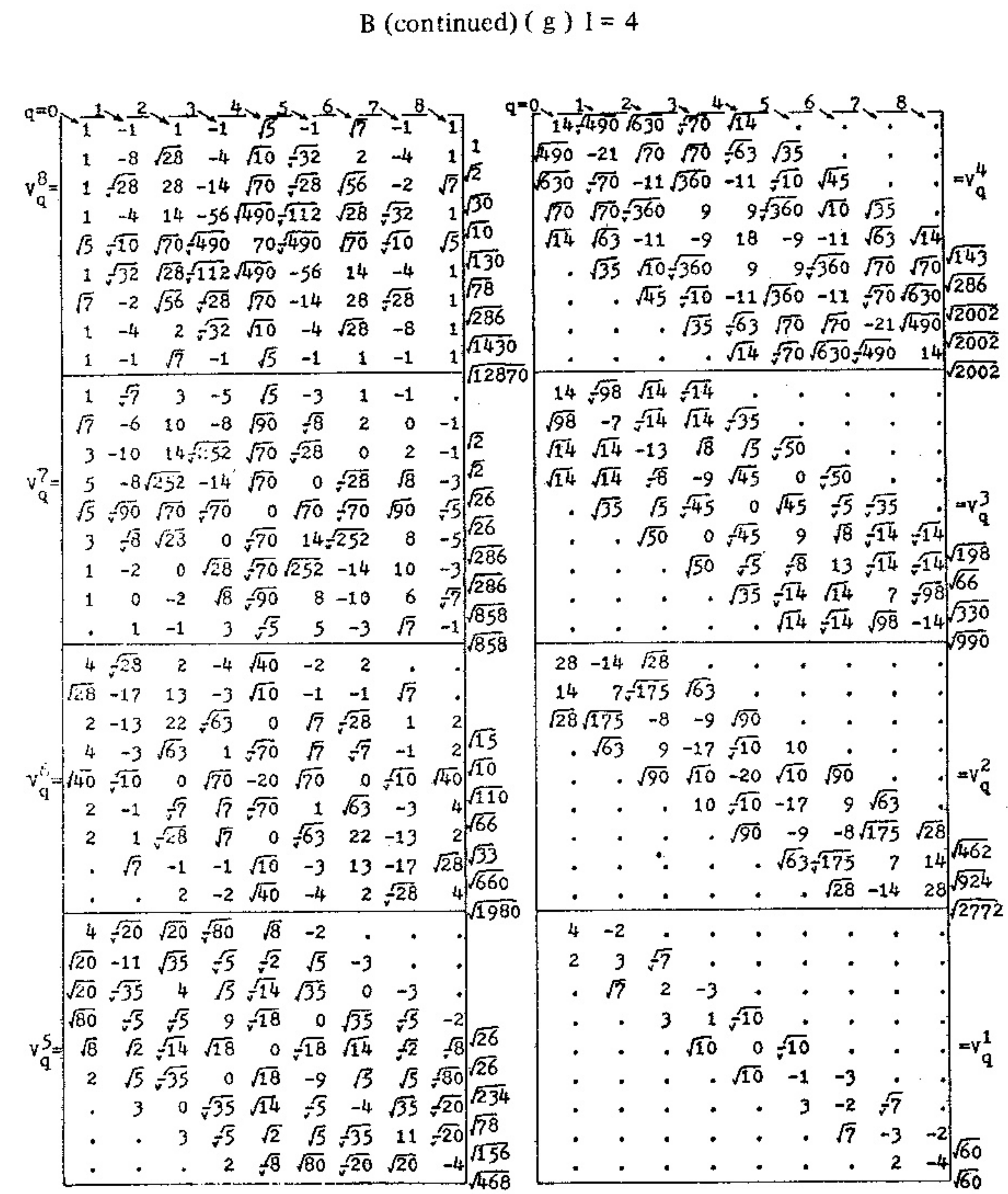

note orthonormality of 45° slant rows!

Easy to fit tensors to any matrix!

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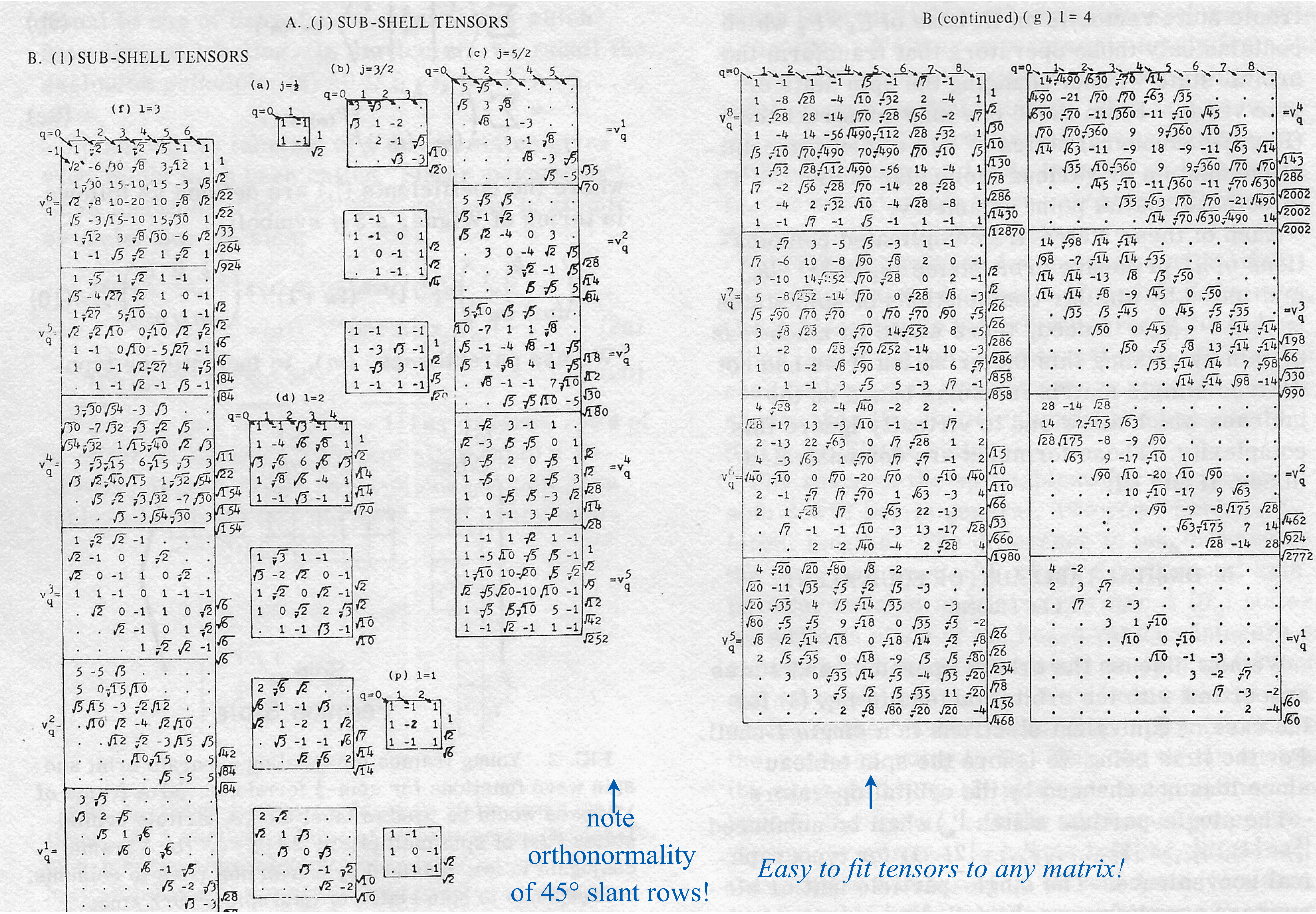

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Start with highest angular momentum (L=2) p^3 state: $\left|{}^2D, L=2\right\rangle = \begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array}$ (Fermi spin-mate $\begin{array}{|c|c|}\hline \uparrow&\uparrow\\\hline \downarrow\\\cline{1-1}\end{array}$)

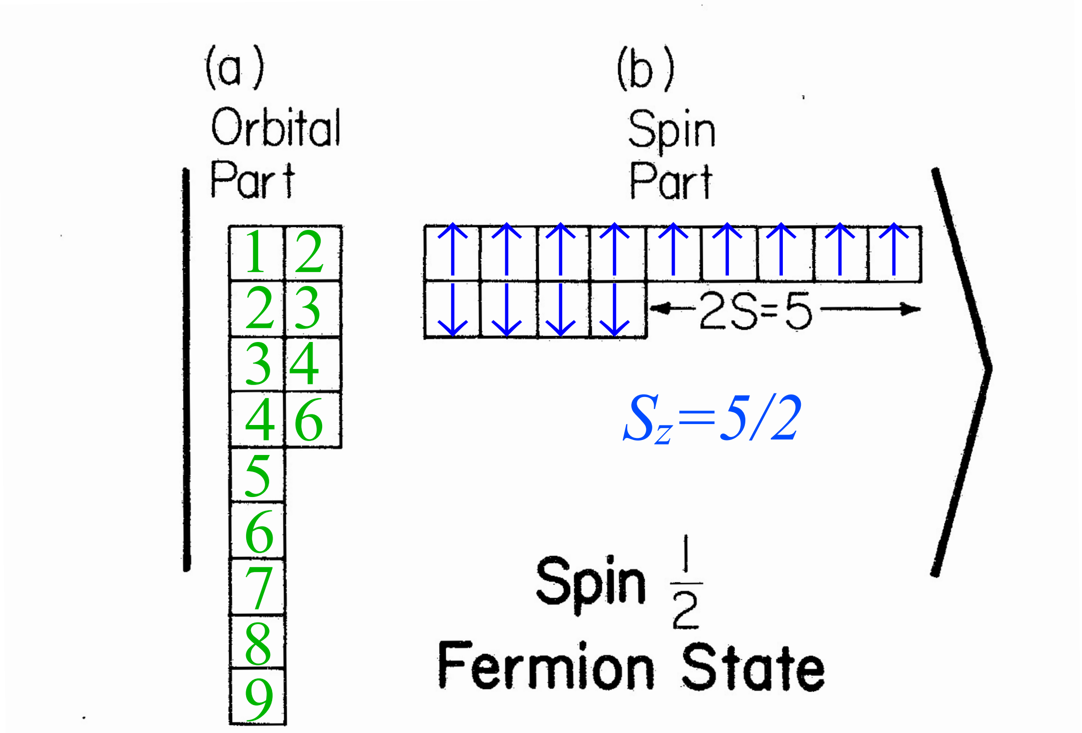

FIG. 2. Young frames for labeling separate orbit and spin wave functions for spin-$\frac{1}{2}$ fermions. (a) A frame of 13 boxes would be used to label the 13-particle orbital states (^6L) of spin multiplicity $2S+1=6$. (b) A frame conjugate to (a), obtained by converting rows to columns, corresponds to spin states of total spin $S=5/2$ since only five of the spin boxes are "unpaired."

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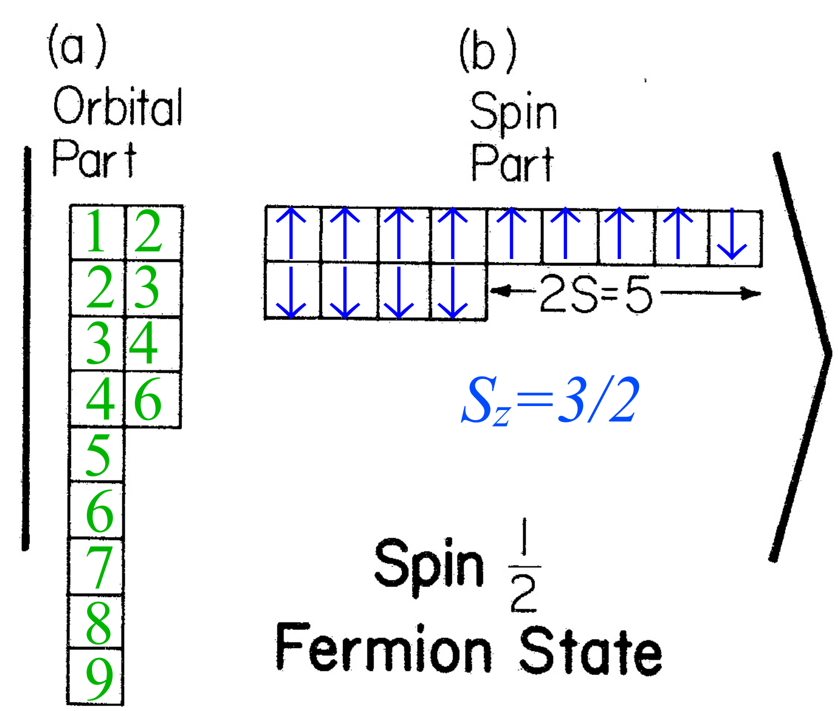
Then apply lowering operator $L_- \equiv \sqrt{2}(E_{21} + E_{32})$



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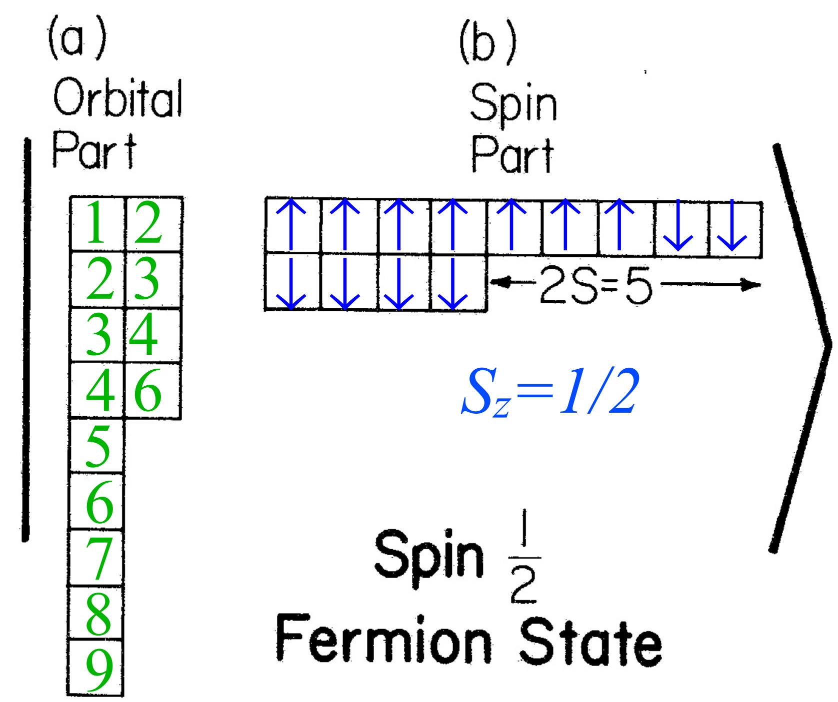
Here this is done using Tableau "Jawbone" formula.



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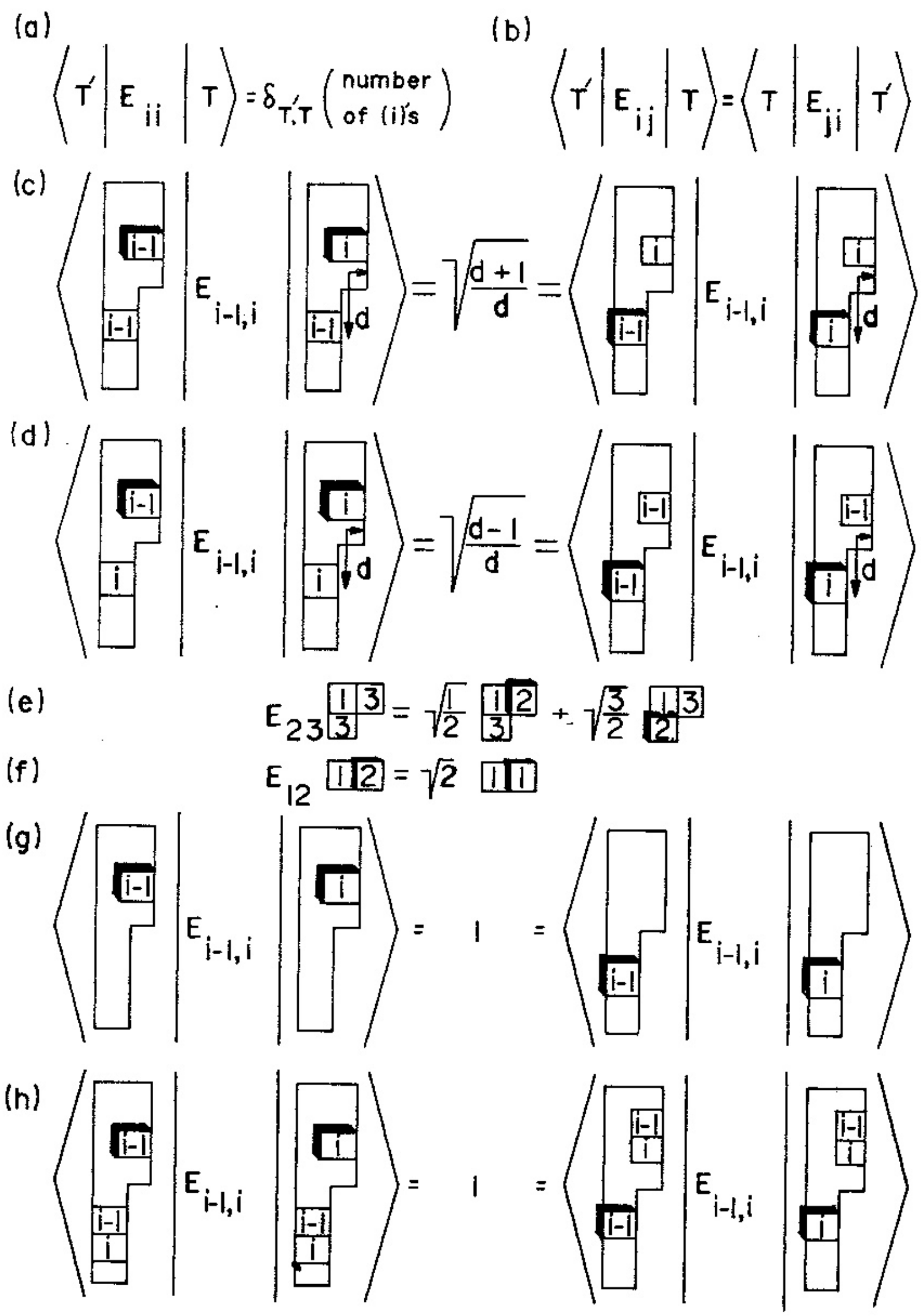

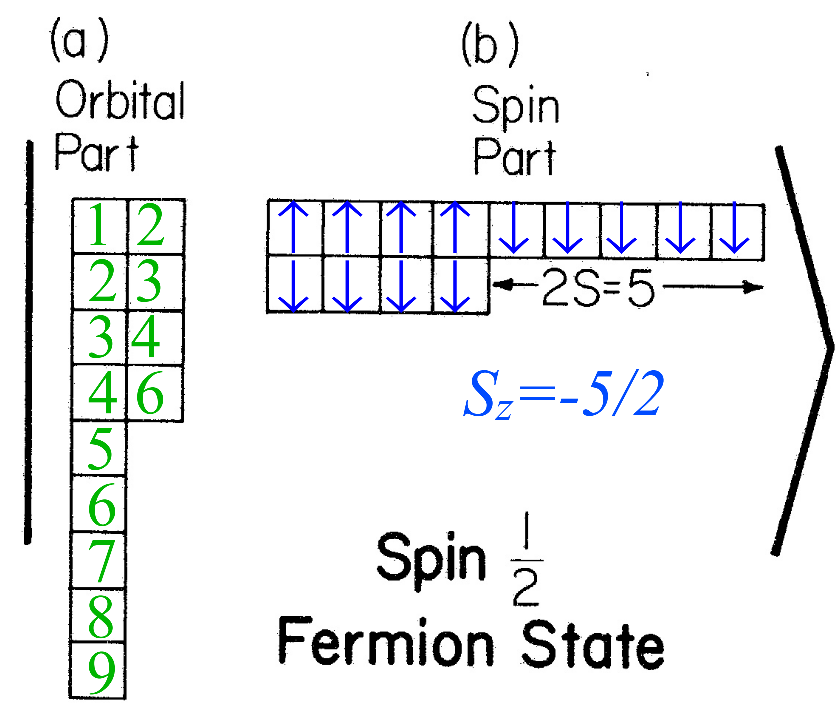

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Then apply lowering operator $L_- \equiv \sqrt{2}(E_{21}+E_{32})$ $\qquad \left|{}^2D^{L=2}_{M=1}\right\rangle = \frac{1}{2}L_-\left|{}^2D^{L=2}_{M=2}\right\rangle = \frac{1}{2}\sqrt{2}(E_{21}+E_{32})\left|\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 \\ \cline{1-1}\end{array}\right\rangle$

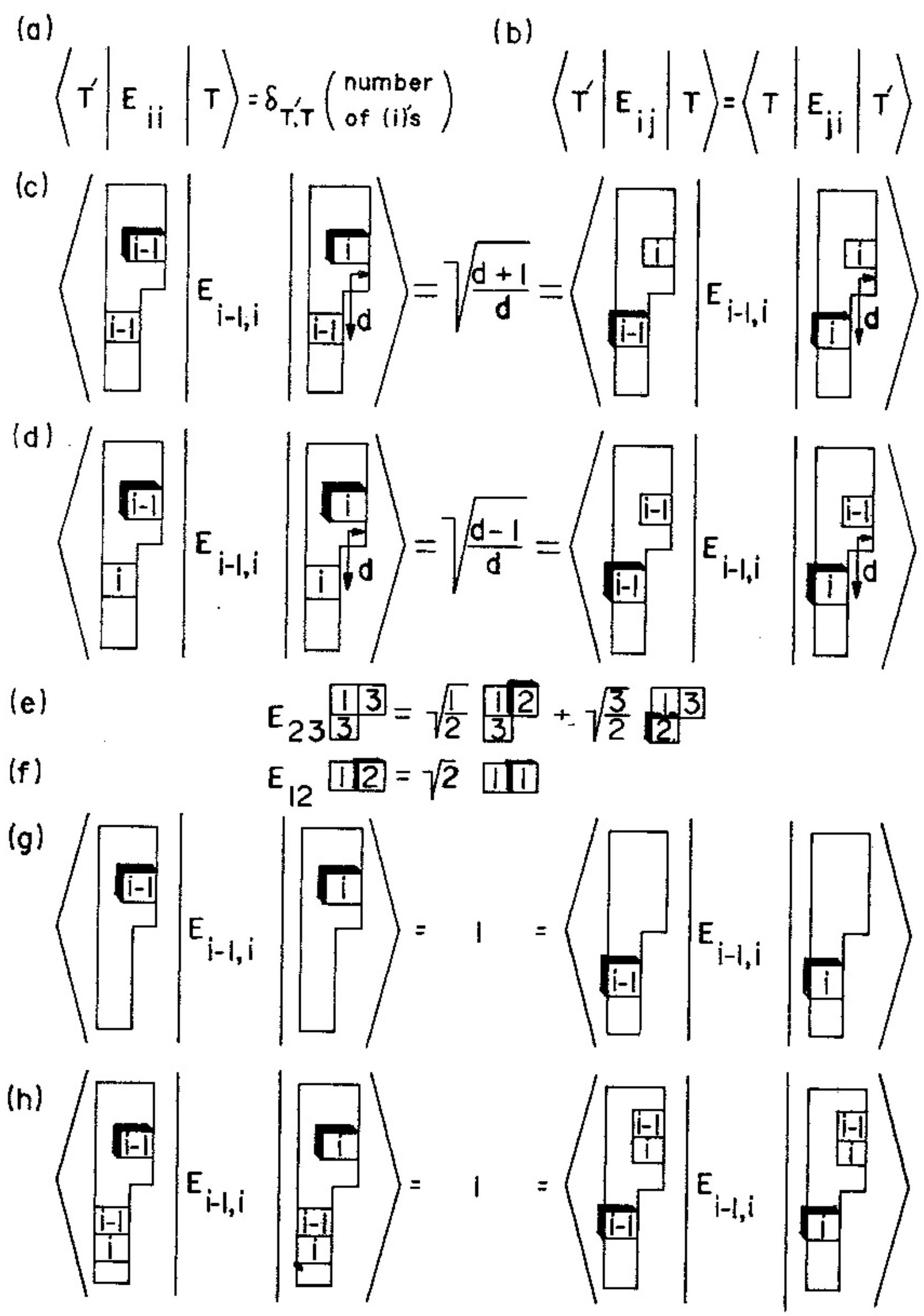


FIG. 3. Simplified jawbone formula for electronic orbital operators. (a) Number operators E_{ii} are diagonal. (The only eigenvalues for orbital states are 0, 1, and 2.). (b) Raising and lowering operators are simply transposes of each other. (c)–(h) $E_{i-1,i}$ acting on a tableau state gives zero unless there is an (i) in a column of the tableau that doesn't already have an $(i-1)$, too. Then it gives back a new state with the (i) changed to $(i-1)$ and a factor (matrix element) that depends on where the other (i)'s and $(i-1)$'s are located. [Boxes not outlined in the figure contain numbers not equal to (i) or $(i-1)$.] Cases (c) and (d) involved the "city block" distance d which is the denominator of the matrix element. The numerator is one larger $(d+1)$ or smaller $(d-1)$, depending on whether the involved tableaus favor the larger or smaller state number (i or $i-1$) with a higher position. The special cases of $(d=1)$ shown in (f) always pick the larger (and nonzero) choice of $d+1=2$. All other nonzero matrix elements are equal to unity.

Tableau calculation of 3-electron ℓ=1 orbital p^3-states and their $\mathbf{V}^k{}_q$ matrices

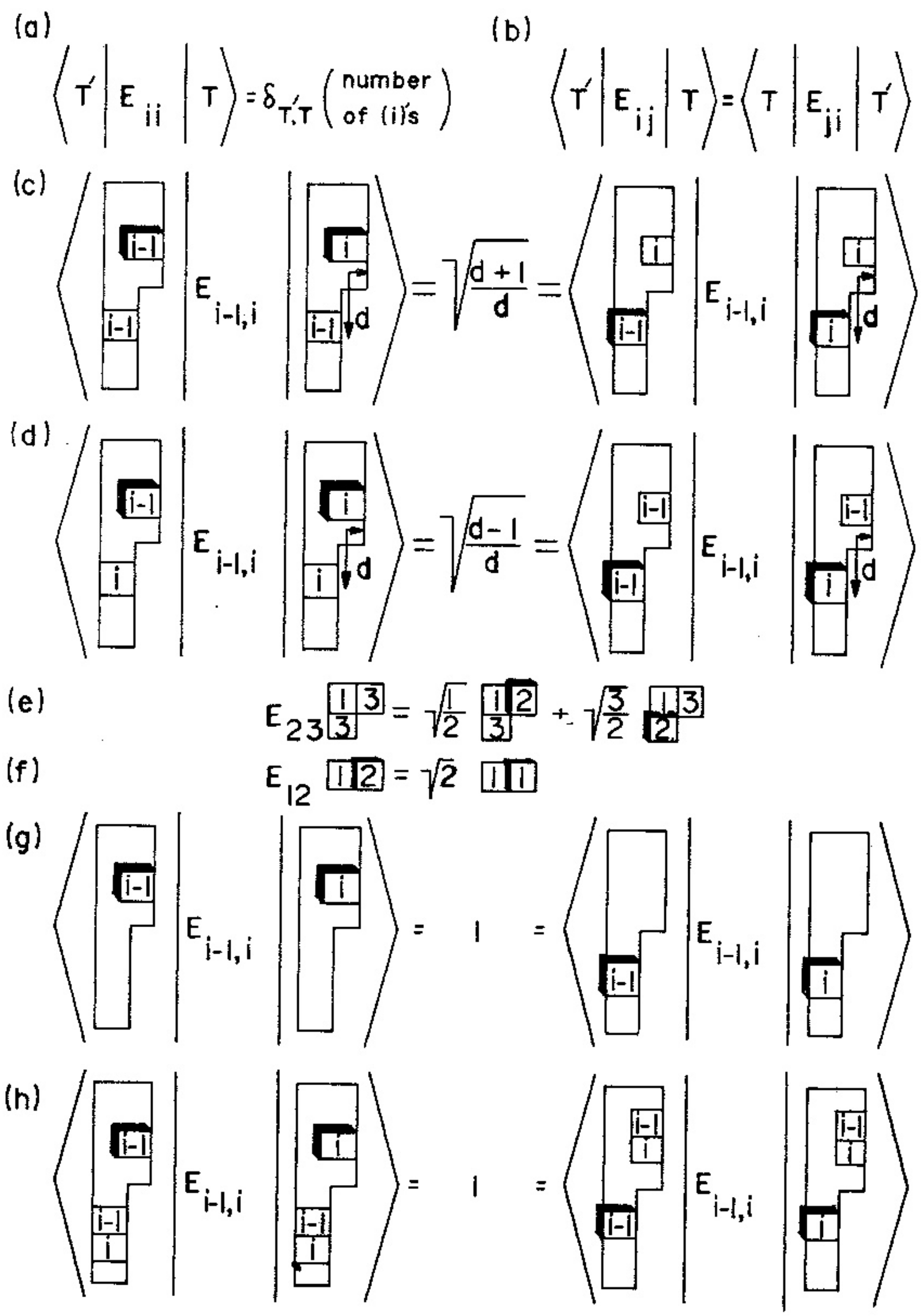
Start with highest angular momentum (L=2) p^3 state: $\left|{}^2D,{}^{L=2}_{M=2}\right\rangle = \begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array}$ (Fermi spin-mate $\begin{array}{|c|c|}\hline \uparrow&\uparrow\\\hline \downarrow\\\cline{1-1}\end{array}$)

Then apply lowering operator $L_- \equiv \sqrt{2}(E_{21}+E_{32})$

$$\left|{}^2D^{L=2}_{M=1}\right\rangle = \tfrac{1}{2}L_-\left|{}^2D^{L=2}_{M=2}\right\rangle = \tfrac{1}{2}\sqrt{2}(E_{21}+E_{32})\left|\begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array}\right\rangle$$

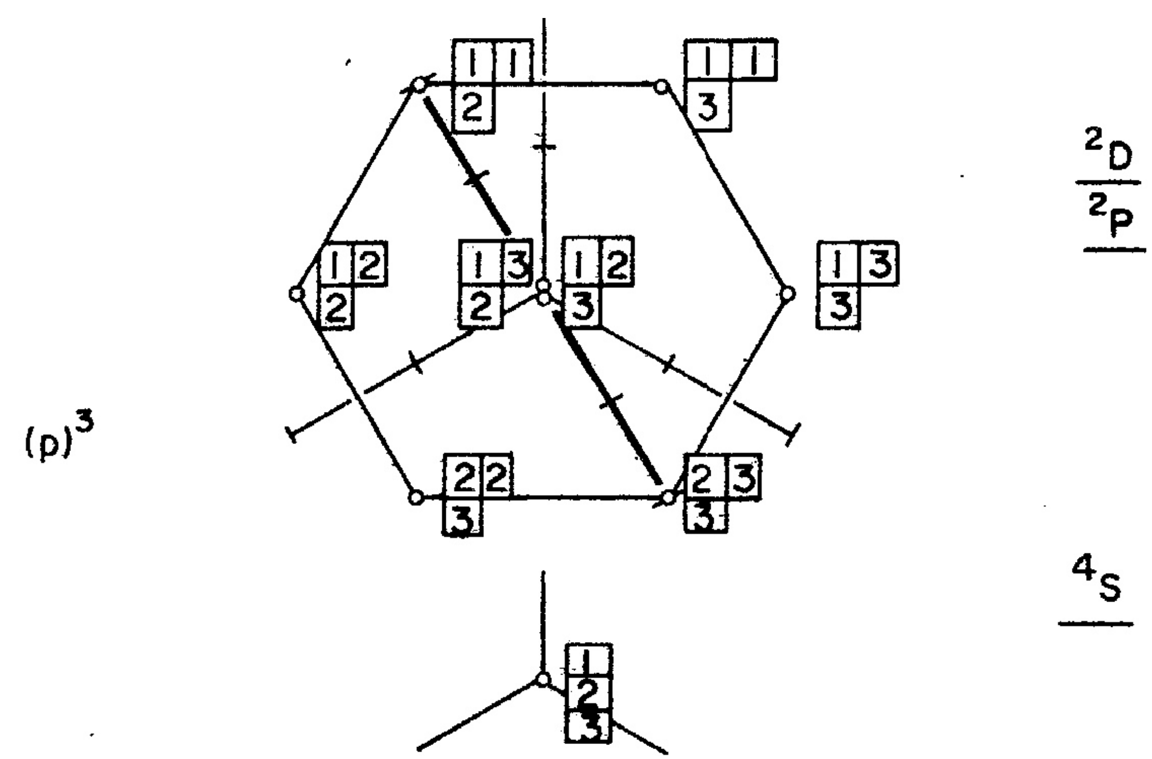
Here this is done using Tableau "Jawbone" formula.

$$= = \frac{1}{\sqrt{2}}\left(\left|\begin{array}{|c|c|}\hline 1&2\\\hline 2\\\cline{1-1}\end{array}\right\rangle + \left|\begin{array}{|c|c|}\hline 1&1\\\hline 3\\\cline{1-1}\end{array}\right\rangle\right)$$



Orthogonal to this is a ^{2}P (M=1) state

$$\left|{}^2P^{L=1}_{M=1}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{array}{|c|c|}\hline 1&2\\\hline 2\\\cline{1-1}\end{array}\right\rangle - \left|\begin{array}{|c|c|}\hline 1&1\\\hline 3\\\cline{1-1}\end{array}\right\rangle\right)$$



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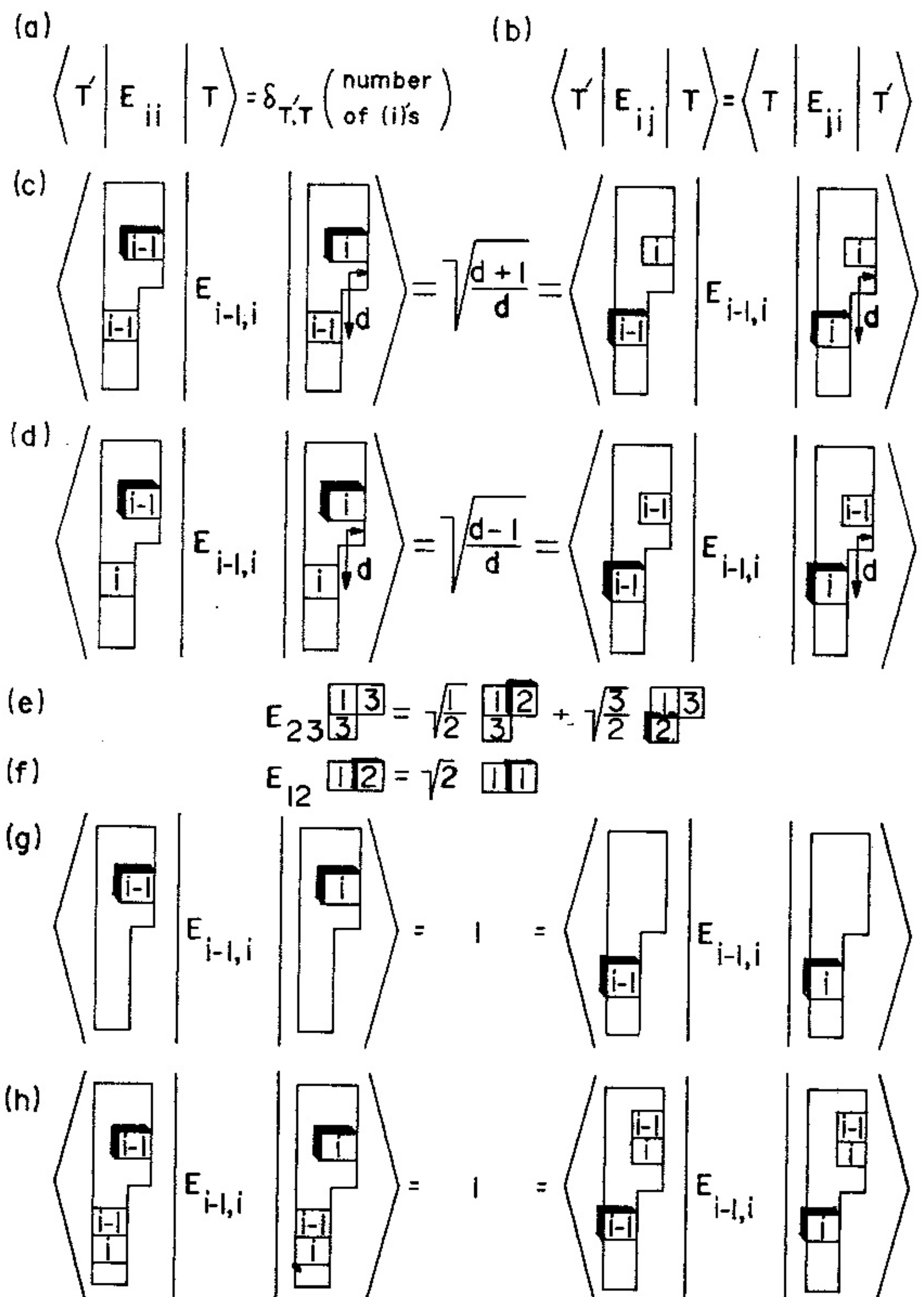


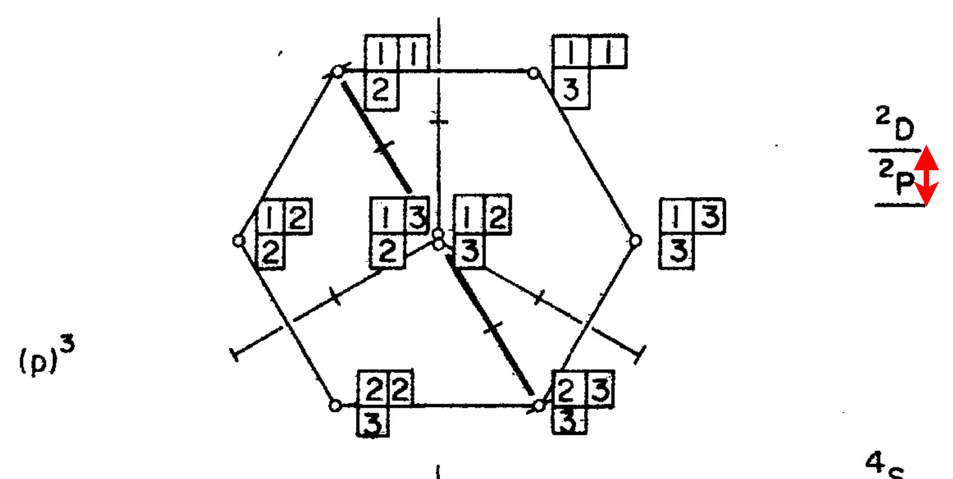
Orthogonal to this is a ${}^2P$ (M=1) state

$$\left|{}^2P^{L=1}_{M=1}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

Next we calculate 2^n-pole moments the pair:

$$\left\langle {}^2P^{L=1}_{M=1}\right|V^k_0\left|{}^2D^{L=2}_{M=1}\right\rangle =$$

$$\frac{1}{\sqrt{2}}\left(\left\langle\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right| + \left\langle\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right|\right)\left[\binom{k}{11}E_{11}+\binom{k}{22}E_{22}+\binom{k}{33}E_{33}\right]\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$



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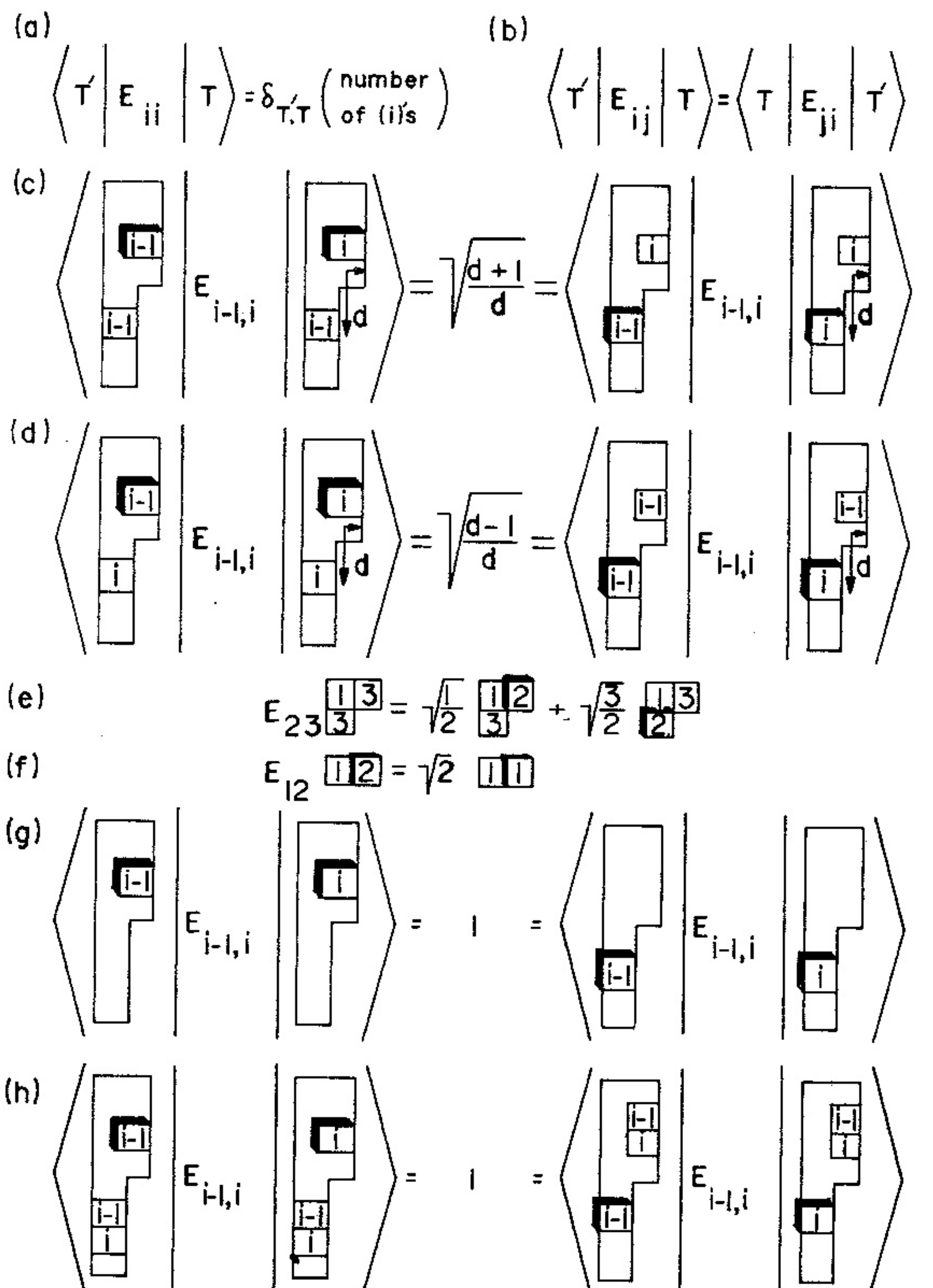

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$$\left\langle {}^2P^{L=1}_{M=1}\right|V^k_0\left|{}^2D^{L=2}_{M=1}\right\rangle =$$

$$\frac{1}{\sqrt{2}}\left(\left\langle\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right| + \left\langle\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right|\right)\left[\left(\begin{smallmatrix}k\\11\end{smallmatrix}\right)E_{11}+\left(\begin{smallmatrix}k\\22\end{smallmatrix}\right)E_{22}+\left(\begin{smallmatrix}k\\33\end{smallmatrix}\right)E_{33}\right]\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

$$= \tfrac{1}{2}\left[-\left(\begin{smallmatrix}2\\11\end{smallmatrix}\right)E_{11}+2\left(\begin{smallmatrix}2\\22\end{smallmatrix}\right)E_{22}-\left(\begin{smallmatrix}2\\33\end{smallmatrix}\right)\right] = -\sqrt{\tfrac{3}{2}} \quad \text{for}: k=2$$

$$= \tfrac{1}{2}\left[-\left(\begin{smallmatrix}1\\11\end{smallmatrix}\right)E_{11}+2\left(\begin{smallmatrix}1\\22\end{smallmatrix}\right)E_{22}-\left(\begin{smallmatrix}1\\33\end{smallmatrix}\right)\right] = 0 \quad \text{for}: k=1$$

$$= \tfrac{1}{2}\left[-\left(\begin{smallmatrix}0\\11\end{smallmatrix}\right)E_{11}+2\left(\begin{smallmatrix}0\\22\end{smallmatrix}\right)E_{22}-\left(\begin{smallmatrix}0\\33\end{smallmatrix}\right)\right] = 0 \quad \text{for}: k=0$$

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Comparison calculation of p^3-$\mathbf{V}^k_q$ vs. calculation by cfp (fractional parentage)

$$\langle p^3\,{}^2P\,1|\,V^2_0|p^3\,{}^2D\,1\rangle = C^{221}_{011}\left[(p^2D]\!]p^3D)(p^2D]\!]p^3P)\sqrt{(15)}\begin{Bmatrix}1&2&1\\2&2&1\end{Bmatrix} - (p^2P]\!]p^3D)(p^2P]\!]p^3P)\sqrt{(15)}\begin{Bmatrix}1&2&1\\2&1&1\end{Bmatrix}\right]\langle 1||\,2||1\rangle$$

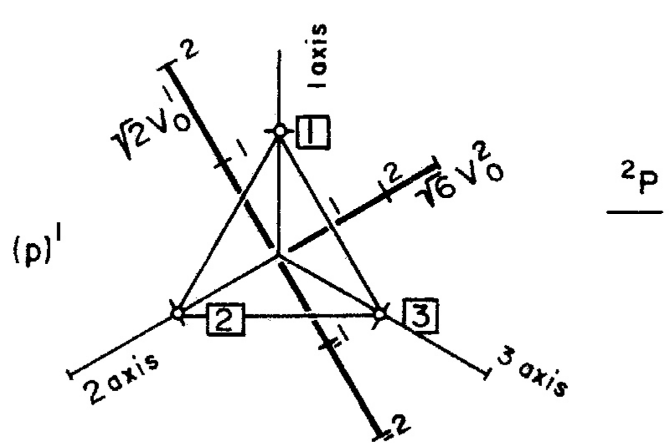
$$= -\sqrt{\tfrac{3}{2}}. \qquad (20)$$

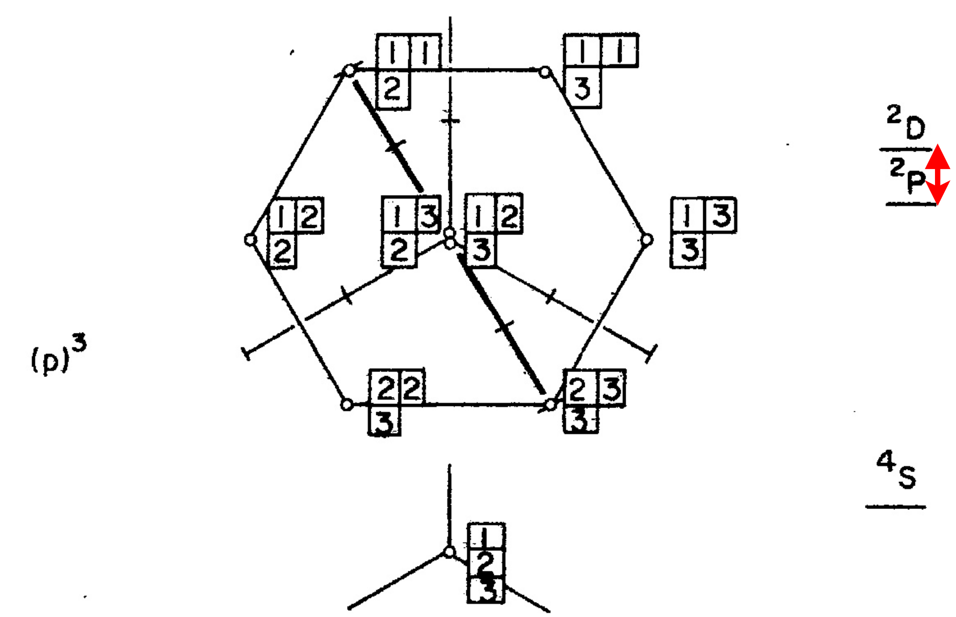
Versus:

$$\left\langle {}^2P^{L=1}_{M=1}\middle|V^k_0\middle|{}^2D^{L=2}_{M=1}\right\rangle =$$

$$\frac{1}{\sqrt{2}}\left(\left\langle \begin{smallmatrix}1&2\\2&\end{smallmatrix}\right| + \left\langle \begin{smallmatrix}1&1\\3&\end{smallmatrix}\right|\right)\left[\binom{k}{11}E_{11}+\binom{k}{22}E_{22}+\binom{k}{33}E_{33}\right]\left(\left|\begin{smallmatrix}1&2\\2&\end{smallmatrix}\right\rangle - \left|\begin{smallmatrix}1&1\\3&\end{smallmatrix}\right\rangle\right)$$

$$= \quad \tfrac{1}{2}\left[-\binom{2}{11}E_{11}+2\binom{2}{22}E_{22}-\binom{2}{33}\right] \quad = -\sqrt{\tfrac{3}{2}} \text{ for : } k=2$$





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Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

	$\lvert{}^{1\,1}_{2}\rangle$	$\lvert{}^{1\,2}_{2}\rangle$	$\lvert{}^{1\,1}_{3}\rangle$	$\lvert{}^{1\,2}_{3}\rangle$	$\lvert{}^{1\,3}_{2}\rangle$	$\lvert{}^{1\,3}_{3}\rangle$	$\lvert{}^{2\,2}_{3}\rangle$	$\lvert{}^{2\,3}_{3}\rangle$
	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
$\langle{}^{1\,1}_{2}\rvert$	$2^{(11)}+1^{(22)}$	$1^{(12)}$	$1^{(23)}$	$-\sqrt{\frac{1}{2}}^{(13)}$	$\sqrt{\frac{3}{2}}^{(13)}$			
$\langle{}^{1\,2}_{2}\rvert$		$1^{(11)}+2^{(22)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$-1^{(13)}$	
$\langle{}^{1\,1}_{3}\rvert$			$2^{(11)}+1^{(33)}$	$\sqrt{2}^{(12)}$		$1^{(13)}$		
$\langle{}^{1\,2}_{3}\rvert$				$1^{(11)}+1^{(22)}+1^{(33)}$		$\sqrt{\frac{1}{2}}^{(23)}$	$\sqrt{2}^{(12)}$	$\sqrt{\frac{1}{2}}^{(13)}$ $=\langle E_{ij}\rangle$
$\langle{}^{1\,3}_{2}\rvert$					$1^{(11)}+1^{(22)}+1^{(33)}$	$\sqrt{\frac{3}{2}}^{(23)}$		$\sqrt{\frac{3}{2}}^{(13)}$
$\langle{}^{1\,3}_{3}\rvert$						$1^{(11)}+2^{(33)}$		$1^{(12)}$
$\langle{}^{2\,2}_{3}\rvert$							$2^{(22)}+1^{(33)}$	$1^{(23)}$
$\langle{}^{2\,3}_{3}\rvert$								$1^{(22)}+2^{(33)}$

notation:
(jk) numbers tell
which E_{jk} gave that entry

Diagonal examples in *n-particle* notation:

$$\sqrt{3}\mathbf{V}^0_0 = E_{11}+E_{22}+E_{33}$$

$$\sqrt{2}\mathbf{V}^1_0 = E_{11} - E_{33} \equiv L_z$$

$$\sqrt{6}\mathbf{V}^2_0 = E_{11}-2E_{22}+E_{33}$$

Off-Diagonal examples in *n-particle* notation:

$$\mathbf{V}^2_2 = E_{13}\ ,\quad -2\mathbf{V}^2_1 = \sqrt{2}(E_{12}-E_{23})\ ,\quad 2\mathbf{V}^2_{-1} = \sqrt{2}(E_{21}-E_{32})\ ,\quad 2\mathbf{V}^2_{-2} = E_{31}\ ,$$

$$-2\mathbf{V}^1_1 = \sqrt{2}(E_{12}+E_{23}) \equiv L_+,\quad 2\mathbf{V}^1_{-1} = \sqrt{2}(E_{21}+E_{32}) \equiv L_-\ .$$

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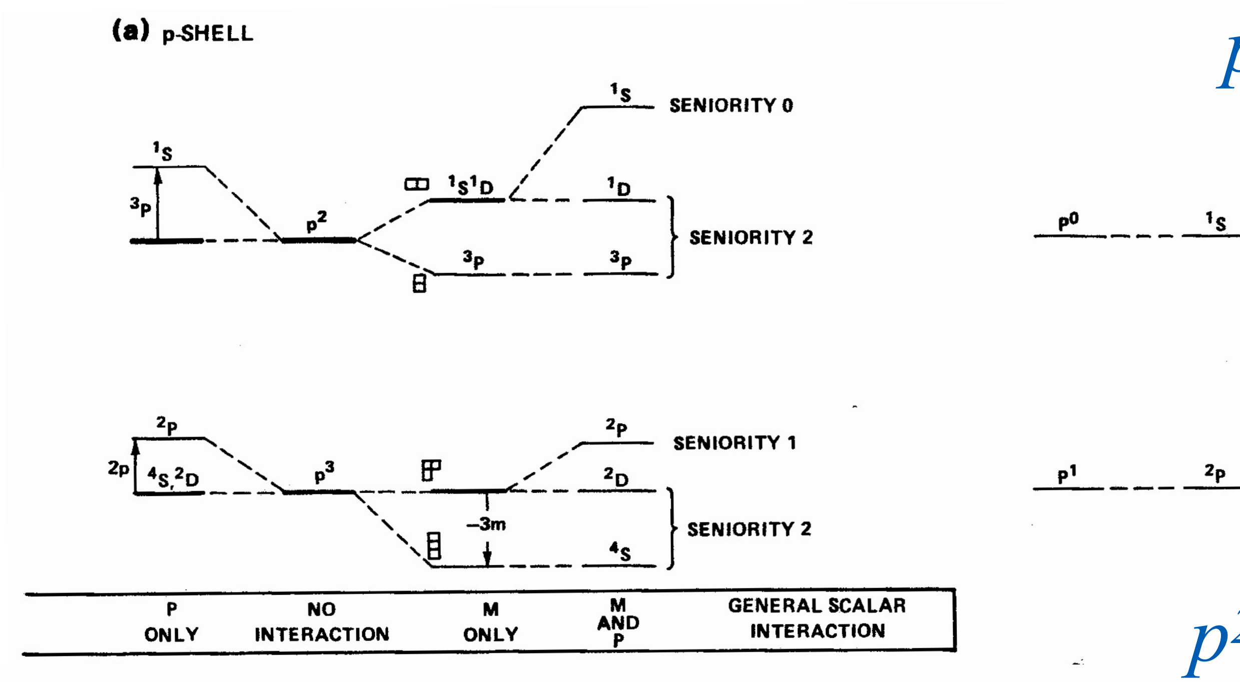
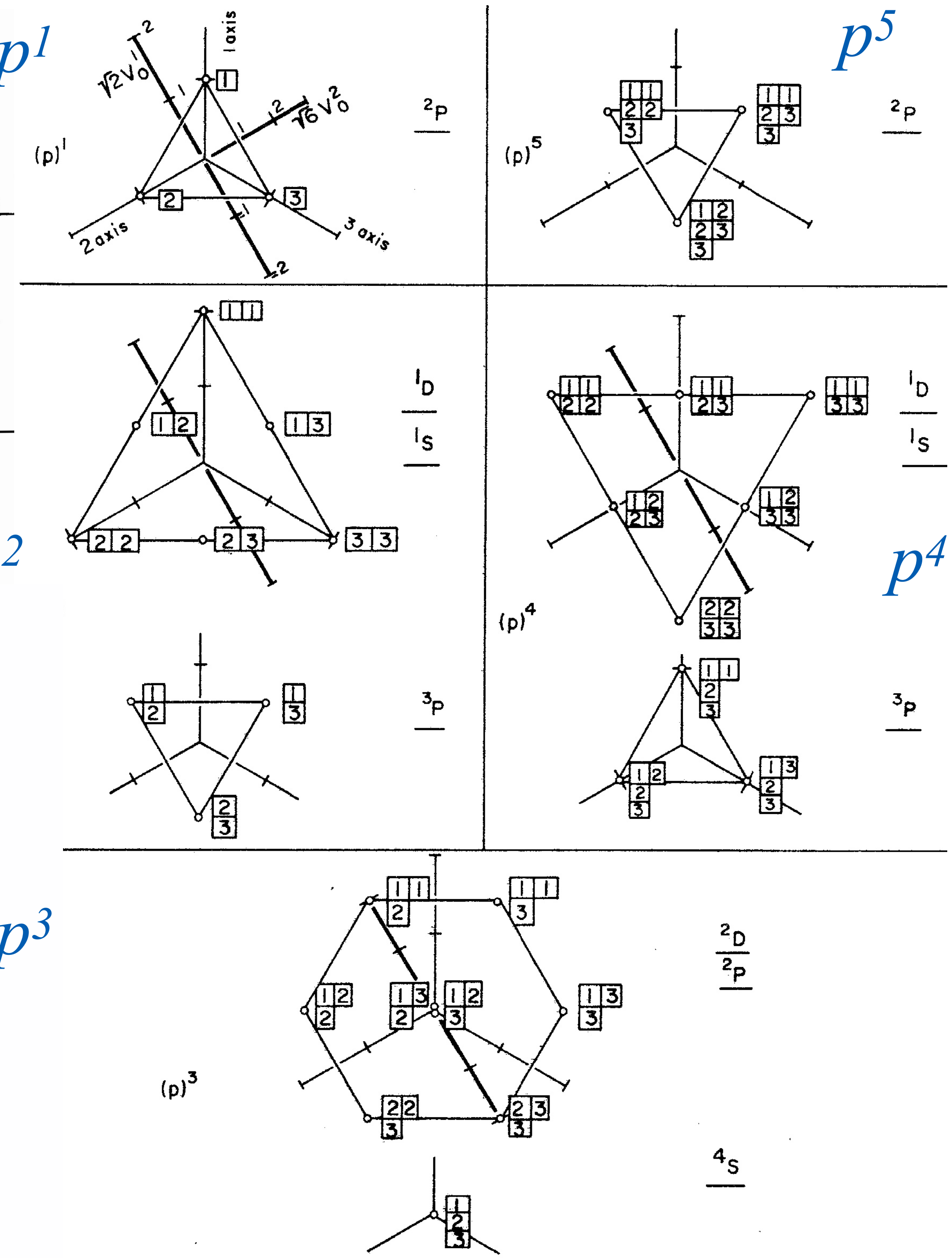
p^2

p^3



p^1 *p^5* *p^2* *p^4* *p^3*



Excerpts from unpublished Ch. 9 intended for Vol II of Principles of Symmetry, Dynamics and Spectroscopy

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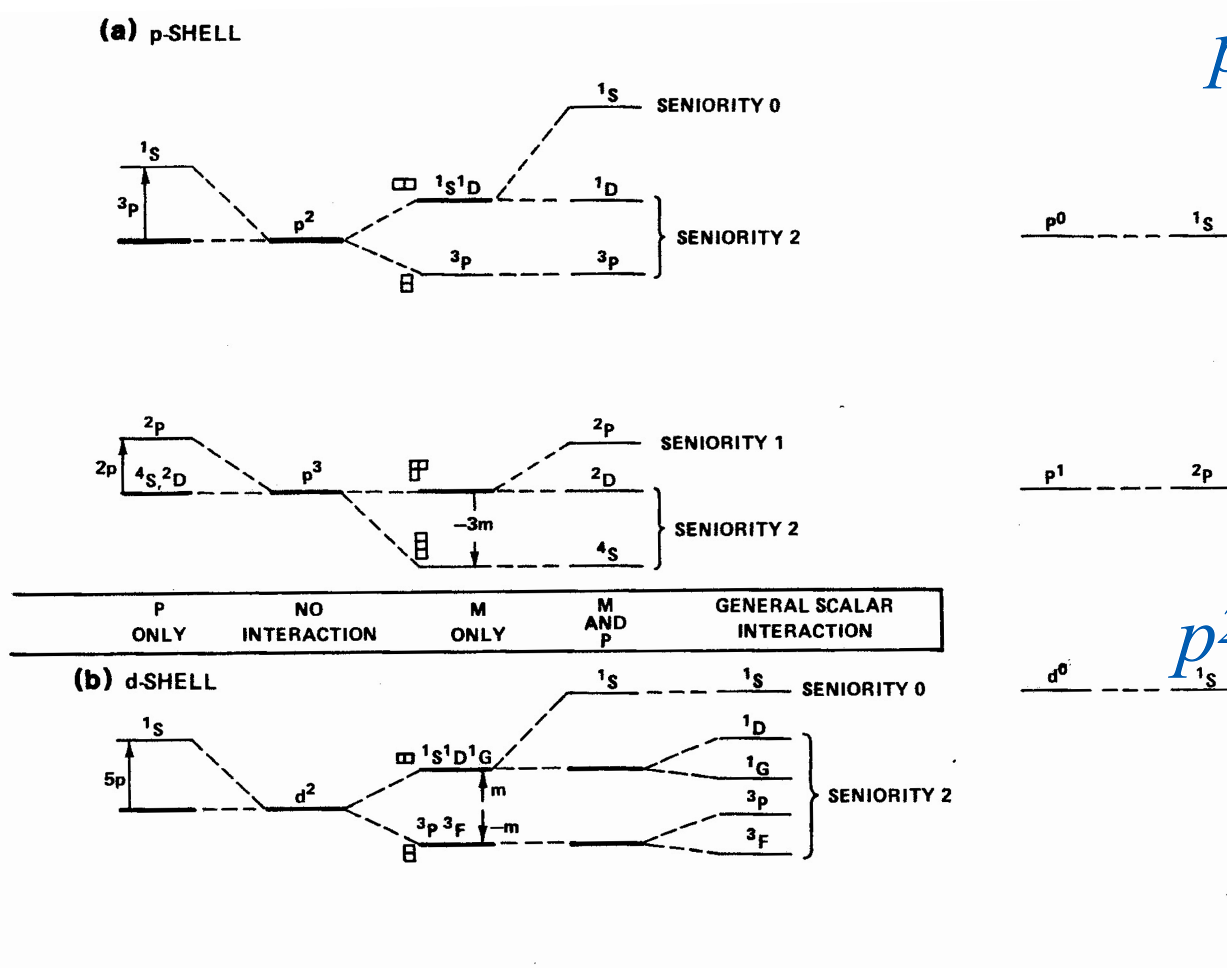
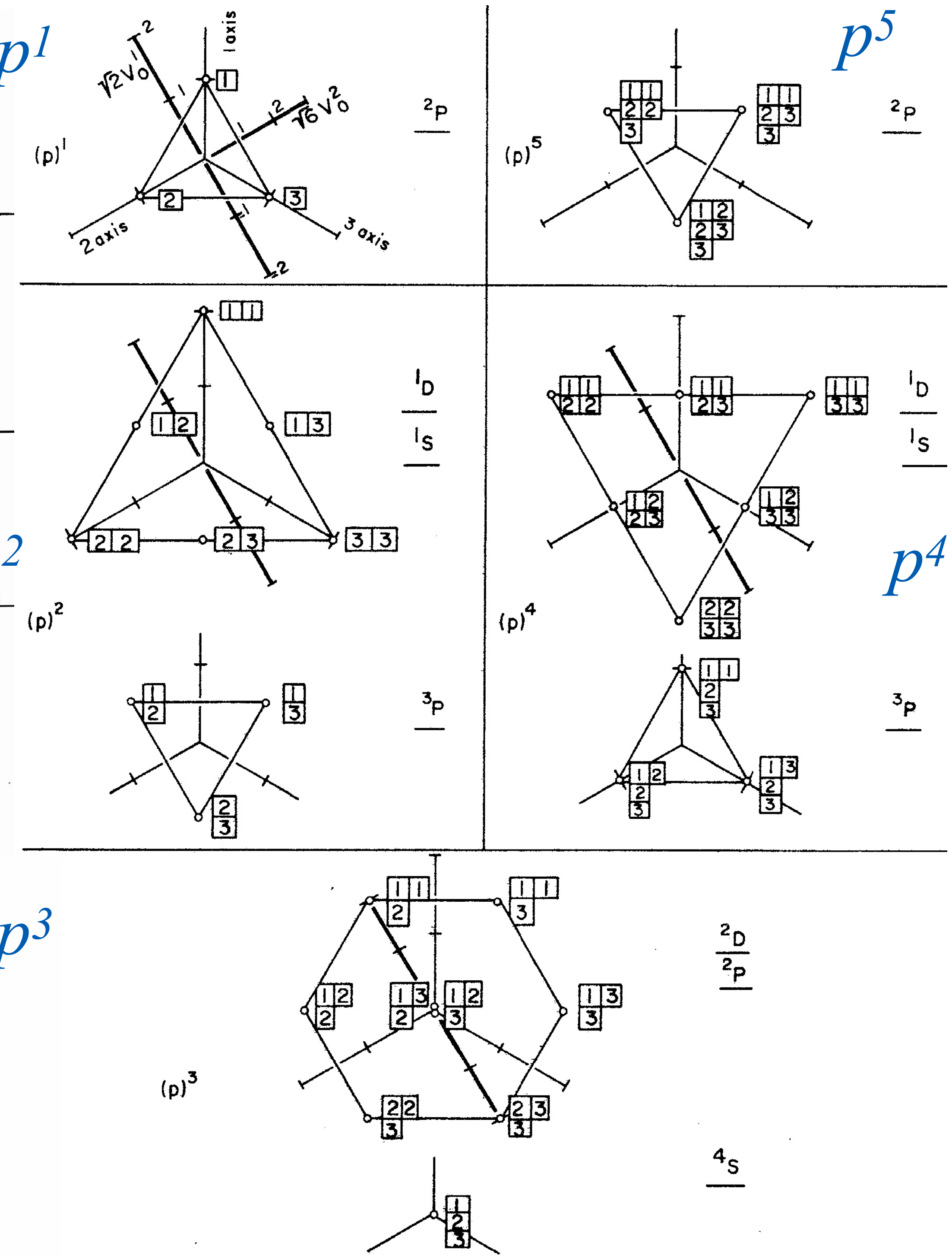
p^2

p^3

d^2



p^1 *p^5* *p^2* *p^4* *p^3*



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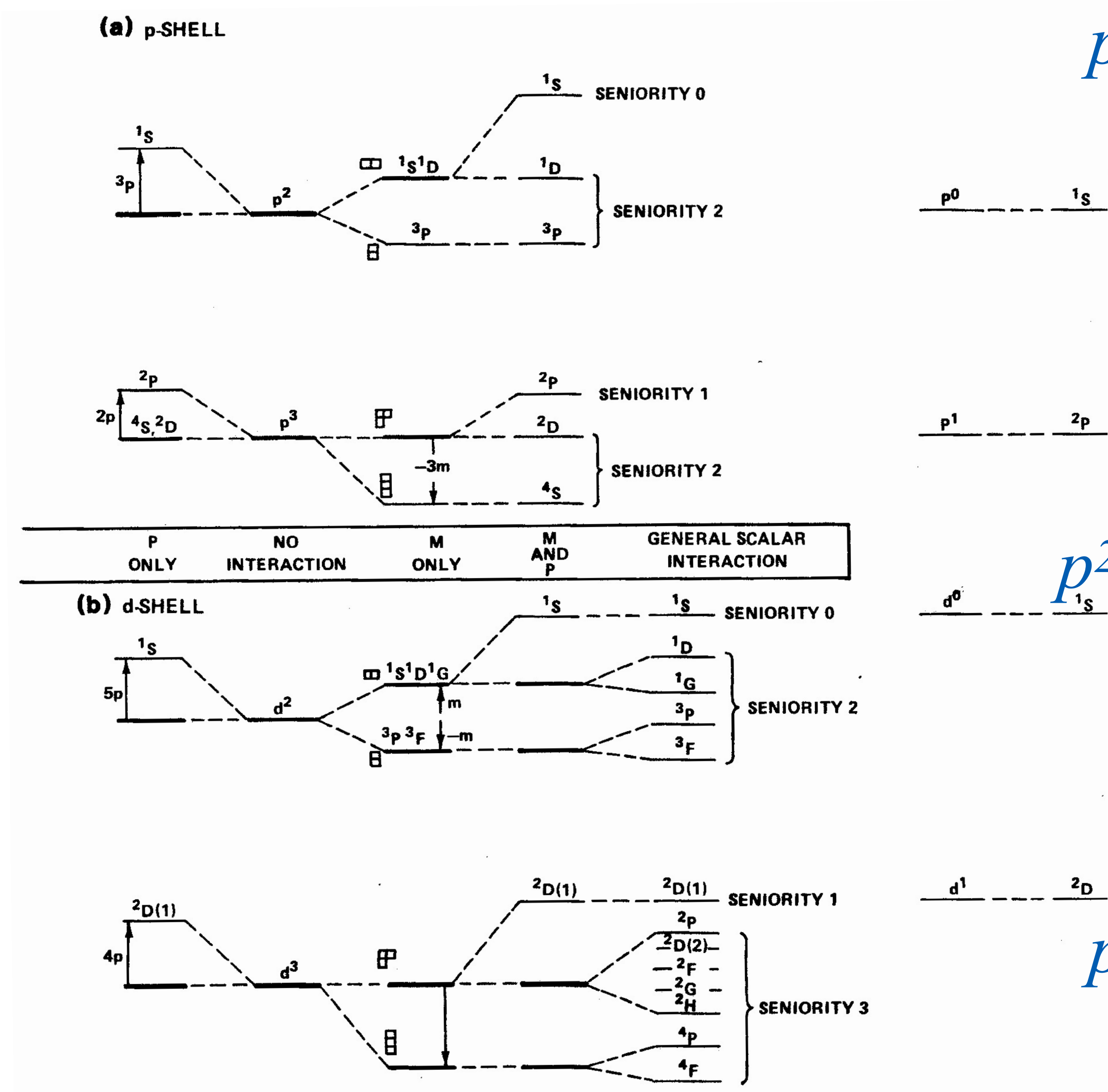
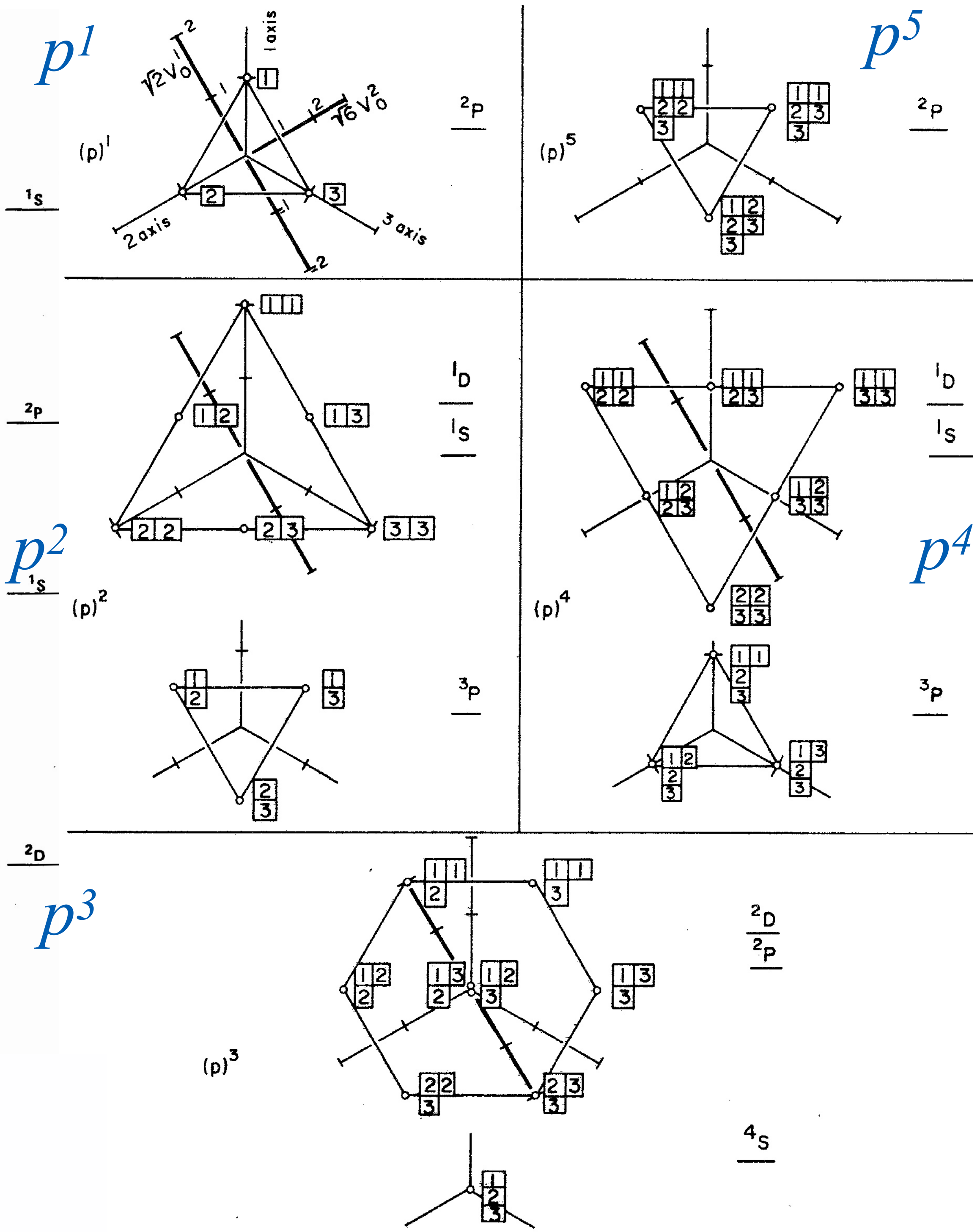
p^2

p^3

d^2

d^3





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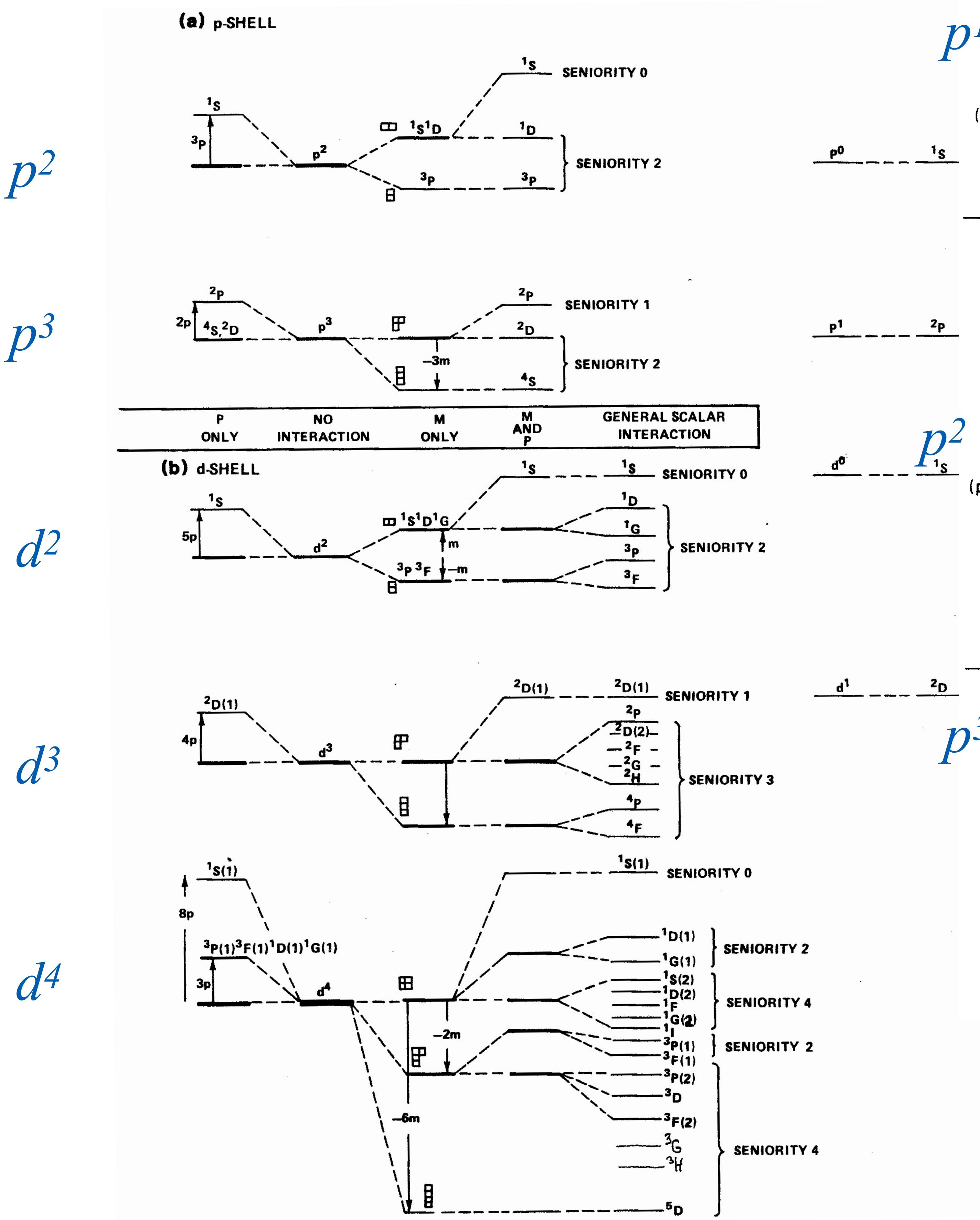

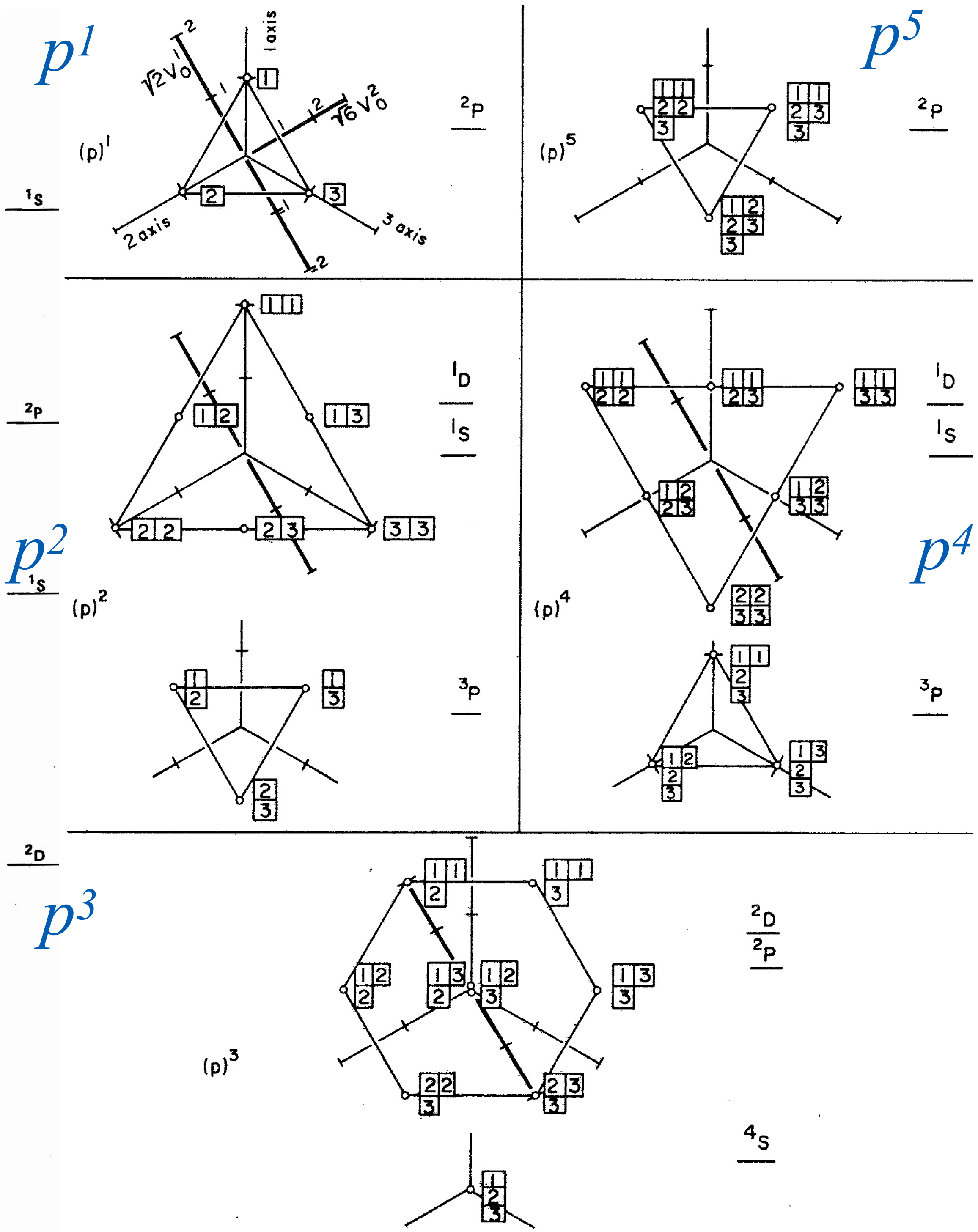

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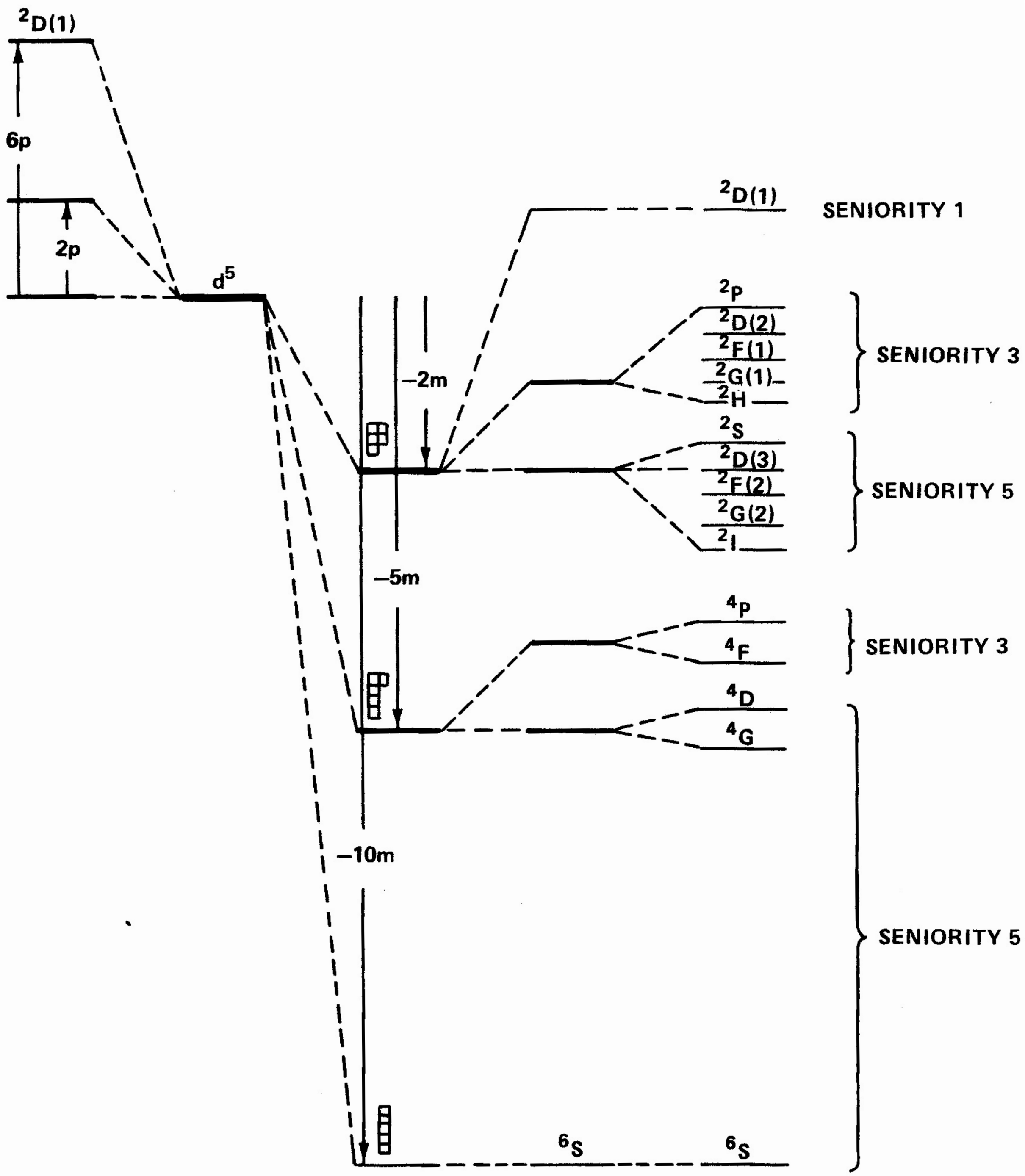
d^5



Eigenstates of P and M are said to be states of definite SENIORITY. The guantum number ν of SENIORITY is equal to the number of unpaired particles in the state. Examples of states made entirely of paired particles are $|p^2\ {}^1S\rangle$, $|d^2\ {}^1S\rangle$, $|d^4\ {}^1S\rangle$ . . . The first two examples have exactly one "pair" and their p eigenvalues are 3p and 5p respectively. The state $|d^4\ {}^1S\rangle$ has two pairs, and it takes energy 5p to "break one pair" to make seniority 2 states ${}^1D(1)$ and ${}^1G(1)$. However, then only 3p is needed to break the remaining pair to make any of the seniority 4 states. Note that in each case, seniority ν states show up with the same partners in the ℓ^ν configuration. "Pairs" are like a scalar "core" which does not influence the angular momentum of the ν unpaired particles "outside" it. You will first see a seniority ν group in ℓ^ν, then all over again in $\ell^{\nu+2}$, $\ell^{\nu+4}$, . . . , and so on.

Excerpts from unpublished Ch. 9 intended for Vol II of Principles of Symmetry, Dynamics and Spectroscopy

AMOP reference links on page 2

4.09.18 class 22: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Atomic shell models using intertwining $(S_n)^*(U(m))$ matrix operators

Single particle p^1-orbitals: U(3) triplet
- Elementary U(*N*) commutation
- Elementary state definitions by Boson operators
  - Summary of multi particle commutation relations

Symmetric p^2-orbitals: U(3) sextet
- Sample matrix elements
  - Combining elementary "1-jump" E_{12}, E_{23}, to get "2-jump" operator E_{13}
    - Review:Representation of *Diagonalizing Transform* (DTran *T*)

Relating elementary $\mathbf{E}_{jk}$ matrices to Tensor operator $\mathbf{V}^k{}_q$ *(ℓ=1 atomic p-shell)*
- Condensed form tensor tables for orbital shells *p: ℓ=1, d: ℓ=2, f: ℓ=3, g: ℓ=4.*

Tableau calculation of 3-electron ℓ=1 orbital p^3-states and $\mathbf{V}^k{}_q$ matrices
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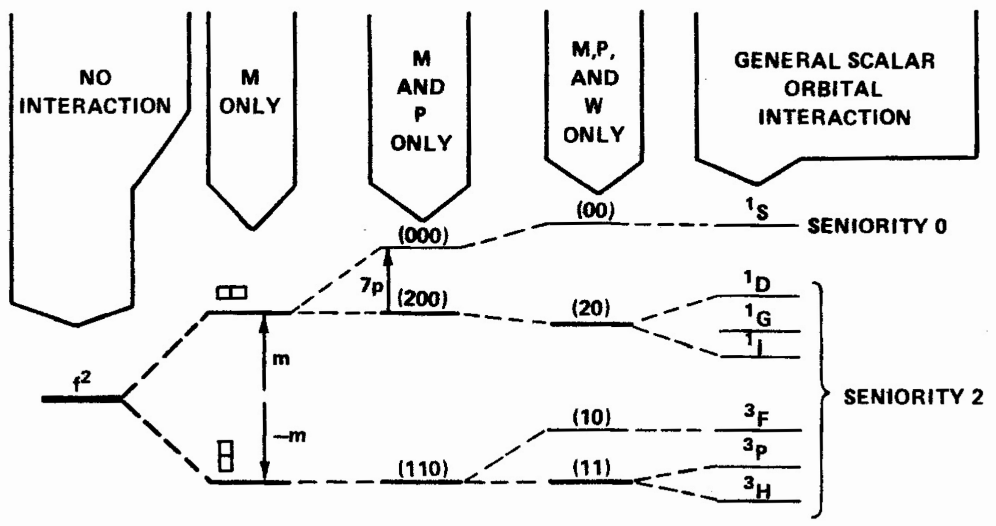
  - Calculate 2^n-pole moments
- Comparison calculation of p^3-$\mathbf{V}^k{}_q$ vs. calculation by cfp (fractional parentage)
  - Complete set of E_{jk} matrix elements for the doublet (spin-½) p^3 orbits

→ Level diagrams for pure atomic shells $p^{n=1\text{-}6}$, $d^{n=1\text{-}5}$, → $f^{n=1\text{-}7}$
- Classical Lie Groups used to label f-shell structure (a rough sketch)

Level diagrams for pure atomic shells $p^{n=1\text{-}3}$, $d^{n=1\text{-}5}$, $f^{n=1\text{-}7}$,

f^2



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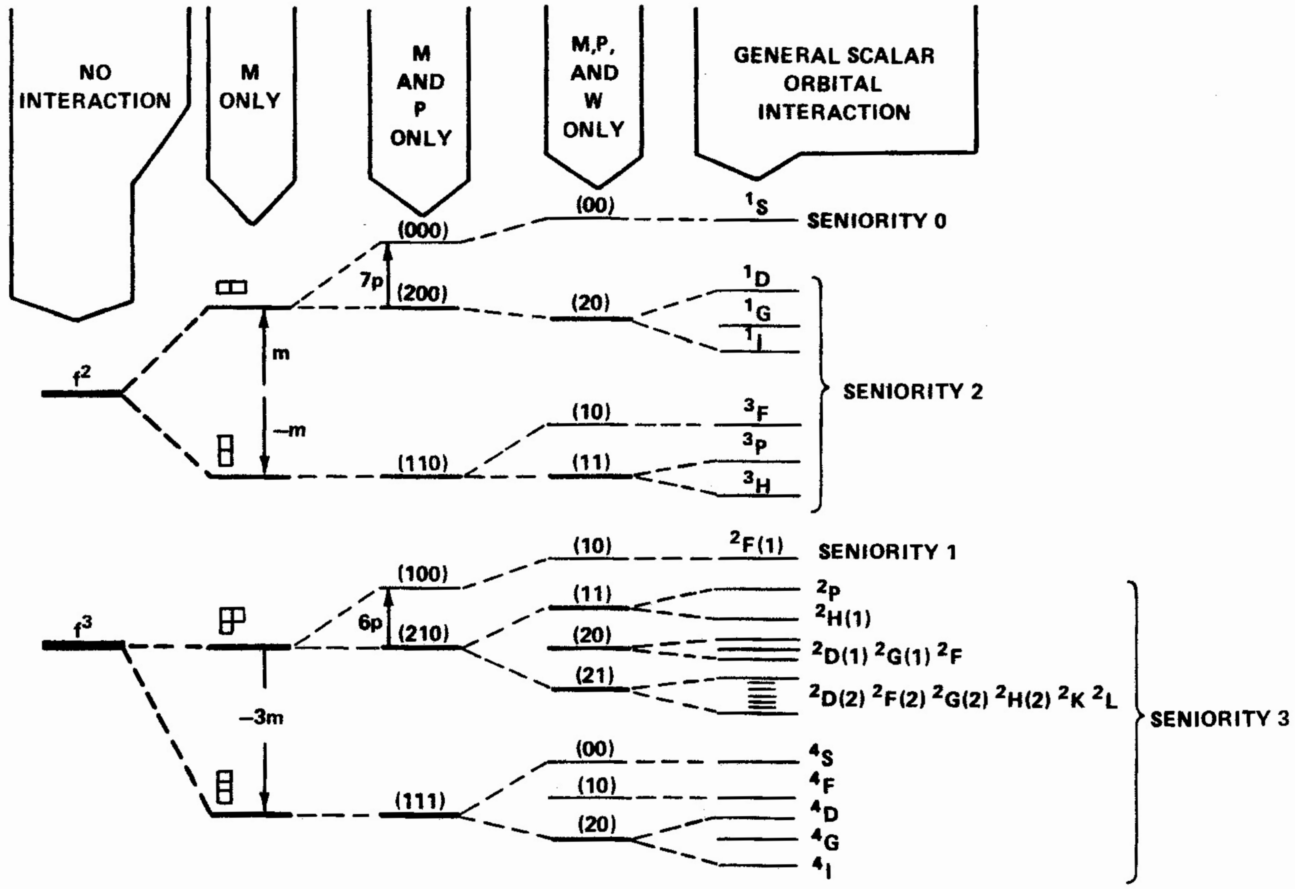
Level diagrams for pure atomic shells $p^{n=1-3}$, $d^{n=1-5}$, $f^{n=1-7}$,

f 2

f 3



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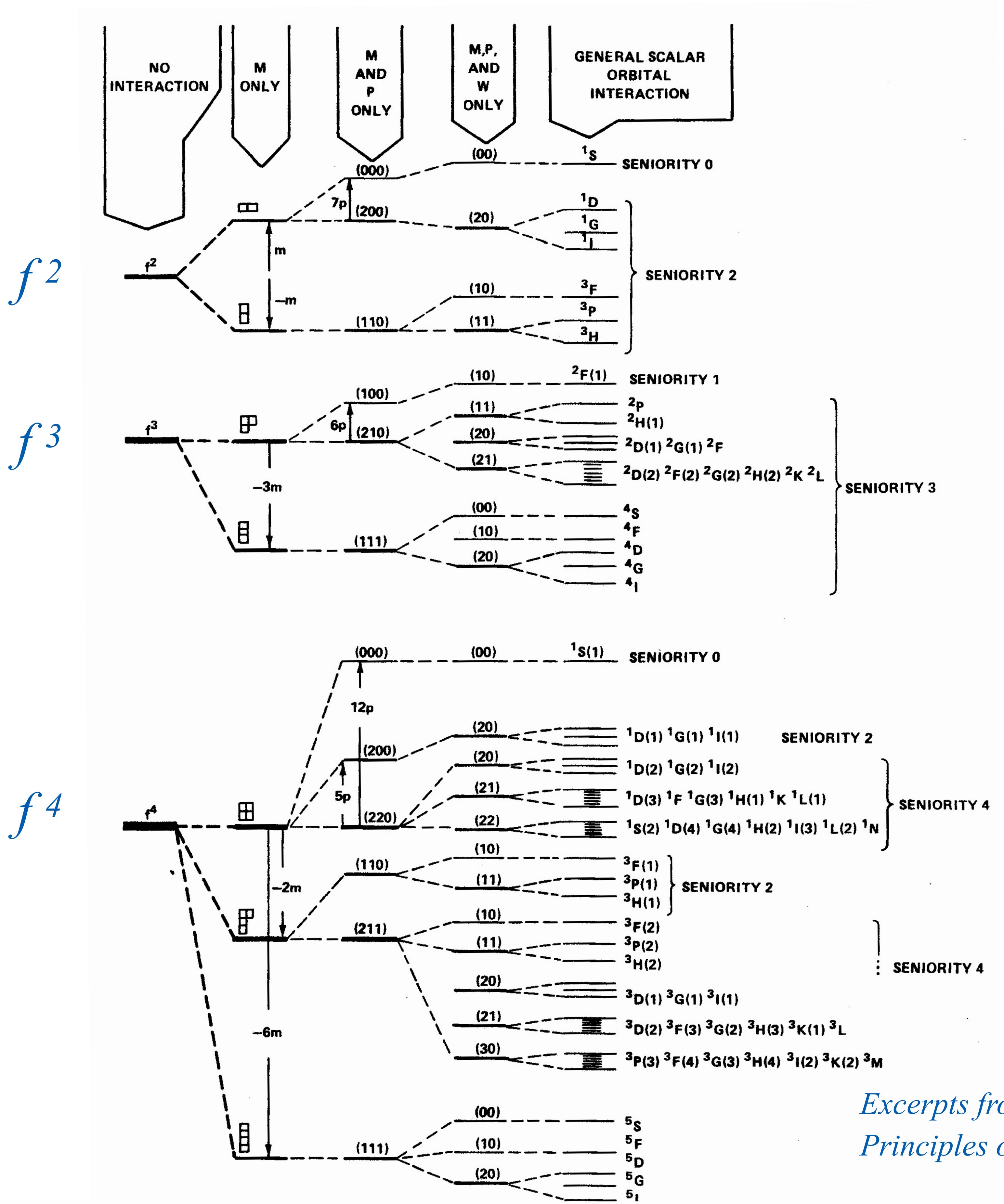

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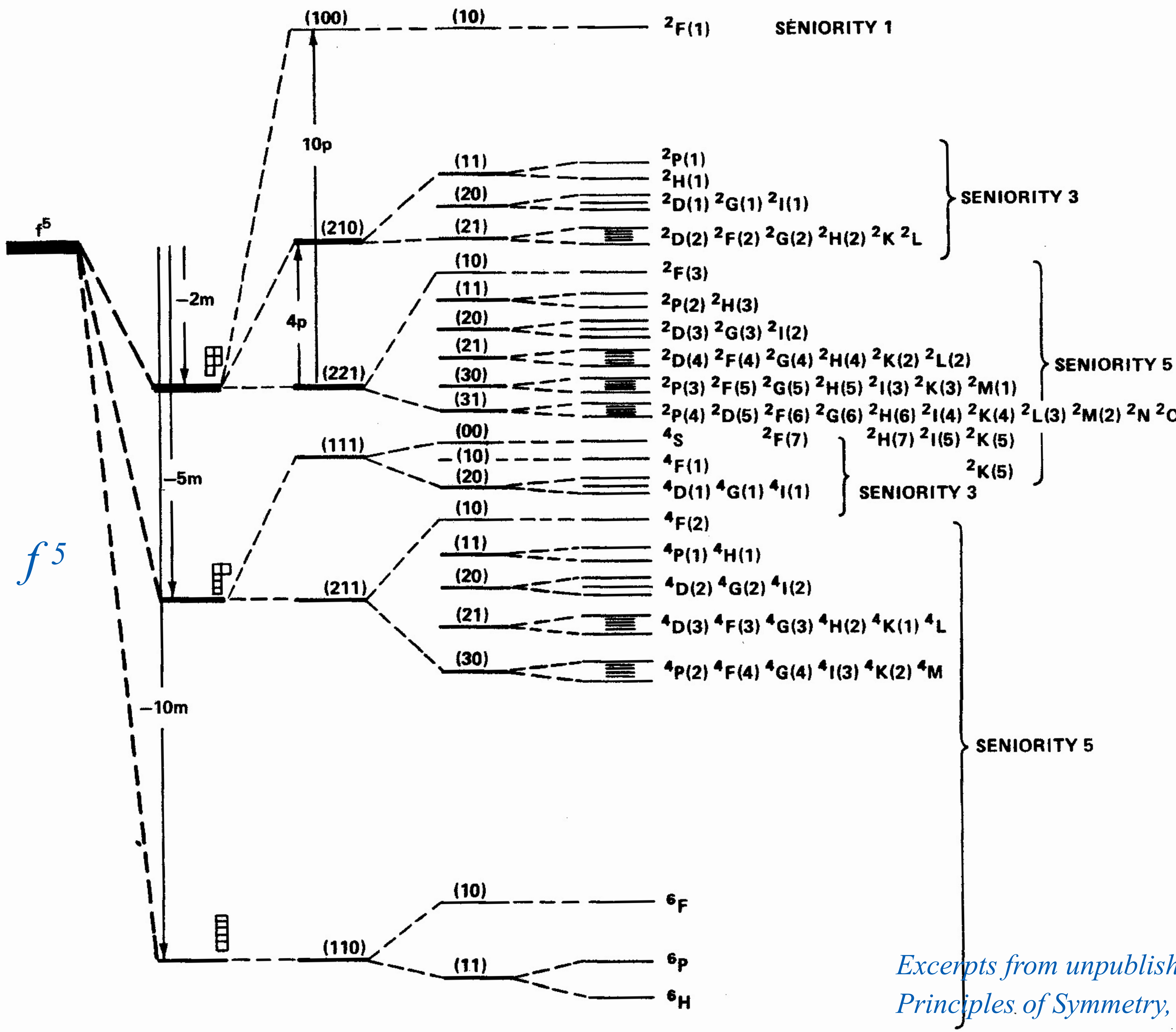

f 5

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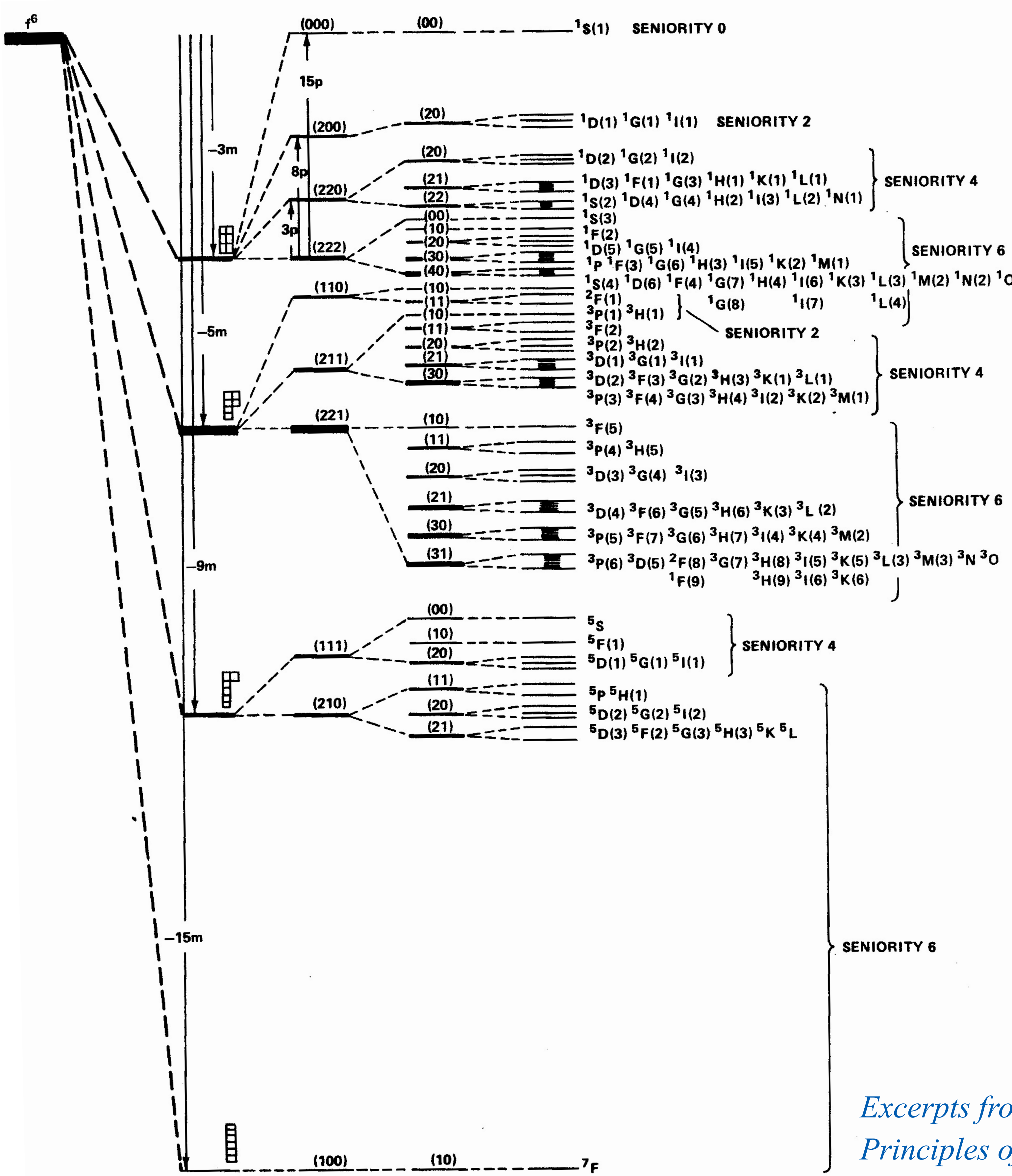
Level diagrams for pure atomic shells $p^{n=1\text{-}3}$, $d^{n=1\text{-}5}$, $f^{n=1\text{-}7}$,

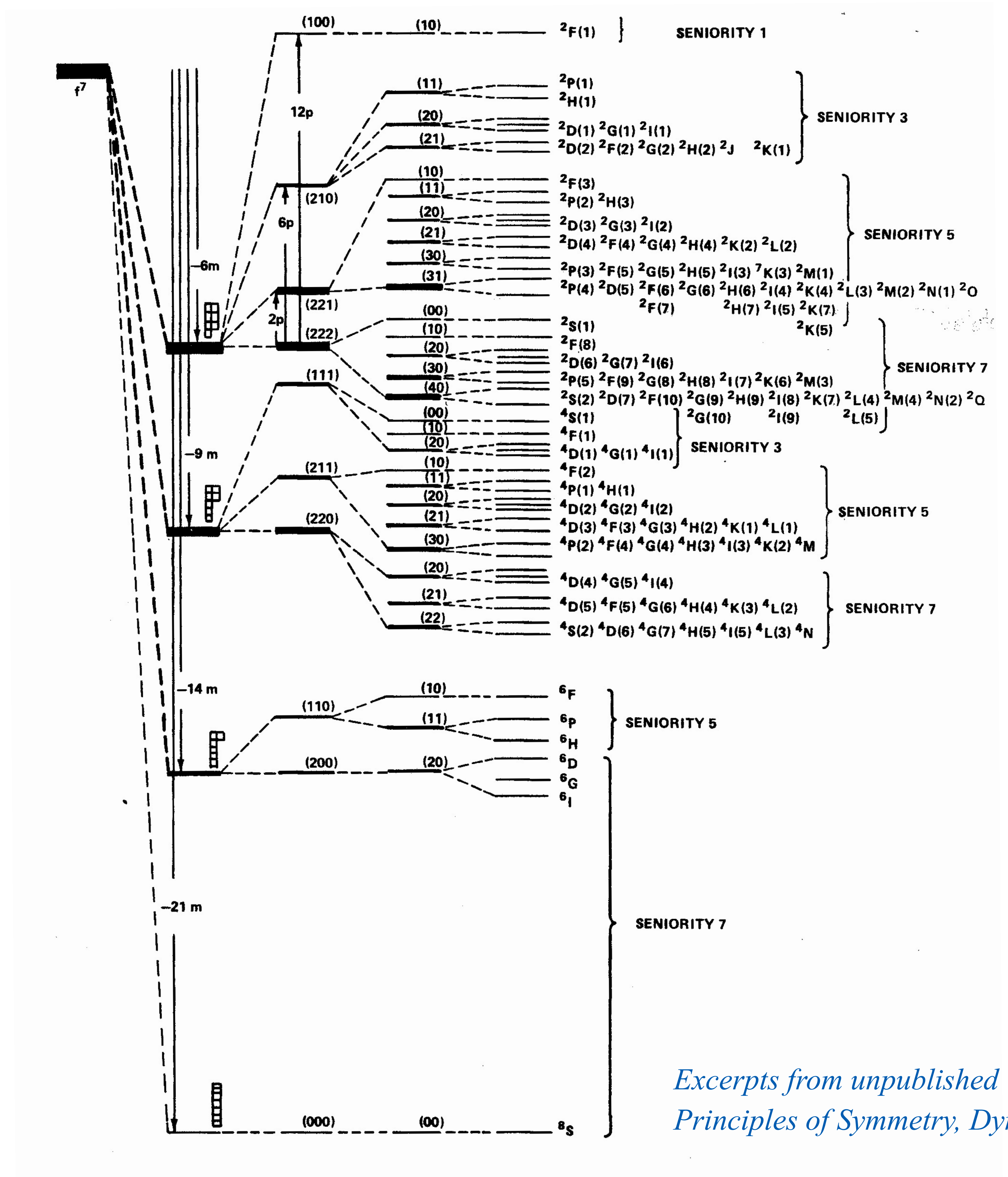
f^6



Excerpts from unpublished Ch. 9 intended for Vol II of Principles of Symmetry, Dynamics and Spectroscopy

Level diagrams for pure atomic shells $p^{n=1\text{-}3}$, $d^{n=1\text{-}5}$, $f^{n=1\text{-}7}$,

$f^{\,7}$



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Level diagrams for pure atomic shells $p^{n=1-6}$, $d^{n=1-5}$, → $f^{n=1-7}$
- → Classical Lie Groups used to label f-shell structure (a rough sketch)

Classical Lie Groups used to label f-shell structure

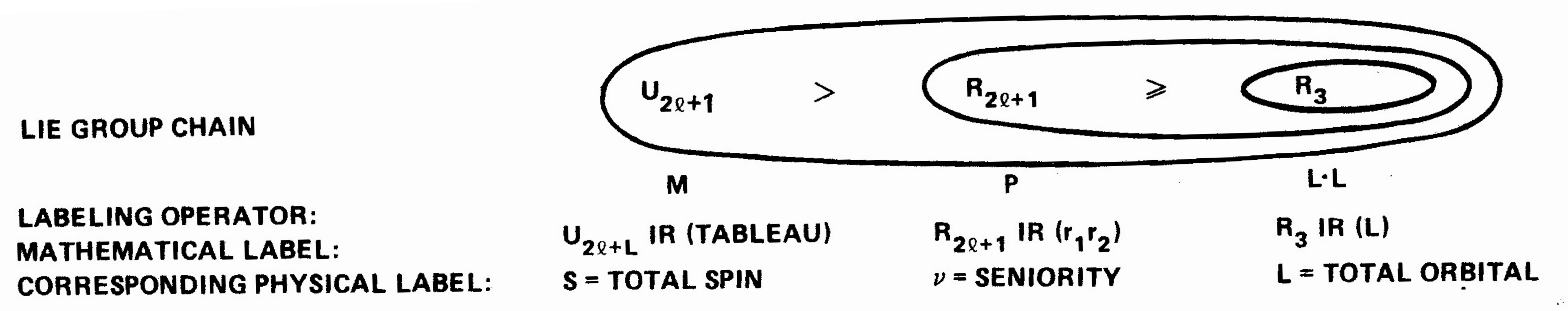

Fig 9.8.4. Labeling scheme for d-shell

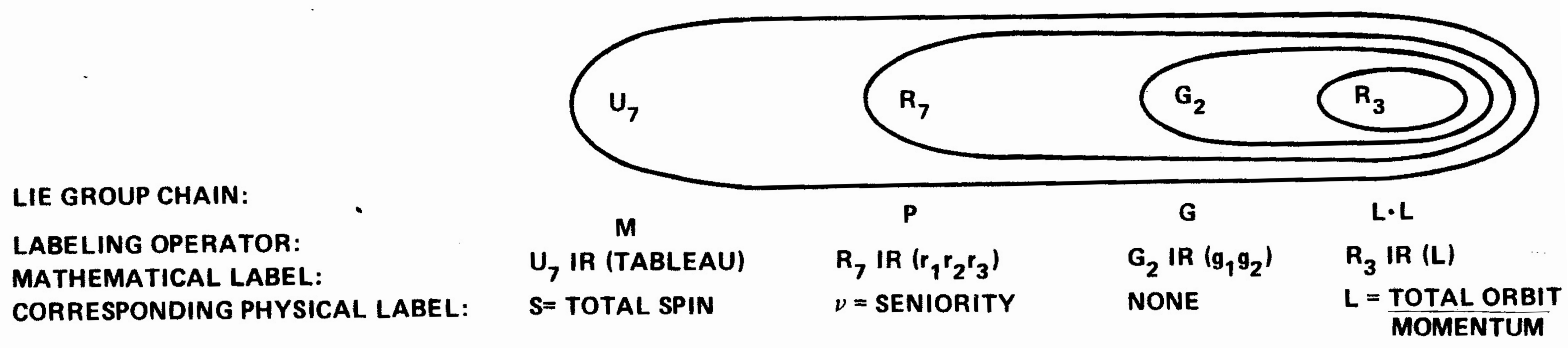

Fig 9.8.5 Labeling scheme for f-shell

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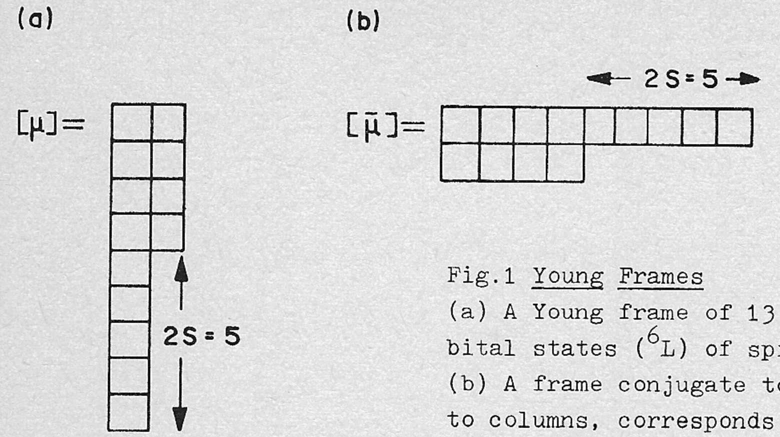

Fig.1 Young Frames

(a) A Young frame of 13 particles corresponding to all orbital states (^6L) of spin multiplicity 2S+1=6

(b) A frame conjugate to (a) obtained by converting rows to columns, corresponds to spin states of total spin S=5/2, since only 5 of the 13 spins are unpaired.(These are represented by the single row of 5 boxes.)

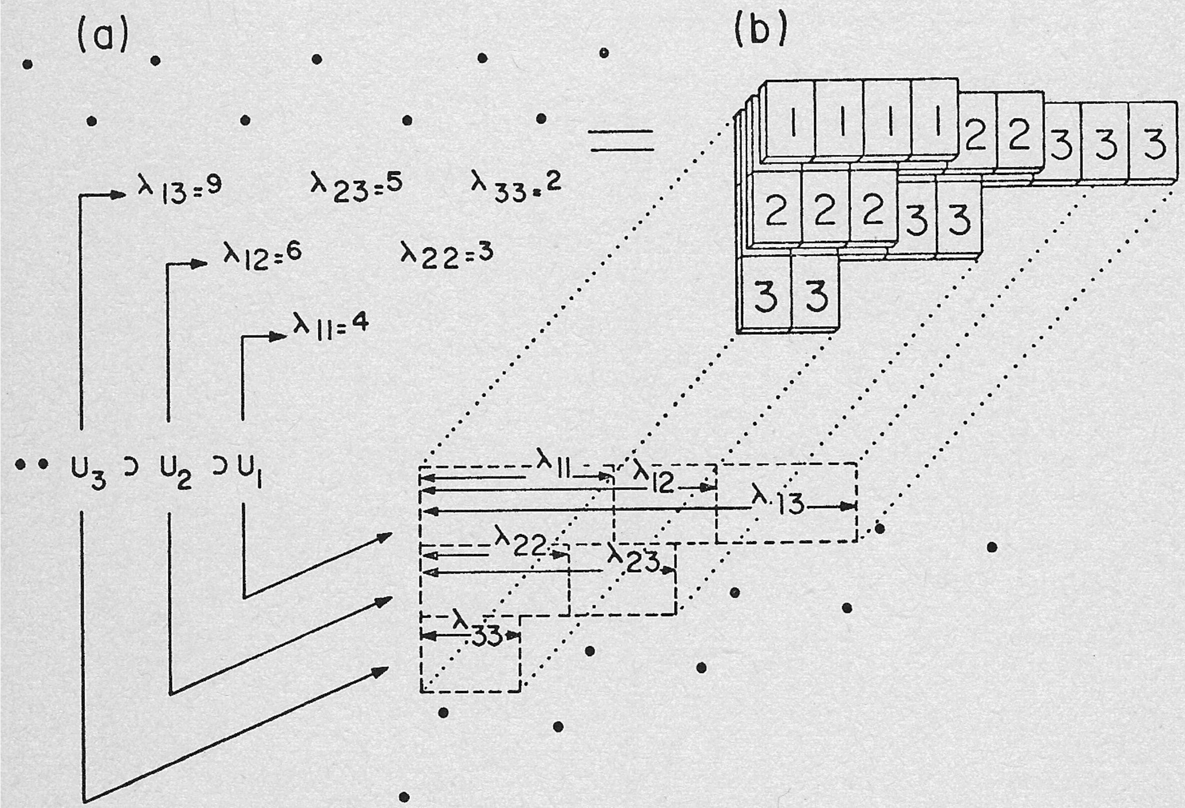

Fig.2 Unitary State Labeling

(a) Gelfand Pattern - The jth row of integers ($\lambda_{1,j}\lambda_{2,j}\cdots$ $\cdots\lambda_{j,j}$) tells to which representation of U_j the state belongs, and similarily for the j-1th row ($\lambda_{1,j-1}\lambda_{2,j-i}\cdots\lambda_{j-1,j-1}$) which labels a unique representation of U_{j-1} contained in ($\lambda_{1,j}\lambda_{2,j}\cdots\lambda_{j,j}$). In this way each state has a unique genealogy chain and labeling.

(b) Young Tableau - Tableaus are a completely equivalent but non-algebraic "picture" of the Gelfand patterns.(When labeled algebraically, it is just an up-side-down Gelfand Pattern.)

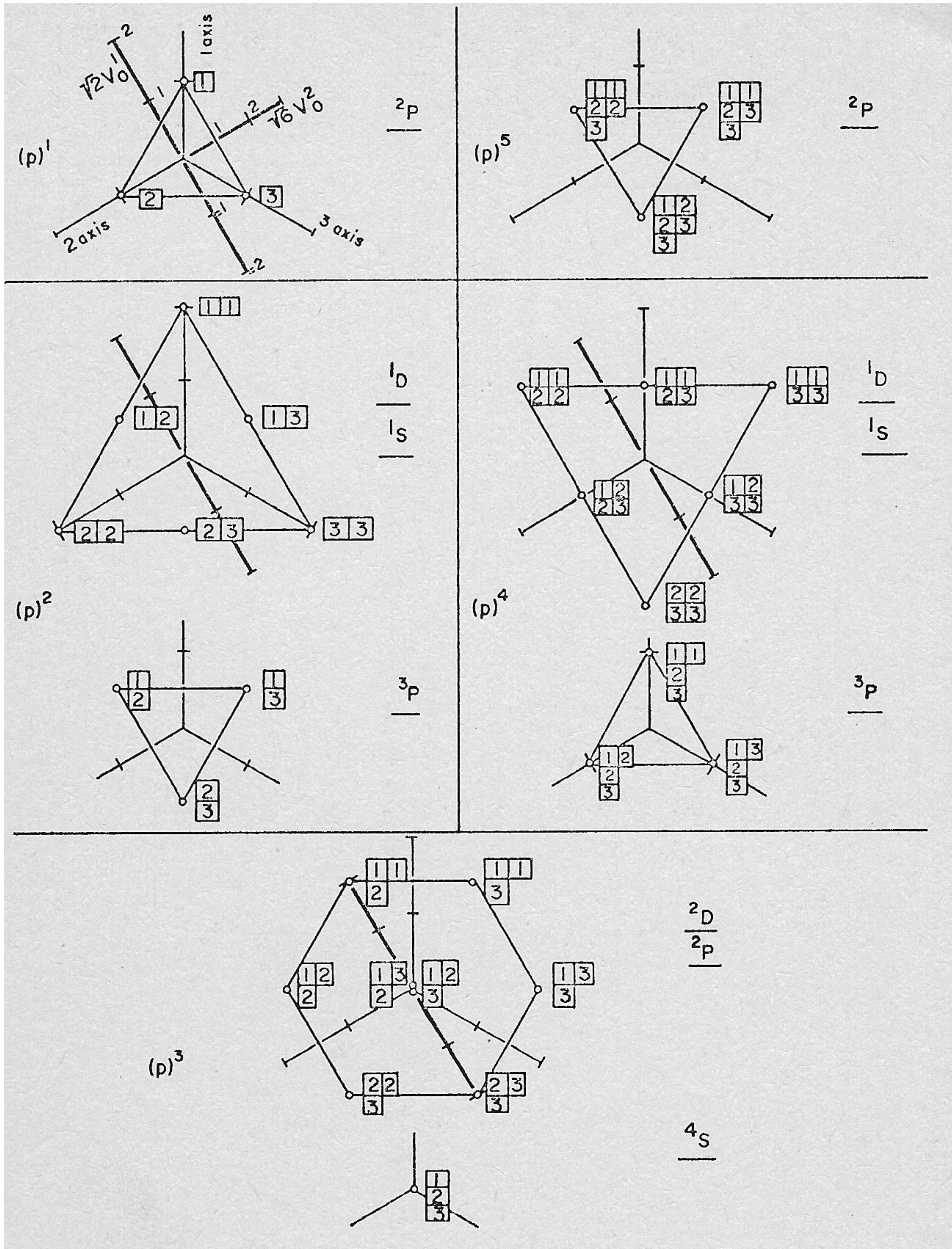

Fig.8 Weight or Moment Diagrams of Atomic $(p)^n$ States
Each tableau is located at point $(x_1\ x_2\ x_3)$ in a cartesian co-ordinate system for which x_n is the number of n's in the tableau. An alternative co-ordinate system is (v_0^2, v_0^1, v_0^0) defined by Eq.16 which gives the z-quadrupole moment, z-magnetic dipole moment, and number of particles, respectively. The last axis (v_0^0) would be pointing straight out of the figure, and each family of states lies in a plane perpendicular to it.

A Unitary Calculus for Electronic Orbitals
William G. Harter and Christopher W. Patterson
Springer-Verlag Lectures in Physics 49 1976

Alternative basis for the theory of complex spectra I
William G. Harter
Physical Review A 8 3 p2819 (1973)

Alternative basis for the theory of complex spectra II
William G. Harter and Christopher W. Patterson
Physical Review A 13 3 p1076-1082 (1976)

Alternative basis for the theory of complex spectra III
William G. Harter and Christopher W. Patterson
Physical Review A ??

$$\left|1,2,3\right\rangle \equiv \left|1\right\rangle_{particle-a} \left|2\right\rangle_{particle-b} \left|3\right\rangle_{particle-c} \equiv \left|1\right\rangle_{a} \left|2\right\rangle_{b} \left|3\right\rangle_{c}$$

Single particle p^1-orbitals: U(3) triplet $\left|p^1 \square\right\rangle$

$$e_{11}=\begin{pmatrix}1&\cdot&\cdot\\ \cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix}, e_{12}=\begin{pmatrix}\cdot&1&\cdot\\ \cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix}, e_{13}=\begin{pmatrix}\cdot&\cdot&1\\ \cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix}, e_{21}=\begin{pmatrix}\cdot&\cdot&\cdot\\ 1&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix}, \ldots e_{33}=\begin{pmatrix}\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\\ 1&\cdot&\cdot\end{pmatrix}.$$

$e_{12}e_{21}=e_{11}$ $|1\rangle\langle 2\|2\rangle\langle 1|=|1\rangle\langle 1|$

$e_{12}e_{22}=e_{12}$ $|1\rangle\langle 2\|2\rangle\langle 2|=|1\rangle\langle 2|$

Elementary matrix algebra $\vdots$

$e_{jk}e_{pq}=\delta_{pk}e_{jq}$ $|j\rangle\langle k\|p\rangle\langle q|=\delta_{pk}|j\rangle\langle q|$

General elementary operator commutation $[E_{jk}, E_{pq}]=\delta_{kp}E_{jq} - \delta_{qj}E_{pk}$
has same form as 1-particle commutation: $[e_{jk}, e_{pq}]=\delta_{kp}e_{jq} - \delta_{qj}e_{pk}$

Elementary-elementary operator commutation algebra

This applies to all of multi-particle representations of E_{jk} and to momentum operators L_x, L_y, and L_z.

Single particle p-orbit (ℓ=1) representation of L_x, L_y, and L_z

$$D^1_{mn}(L_x)=\frac{1}{\sqrt{2}}\begin{pmatrix}\cdot&1&\cdot\\ 1&\cdot&1\\ \cdot&1&\cdot\end{pmatrix},\quad D^1_{mn}(L_y)=\frac{-i}{\sqrt{2}}\begin{pmatrix}\cdot&1&\cdot\\ -1&\cdot&1\\ \cdot&-1&\cdot\end{pmatrix},\quad D^1_{mn}(L_z)=\begin{pmatrix}1&\cdot&\cdot\\ \cdot&0&\cdot\\ \cdot&\cdot&-1\end{pmatrix}$$

Elementary operator form of L_x, L_y, and L_z

$$L_x=\left(E_{12}+E_{23}+E_{21}+E_{32}\right)/\sqrt{2},\quad L_y=-i\left(E_{12}+E_{23}-E_{21}-E_{32}\right)/\sqrt{2},\quad L_z=E_{11}-E_{33}$$

…and of raise-lower operators L_+ and L_-

$$L_+=L_x+i\,L_y=\sqrt{2}\left(E_{12}+E_{23}\right),\quad L_-=L_x-i\,L_y=\sqrt{2}\left(E_{21}+E_{32}\right)=L_+^\dagger,\quad L_z=[L_+,L_-]$$

Symmetric p^2-orbitals: U(3) sextet $\left|p^2\ \boxed{}\boxed{}\right\rangle$

Elementary creation-destruction $a_j\bar{a}_k$ pairs give the [2,0] sextet states $\left\{\left|\boxed{1}\boxed{1}\right\rangle,\left|\boxed{1}\boxed{2}\right\rangle,\left|\boxed{1}\boxed{3}\right\rangle,\left|\boxed{2}\boxed{2}\right\rangle,\left|\boxed{2}\boxed{3}\right\rangle,\left|\boxed{3}\boxed{3}\right\rangle\right\}$

$$E_{12}\left|n_1,n_2\right\rangle = a_1\bar{a}_2\left|n_1,n_2\right\rangle = a_1\sqrt{n_2}\left|n_1,n_2-1\right\rangle = \sqrt{n_1+1}\sqrt{n_2}\left|n_1+1,n_2-1\right\rangle$$

$$E_{23}\left|n_1,n_2,n_3\right\rangle = a_2\bar{a}_3\left|n_1,n_2,n_3\right\rangle = a_2\sqrt{n_3}\left|n_1,n_2,n_3-1\right\rangle = \sqrt{n_2+1}\sqrt{n_3}\left|n_1,n_2+1,n_3-1\right\rangle$$

Apply elementary operations e_{jk} to each particle a, b, c, … in turn.

$$E_{23}\left|3_a3_b3_c\right\rangle = \left|2_a3_b3_c\right\rangle + \left|3_a2_b3_c\right\rangle + \left|3_a3_b2_c\right\rangle = \sqrt{3}\,\frac{\left|2_a3_b3_c\right\rangle + \left|3_a2_b3_c\right\rangle + \left|3_a3_b2\right\rangle}{\sqrt{3}} = \sqrt{3}\left|\boxed{2}\boxed{3}\boxed{3}\right\rangle$$

$$a_2\bar{a}_3\left|n_1=0,n_2=0,n_3=3\right\rangle = a_2\sqrt{3}\left|0,0,2\right\rangle = \sqrt{1}\sqrt{3}\left|0,1,2\right\rangle = E_{23}\left|\boxed{3}\boxed{3}\boxed{3}\right\rangle = \sqrt{3}\left|\boxed{2}\boxed{3}\boxed{3}\right\rangle$$

The e_{jk} procedure shows $a=\mathbf{a}^\dagger$ or $\bar{a}=\mathbf{a}$ factors $\sqrt{n_k}$ or $\sqrt{n_k+1}$ arise by adjusting norms.

$$E_{23}\frac{\left|2_a3_b3_c3_d\right\rangle + \left|3_a2_b3_c3_d\right\rangle + \left|3_a3_b2_c3_d\right\rangle + \left|3_a3_b3_c2_d\right\rangle}{2} = E_{23}\left|\boxed{2}\boxed{3}\boxed{3}\boxed{3}\right\rangle$$

$$= \frac{\left|2_a2_b3_c3_d\right\rangle + \left|2_a2_b3_c3_d\right\rangle + \left|2_a3_b2_c3_d\right\rangle + \left|2_a3_b3_c2_d\right\rangle}{2} \qquad = \sqrt{6}\left[\frac{\left|2_a2_b3_c3_d\right\rangle + \left|2_a3_b2_c3_d\right\rangle + \left|2_a3_b3_c2_d\right\rangle}{\sqrt{6}}\right.$$

$$+ \frac{\left|2_a3_b2_c3_d\right\rangle + \left|3_a2_b2_c3_d\right\rangle + \left|3_a2_b2_c3_d\right\rangle + \left|3_a2_b3_c2_d\right\rangle}{2} \qquad \left. + \frac{\left|3_a2_b2_c3_d\right\rangle + \left|3_a2_b3_c2_d\right\rangle + \left|3_a3_b2_c2_d\right\rangle}{\sqrt{6}}\right]$$

$$+ \frac{\left|2_a3_b3_c2_d\right\rangle + \left|3_a2_b3_c2_d\right\rangle + \left|3_a3_b2_c2_d\right\rangle + \left|3_a3_b2_c2_d\right\rangle}{2} \qquad = \sqrt{6}\left|\boxed{2}\boxed{2}\boxed{3}\boxed{3}\right\rangle$$

$$a_2\bar{a}_3\left|n_1=0,n_2=0,n_3=3\right\rangle = a_2\sqrt{3}\left|0,0,2\right\rangle = \sqrt{1}\sqrt{3}\left|0,1,2\right\rangle = E_{23}\left|\boxed{3}\boxed{3}\boxed{3}\right\rangle = \sqrt{3}\left|\boxed{2}\boxed{3}\boxed{3}\right\rangle$$