AMOP reference links on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

U(2)~O(3)⊃O_h Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for O(3)⊃O_h symmetry breaking

Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure

- *Kronecker product states and operators*
- *Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$*
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Higher-J product states: (J=1)⊗(J=1)=2⊕1⊕0 case

- *Effect of Pauli-Fermi-Dirac symmetry*
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  - *LS to jj Level corralations*
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- *Intro to U(2) Young Tableaus*
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U(2) and U(3) tensor expansion of H operator

- *Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors*
- *Tensor operators for spin-1 states: U(3) generalization of Pauli spinors*
  - *4th rank tensor example with exact splitting of d-orbital*
  - *6th rank tensor example with exact splitting of f-orbital*

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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electron-proton spin-spin interaction gives a simple example of *hyperfine* spectra

Ket-kets for spin-up and spin-dn states and column matrix representations..

$$\left|\uparrow\right\rangle\left|\uparrow\right\rangle = \left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{electron}, \left|\uparrow\right\rangle\left|\downarrow\right\rangle = \left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{electron}, \left|\downarrow\right\rangle\left|\uparrow\right\rangle = \left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{electron}, \left|\downarrow\right\rangle\left|\downarrow\right\rangle = \left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{electron}$$

$$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad \begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

Same spin-1/2 representation applies to either proton or electron kets.

$$D^{1/2}(\alpha\beta\gamma)=\begin{pmatrix}D^{1/2}_{+1/2,+1/2} & D^{1/2}_{+1/2,-1/2}\\ D^{1/2}_{-1/2,+1/2} & D^{1/2}_{-1/2,-1/2}\end{pmatrix}=\begin{pmatrix}e^{\frac{-i(\alpha+\gamma)}{2}}\cos\frac{\beta}{2} & -e^{\frac{-i(\alpha-\gamma)}{2}}\sin\frac{\beta}{2}\\ e^{\frac{i(\alpha-\gamma)}{2}}\sin\frac{\beta}{2} & e^{\frac{i(\alpha+\gamma)}{2}}\cos\frac{\beta}{2}\end{pmatrix}$$

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Kronecker product $D^{\frac{1}{2}}\otimes D^{\frac{1}{2}}$

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(for $\alpha=0=\gamma$)

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$$\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}&0\\0&0&0&1\\0&\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}&0\end{pmatrix}\cdot\begin{pmatrix}
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\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\
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$$\left|\uparrow\right\rangle\left|\uparrow\right\rangle=\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{electron},\left|\uparrow\right\rangle\left|\downarrow\right\rangle=\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{electron},\left|\downarrow\right\rangle\left|\uparrow\right\rangle=\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\end{matrix}\right\rangle^{electron},\left|\downarrow\right\rangle\left|\downarrow\right\rangle=\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{proton}\left|\begin{matrix}\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right\rangle^{electron}$$

$$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\quad\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\quad\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

Same spin-1/2 representation applies to either proton or electron kets.

$$D^{1/2}(\alpha\beta\gamma)=\begin{pmatrix}D^{1/2}_{+1/2,+1/2} & D^{1/2}_{+1/2,-1/2}\\ D^{1/2}_{-1/2,+1/2} & D^{1/2}_{-1/2,-1/2}\end{pmatrix}=\begin{pmatrix}e^{\frac{-i(\alpha+\gamma)}{2}}\cos\frac{\beta}{2} & -e^{\frac{-i(\alpha-\gamma)}{2}}\sin\frac{\beta}{2}\\ e^{\frac{i(\alpha-\gamma)}{2}}\sin\frac{\beta}{2} & e^{\frac{i(\alpha+\gamma)}{2}}\cos\frac{\beta}{2}\end{pmatrix}$$

Kronecker product $D^{\frac{1}{2}}\otimes D^{\frac{1}{2}}$

Applies to *outer product symmetry* $U(2)^{proton}\times U(2)^{electron}$ for NO interaction.

$$\begin{pmatrix}\cos\frac{\beta_p}{2} & -\sin\frac{\beta_p}{2}\\ \sin\frac{\beta_p}{2} & \cos\frac{\beta_p}{2}\end{pmatrix}\otimes\begin{pmatrix}\cos\frac{\beta_e}{2} & -\sin\frac{\beta_e}{2}\\ \sin\frac{\beta_e}{2} & \cos\frac{\beta_e}{2}\end{pmatrix}=\begin{pmatrix}\cos\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & -\cos\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & -\sin\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & \sin\frac{\beta_p}{2}\sin\frac{\beta_e}{2}\\ \cos\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & \cos\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & -\sin\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & -\sin\frac{\beta_p}{2}\cos\frac{\beta_e}{2}\\ \sin\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & -\sin\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & \cos\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & -\cos\frac{\beta_p}{2}\sin\frac{\beta_e}{2}\\ \sin\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & \sin\frac{\beta_p}{2}\cos\frac{\beta_e}{2} & \cos\frac{\beta_p}{2}\sin\frac{\beta_e}{2} & \cos\frac{\beta_p}{2}\cos\frac{\beta_e}{2}\end{pmatrix}$$

Interaction reduces symmetry:

(Only $(\alpha_e,\beta_e,\gamma_e)=(\alpha_p,\beta_p,\gamma_p)$

is allowed!

Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ *to* $U(2)^{e+p}$

$$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ 0 & 0 & 0 & 1\\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0\end{pmatrix}\cdot\begin{pmatrix}\cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2}\\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\ \sin^2\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2}\end{pmatrix}\cdot\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}}\\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}}\\ 0 & 0 & 1 & 0\end{pmatrix}$$

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Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$

$$\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}&0\\0&0&0&1\\0&\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}&0\end{pmatrix}\cdot\begin{pmatrix}\cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2}\\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\ \sin^2\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2}\end{pmatrix}\cdot\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{2}}&0&\frac{1}{\sqrt{2}}\\0&\frac{1}{\sqrt{2}}&0&\frac{-1}{\sqrt{2}}\\0&0&1&0\end{pmatrix}=\begin{pmatrix}\sin^2\frac{\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \sin^2\frac{\beta}{2} & 0\\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} & 0\\ \sin^2\frac{\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \cos^2\frac{\beta}{2} & 0\\ 0&0&0&1\end{pmatrix}=\left(\begin{array}{c|c}D^{J=1}_{(0\beta0)} & \\ \hline & D^{J=0}\end{array}\right)$$

...and "irreducible" becomes "reducible"...

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3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

U(2)~O(3)⊃O_h Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for O(3)⊃O_h symmetry breaking

Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure

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U(2) and U(3) tensor expansion of H operator

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- *Tensor operators for spin-1 states: U(3) generalization of Pauli spinors*
  - *4th rank tensor example with exact splitting of d-orbital*
  - *6th rank tensor example with exact splitting of f-orbital*

Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix} \cdot \begin{pmatrix} \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2} \\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} \\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} \\ \sin^2\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} \sin^2\frac{\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \sin^2\frac{\beta}{2} & 0 \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} & 0 \\ \sin^2\frac{\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \cos^2\frac{\beta}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|c} D^{J=1}_{(0\beta 0)} & \\ \hline & D^{J=0} \end{array}\right)$$

Clebsch-Gordan coefficients(CGC)

$$C^{\frac{1}{2}\ \frac{1}{2}\ J}_{m_p\ m_e\ M} \equiv \left\langle \begin{matrix} \frac{1}{2} & \frac{1}{2} \\ m_p & m_e \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right\rangle$$

reduce $D^{1/2}\otimes D^{1/2}$ to $D^{1}\oplus D^{0}$

$\frac{1}{2}\otimes\frac{1}{2}$	$J=1$ $M=1$	1 0	1 -1	0 0
$\frac{1}{2},\frac{1}{2}$	1	0	0	0
$\frac{1}{2},\frac{-1}{2}$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$\frac{-1}{2},\frac{1}{2}$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{-1}{\sqrt{2}}$
$\frac{-1}{2},\frac{-1}{2}$	0	0	1	0

$$= \left\langle C^{\frac{1}{2}\ \frac{1}{2}}_{m_p\ m_e} \middle| \begin{matrix} J \\ M \end{matrix} \right\rangle$$

$$\sum_{m_1 m_1'} \sum_{m_2 m_2'} C^{\frac{1}{2}\ \frac{1}{2}\ J}_{m_1\ m_1'\ M} D^{\frac{1}{2}}_{m_1 m_2} D^{\frac{1}{2}}_{m_1' m_2'} C^{\frac{1}{2}\ \frac{1}{2}\ J'}_{m_2\ m_2'\ M'} = \delta^{JJ'} D^{J}_{M\,M'}$$

Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$

$$\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}&0\\0&0&0&1\\0&\frac{1}{\sqrt{2}}&\frac{-1}{\sqrt{2}}&0\end{pmatrix}\cdot\begin{pmatrix}\cos^2\frac{\beta}{2}&-\sin\frac{\beta}{2}\cos\frac{\beta}{2}&-\sin\frac{\beta}{2}\cos\frac{\beta}{2}&\sin^2\frac{\beta}{2}\\\sin\frac{\beta}{2}\cos\frac{\beta}{2}&\cos^2\frac{\beta}{2}&-\sin^2\frac{\beta}{2}&-\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\\sin\frac{\beta}{2}\cos\frac{\beta}{2}&-\sin^2\frac{\beta}{2}&\cos^2\frac{\beta}{2}&-\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\\sin^2\frac{\beta}{2}&\sin\frac{\beta}{2}\cos\frac{\beta}{2}&\sin\frac{\beta}{2}\cos\frac{\beta}{2}&\cos^2\frac{\beta}{2}\end{pmatrix}\cdot\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{2}}&0&\frac{1}{\sqrt{2}}\\0&\frac{1}{\sqrt{2}}&0&\frac{-1}{\sqrt{2}}\\0&0&1&0\end{pmatrix}=\begin{pmatrix}\sin^2\frac{\beta}{2}&\frac{-\sin\beta}{\sqrt{2}}&\sin^2\frac{\beta}{2}&0\\\frac{\sin\beta}{\sqrt{2}}&\cos\beta&\frac{-\sin\beta}{\sqrt{2}}&0\\\sin^2\frac{\beta}{2}&\frac{\sin\beta}{\sqrt{2}}&\cos^2\frac{\beta}{2}&0\\0&0&0&1\end{pmatrix}=\left(\begin{array}{c|c}D^{J=1}_{(0\beta0)}&\\\hline&D^{J=0}\end{array}\right)$$

$$\begin{array}{c|ccc|c}\frac{1}{2}\otimes\frac{1}{2}&J=1&1&1&0\\&M=1&0&-1&0\\\hline\frac{1}{2},\frac{1}{2}&1&0&0&0\\\frac{1}{2},\frac{-1}{2}&0&\frac{1}{\sqrt{2}}&0&\frac{1}{\sqrt{2}}\\\frac{-1}{2},\frac{1}{2}&0&\frac{1}{\sqrt{2}}&0&\frac{-1}{\sqrt{2}}\\\frac{-1}{2},\frac{-1}{2}&0&0&1&0\\\hline\end{array}=\left\langle C^{\frac{1}{2}\;\frac{1}{2}}_{m_p\;m_e}\middle|\begin{matrix}J\\M\end{matrix}\right\rangle$$

Clebsch-Gordan coefficients(CGC)

$$C^{\frac{1}{2}\;\frac{1}{2}\;J}_{m_p\;m_e\;M}\equiv\left\langle\begin{array}{cc|c}\frac{1}{2}&\frac{1}{2}&J\\m_p&m_e&M\end{array}\right\rangle$$

reduce $D^{1/2}\otimes D^{1/2}$ to $D^{1}\oplus D^{0}$

$$\sum_{m_1m_1'}\sum_{m_2m_2'}C^{\frac{1}{2}\;\frac{1}{2}\;J}_{m_1\;m_1'\;M}D^{\frac{1}{2}}_{m_1m_2}D^{\frac{1}{2}}_{m_1'm_2'}C^{\frac{1}{2}\;\frac{1}{2}\;J'}_{m_2\;m_2'\;M'}=\delta^{JJ'}D^{J}_{M\,M'}$$

$$\left|\begin{matrix}J\\M\end{matrix}^{(1/2\otimes1/2)}\right\rangle=\sum_{m_1,m_2}C^{1/2\;1/2\;J}_{m_1\;\;m_2\;\;M}\left|\begin{matrix}1/2\\m_1\end{matrix}\right\rangle\left|\begin{matrix}1/2\\m_2\end{matrix}\right\rangle$$

Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt2} & \frac{1}{\sqrt2} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & 0 \end{pmatrix} \cdot \begin{pmatrix} \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2} \\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} \\ \sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\sin^2\frac{\beta}{2} & \cos^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2} \\ \sin^2\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt2} & 0 & \frac{1}{\sqrt2} \\ 0 & \frac{1}{\sqrt2} & 0 & \frac{-1}{\sqrt2} \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} \sin^2\frac{\beta}{2} & \frac{-\sin\beta}{\sqrt2} & \sin^2\frac{\beta}{2} & 0 \\ \frac{\sin\beta}{\sqrt2} & \cos\beta & \frac{-\sin\beta}{\sqrt2} & 0 \\ \sin^2\frac{\beta}{2} & \frac{\sin\beta}{\sqrt2} & \cos^2\frac{\beta}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|c} D^{J=1}_{(0\beta0)} & \\ \hline & D^{J=0} \end{array}\right)$$

Clebsch-Gordan coefficients(CGC)

$$C^{\frac12\;\frac12\;J}_{m_p\;m_e\;M} \equiv \left\langle \begin{matrix} \frac12 & \frac12 \\ m_p & m_e \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right\rangle$$

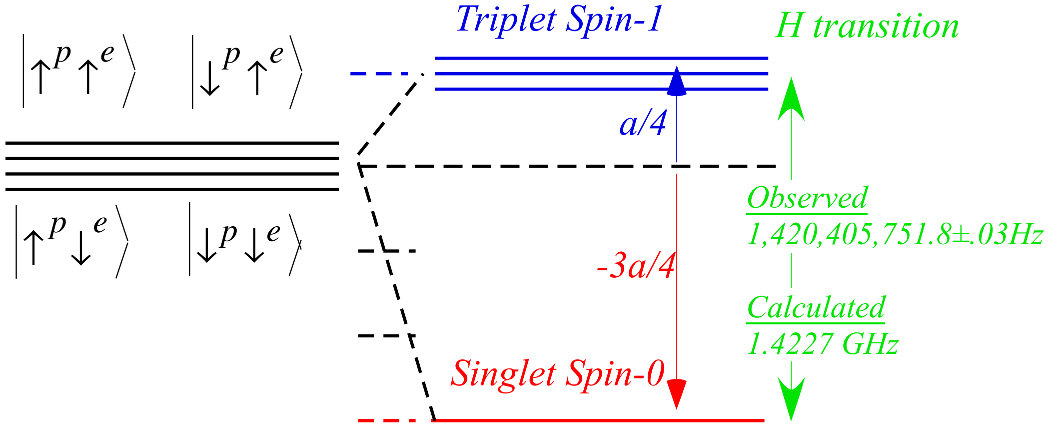
reduce $D^{1/2}\otimes D^{1/2}$ to $D^{1}\oplus D^{0}$

$$\begin{array}{c|ccc|c} \frac12\otimes\frac12 & J{=}1 & 1 & 1 & 0 \\ & M{=}1 & 0 & -1 & 0 \\ \hline \frac12,\frac12 & 1 & 0 & 0 & 0 \\ \frac12,\frac{-1}{2} & 0 & \frac{1}{\sqrt2} & 0 & \frac{1}{\sqrt2} \\ \frac{-1}{2},\frac12 & 0 & \frac{1}{\sqrt2} & 0 & \frac{-1}{\sqrt2} \\ \frac{-1}{2},\frac{-1}{2} & 0 & 0 & 1 & 0 \\ \hline \end{array} = \left\langle C^{\frac12\;\frac12}_{m_p\;m_e} \middle| \begin{matrix} J \\ M \end{matrix} \right\rangle$$

$$\sum_{m_1m_1'}\sum_{m_2m_2'} C^{\frac12\;\frac12\;J}_{m_1\;m_1'\;M}\, D^{\frac12}_{m_1m_2}\, D^{\frac12}_{m_1'm_2'}\, C^{\frac12\;\frac12\;J'}_{m_2\;m_2'\;M'} = \delta^{JJ'} D^{J}_{M\,M'}$$

$$\left(\frac12\right)\otimes\left(\frac12\right) = (1)\oplus(0)$$

$$\left| \begin{matrix} J \\ M \end{matrix} (1/2\otimes1/2) \right\rangle = \sum_{m_1,m_2} C^{1/2\;1/2\;J}_{m_1\;\;m_2\;\;M} \left| \begin{matrix} 1/2 \\ m_1 \end{matrix} \right\rangle \left| \begin{matrix} 1/2 \\ m_2 \end{matrix} \right\rangle$$



$$\left| \begin{matrix} 1 \\ +1 \end{matrix} \right\rangle = \left|\uparrow^p\uparrow^e\right\rangle$$

$$\left| \begin{matrix} 1 \\ 0 \end{matrix} \right\rangle = \left(\left|\uparrow^p\downarrow^e\right\rangle + \left|\downarrow^p\uparrow^e\right\rangle\right)/\sqrt2$$

$$\left| \begin{matrix} 1 \\ -1 \end{matrix} \right\rangle = \left|\downarrow^p\downarrow^e\right\rangle$$

$$\left| \begin{matrix} 0 \\ 0 \end{matrix} \right\rangle = \left(\left|\uparrow^p\downarrow^e\right\rangle - \left|\downarrow^p\uparrow^e\right\rangle\right)/\sqrt2$$

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$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

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    - *4th rank tensor example with exact splitting of d-orbital*
    - *6th rank tensor example with exact splitting of f-orbital*

Hydrogen hyperfine structure: Fermi-contact interaction

Racah's trick for energy eigenvalues

$$a_{ep}\mathbf{J}^{proton}\bullet\mathbf{J}^{electron}=\frac{a_{ep}}{2}\left[\left(\mathbf{J}^{proton}+\mathbf{J}^{electron}\right)^2-\left(\mathbf{J}^{proton}\right)^2-\left(\mathbf{J}^{electron}\right)^2\right]$$

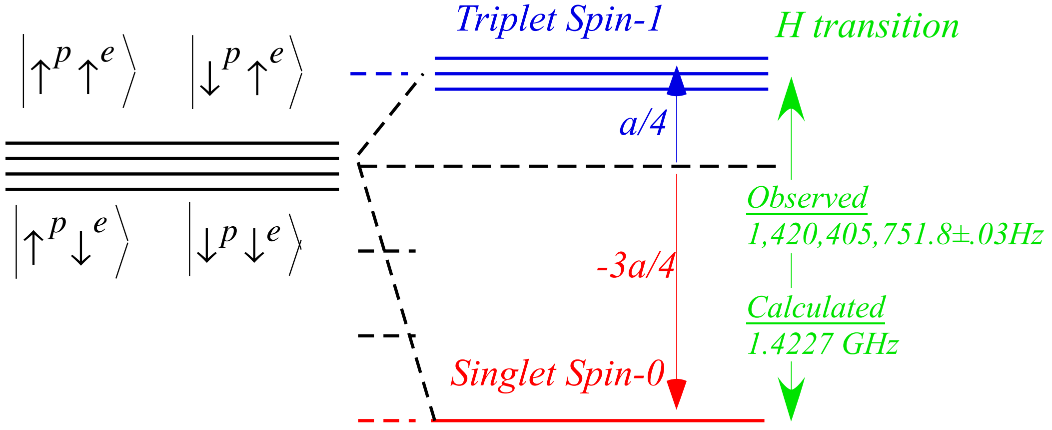
$$=\frac{a_{ep}}{2}\left[\left(\mathbf{J}^{total}\right)^2-\left(\mathbf{J}^{proton}\right)^2-\left(\mathbf{J}^{electron}\right)^2\right].$$

$$\left\langle \begin{matrix} J \\ M \end{matrix} (1/2\otimes 1/2)\right| H_{contact} \left| \begin{matrix} J \\ M \end{matrix} (1/2\otimes 1/2)\right\rangle = \frac{a_{ep}}{2}\left[J(J+1)-\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)-\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)\right]$$

$$=\begin{cases} a_{ep}/4 \ \textit{for the}\ (J=1) & \text{triplet state,} \\ -3a_{ep}/4 \ \textit{for the}\ (J=0) & \text{singlet state.} \end{cases}$$

$$\left|\begin{matrix} J \\ M \end{matrix} (1/2\otimes 1/2)\right\rangle = \sum_{m_1,m_2} C^{1/2\ 1/2\ J}_{m_1\ \ m_2\ \ M}\left|\begin{matrix} 1/2 \\ m_1 \end{matrix}\right\rangle\left|\begin{matrix} 1/2 \\ m_2 \end{matrix}\right\rangle$$

$$\left(\frac{1}{2}\right)\otimes\left(\frac{1}{2}\right)=(1)\oplus(0)$$



$$\left|\begin{matrix} 1 \\ +1 \end{matrix}\right\rangle = \left|\uparrow^p\uparrow^e\right\rangle$$

$$\left|\begin{matrix} 1 \\ 0 \end{matrix}\right\rangle = \left(\left|\uparrow^p\downarrow^e\right\rangle+\left|\downarrow^p\uparrow^e\right\rangle\right)/\sqrt{2}$$

$$\left|\begin{matrix} 1 \\ -1 \end{matrix}\right\rangle = \left|\downarrow^p\downarrow^e\right\rangle$$

$$\left|\begin{matrix} 0 \\ 0 \end{matrix}\right\rangle = \left(\left|\uparrow^p\downarrow^e\right\rangle-\left|\downarrow^p\uparrow^e\right\rangle\right)/\sqrt{2}$$

Hydrogen hyperfine structure: Fermi-contact interaction + B-field

$$H_{1s-B-field} = -a_p B_z J_z^{proton} + a_e B_z J_z^{electron} + a_{ep} \mathbf{J}^{proton} \bullet \mathbf{J}^{electron}$$

	$g-factor$	$Bohr-magneton$	$gyromagnetic\ factor$
$electron$	g_e $=2.0023$	$\mu_e = \frac{e\hbar}{2m_e}$ $=9.27401 \cdot 10^{-24} \frac{J}{T}$	$a_e = g_e \mu_e$ $=1.8570 \cdot 10^{-23} \frac{J}{T}$
$proton$	g_p $=5.585$	$\mu_p = \frac{e\hbar}{2m_p}$ $=5.05078 \cdot 10^{-27} \frac{J}{T}$	$a_p = g_p \mu_p$ $=2.8209 \cdot 10^{-26} \frac{J}{T}$

$Magnetic\ constant:\ \mu_0 / 4\pi = 10^{-7}\, N / A^2$

$Fermi-contact\ factor$
$a_{ep} = \mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} a_e a_p = 9.427 \cdot 10^{-25}\, J$
$\mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} \frac{a_e a_p}{h} = 1.4227 \cdot 10^9\, Hz$
$\mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} \frac{a_e a_p}{hc} = 4.746 m^{-1}$
$= \frac{1}{21.1} cm^{-1}$

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$$\begin{array}{c|c|c|c|c|}
 & \left|\uparrow^p\uparrow^e\right\rangle & \left|\uparrow^p\downarrow^e\right\rangle & \left|\downarrow^p\uparrow^e\right\rangle & \left|\downarrow^p\downarrow^e\right\rangle \\ \hline
\left\langle\uparrow^p\uparrow^e\right| & \frac{1}{2}\left(a_e-a_p\right)B_z & \cdot & \cdot & \cdot \\ \hline
\left\langle\uparrow^p\downarrow^e\right| & \cdot & \frac{-1}{2}\left(a_e+a_p\right)B_z & 0 & \cdot \\
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\left\langle\downarrow^p\downarrow^e\right| & \cdot & \cdot & \cdot & \frac{-1}{2}\left(a_e-a_p\right)B_z
\end{array}$$

$$\left\langle a_{ep}\mathbf{J}^{proton} \bullet \mathbf{J}^{electron}\right\rangle =$$

$$\begin{array}{c|c|c|c|c|}
 & \left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}0\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle \\ \hline
\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| & \frac{a_{ep}}{4} & \cdot & \cdot & \cdot \\ \hline
\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| & \cdot & \frac{a_{ep}}{4} & 0 & \cdot \\
\left\langle\begin{smallmatrix}0\\0\end{smallmatrix}\right| & \cdot & 0 & \frac{-3a_{ep}}{4} & \cdot \\ \hline
\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right| & \cdot & \cdot & \cdot & \frac{a_{ep}}{4}
\end{array}$$

Hydrogen hyperfine structure: Fermi-contact interaction + B-field

$$H_{1s-B-field} = -a_p B_z J_z^{proton} + a_e B_z J_z^{electron} + a_{ep}\mathbf{J}^{proton} \bullet \mathbf{J}^{electron}$$

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$= \frac{1}{21.1} cm^{-1}$

$$\begin{array}{c|ccc|c}
\frac{1}{2}\otimes\frac{1}{2} & \begin{matrix}J{=}1\\ M{=}1\end{matrix} & \begin{matrix}1\\0\end{matrix} & \begin{matrix}1\\-1\end{matrix} & \begin{matrix}0\\0\end{matrix} \\
\hline
\frac{1}{2},\frac{1}{2} & 1 & 0 & 0 & 0 \\
\frac{1}{2},\frac{-1}{2} & 0 & \frac{1}{\sqrt{2}} & & \frac{1}{\sqrt{2}} \\
\frac{-1}{2},\frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & & \frac{-1}{\sqrt{2}} \\
\frac{-1}{2},\frac{-1}{2} & 0 & 0 & 1 & 0 \\
\hline
\end{array} = \left\langle C^{\frac{1}{2}\ \frac{1}{2}}_{m_p\ m_e} \middle| \begin{matrix}J\\M\end{matrix} \right\rangle$$

$$\left\langle -a_p B_z J_z^{proton} + a_e B_z J_z^{electron} \right\rangle =$$

$$\begin{array}{c|c:c:c:c|}
 & |\uparrow^p\uparrow^e\rangle & |\uparrow^p\downarrow^e\rangle & |\downarrow^p\uparrow^e\rangle & |\downarrow^p\downarrow^e\rangle \\
\hdashline
\langle\uparrow^p\uparrow^e| & \frac{1}{2}(a_e - a_p)B_z & \cdot & \cdot & \cdot \\
\hdashline
\langle\uparrow^p\downarrow^e| & \cdot & \frac{-1}{2}(a_e + a_p)B_z & 0 & \cdot \\
\langle\downarrow^p\uparrow^e| & \cdot & 0 & \frac{1}{2}(a_e + a_p)B_z & \cdot \\
\hdashline
\langle\downarrow^p\downarrow^e| & \cdot & \cdot & \cdot & \frac{-1}{2}(a_e - a_p)B_z
\end{array}$$

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$$\begin{array}{c|c:c:c:c|}
 & \left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}0\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle \\
\hdashline
\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| & \frac{a_{ep}}{4} & \cdot & \cdot & \cdot \\
\hdashline
\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| & \cdot & \frac{a_{ep}}{4} & 0 & \cdot \\
\left\langle\begin{smallmatrix}0\\0\end{smallmatrix}\right| & \cdot & 0 & \frac{-3a_{ep}}{4} & \cdot \\
\hdashline
\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right| & \cdot & \cdot & \cdot & \frac{a_{ep}}{4}
\end{array}$$

Hydrogen hyperfine structure: Fermi-contact interaction + B-field

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$= \frac{1}{21.1} cm^{-1}$

$$\begin{array}{c|cccc}
\frac{1}{2}\otimes\frac{1}{2} & J{=}1 & 1 & 1 & 0 \\
 & M{=}1 & 0 & -1 & 0 \\
\hline
\frac{1}{2},\frac{1}{2} & 1 & 0 & 0 & 0 \\
\frac{1}{2},\frac{-1}{2} & 0 & \frac{1}{\sqrt{2}} & & \frac{1}{\sqrt{2}} \\
\frac{-1}{2},\frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & & \frac{-1}{\sqrt{2}} \\
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\hline
\end{array} = \left\langle C^{\frac{1}{2}\ \frac{1}{2}}_{m_p\ m_e} \middle| \begin{matrix} J \\ M \end{matrix} \right\rangle$$

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$$\begin{array}{c|c|c|c|c|}
 & \left|\uparrow^p\uparrow^e\right\rangle & \left|\uparrow^p\downarrow^e\right\rangle & \left|\downarrow^p\uparrow^e\right\rangle & \left|\downarrow^p\downarrow^e\right\rangle \\
\hline
\left\langle\uparrow^p\uparrow^e\right| & \frac{1}{2}\left(a_e - a_p\right)B_z & \cdot & \cdot & \cdot \\
\hline
\left\langle\uparrow^p\downarrow^e\right| & \cdot & \frac{-1}{2}\left(a_e + a_p\right)B_z & 0 & \cdot \\
\left\langle\downarrow^p\uparrow^e\right| & \cdot & 0 & \frac{1}{2}\left(a_e + a_p\right)B_z & \cdot \\
\hline
\left\langle\downarrow^p\downarrow^e\right| & \cdot & \cdot & \cdot & \frac{-1}{2}\left(a_e - a_p\right)B_z
\end{array}$$

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 & \left|\uparrow^p\uparrow^e\right\rangle & \left|\uparrow^p\downarrow^e\right\rangle & \left|\downarrow^p\uparrow^e\right\rangle & \left|\downarrow^p\downarrow^e\right\rangle \\
\hline
\left\langle\uparrow^p\uparrow^e\right| & \frac{a_{ep}}{4} & \cdot & \cdot & \cdot \\
\hline
\left\langle\uparrow^p\downarrow^e\right| & \cdot & \frac{-a_{ep}}{4} & \frac{a_{ep}}{2} & \cdot \\
\left\langle\downarrow^p\uparrow^e\right| & \cdot & \frac{a_{ep}}{2} & \frac{-a_{ep}}{4} & \cdot \\
\hline
\left\langle\downarrow^p\downarrow^e\right| & \cdot & \cdot & \cdot & \frac{a_{ep}}{4}
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 & \left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}0\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle \\
\hline
\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| & \frac{1}{2}\left(a_e - a_p\right)B_z & \cdot & \cdot & \cdot \\
\hline
\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| & \cdot & 0 & \frac{-1}{2}\left(a_e + a_p\right)B_z & \cdot \\
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\hline
\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right| & \cdot & \cdot & \cdot & \frac{-1}{2}\left(a_e - a_p\right)B_z
\end{array}$$

$$\left\langle a_{ep}\mathbf{J}^{proton}\bullet\mathbf{J}^{electron}\right\rangle =$$

$$\begin{array}{c|c|c|c|c|}
 & \left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}0\\0\end{smallmatrix}\right\rangle & \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle \\
\hline
\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| & \frac{a_{ep}}{4} & \cdot & \cdot & \cdot \\
\hline
\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| & \cdot & \frac{a_{ep}}{4} & 0 & \cdot \\
\left\langle\begin{smallmatrix}0\\0\end{smallmatrix}\right| & \cdot & 0 & \frac{-3a_{ep}}{4} & \cdot \\
\hline
\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right| & \cdot & \cdot & \cdot & \frac{a_{ep}}{4}
\end{array}$$

AMOP
reference links
on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure

Kronecker product states and operators

Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ *to* $U(2)^{e+p}$

Elementary ½ × ½ Clebsch-Gordan coefficients

Hydrogen hyperfine levels: Fermi-contact interaction, Racah's trick for energy eigenvalues

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Higher-J product states: $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$ *case*

Effect of Pauli-Fermi-Dirac symmetry

General U(2) Clebsch-Gordan-Wigner-3j coupling coefficient formula

LS to jj Level corralations

Angular momentum uncertainty cones related to 3j coefficients

Multi-spin $(1/2)^N$ *product states Magic squares*

Intro to U(2) Young Tableaus

Intro to U(3) and higher Young Tableaus and Lab-Bod or Particle-State summitry

U(2) and U(3) tensor expansion of H operator

Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors

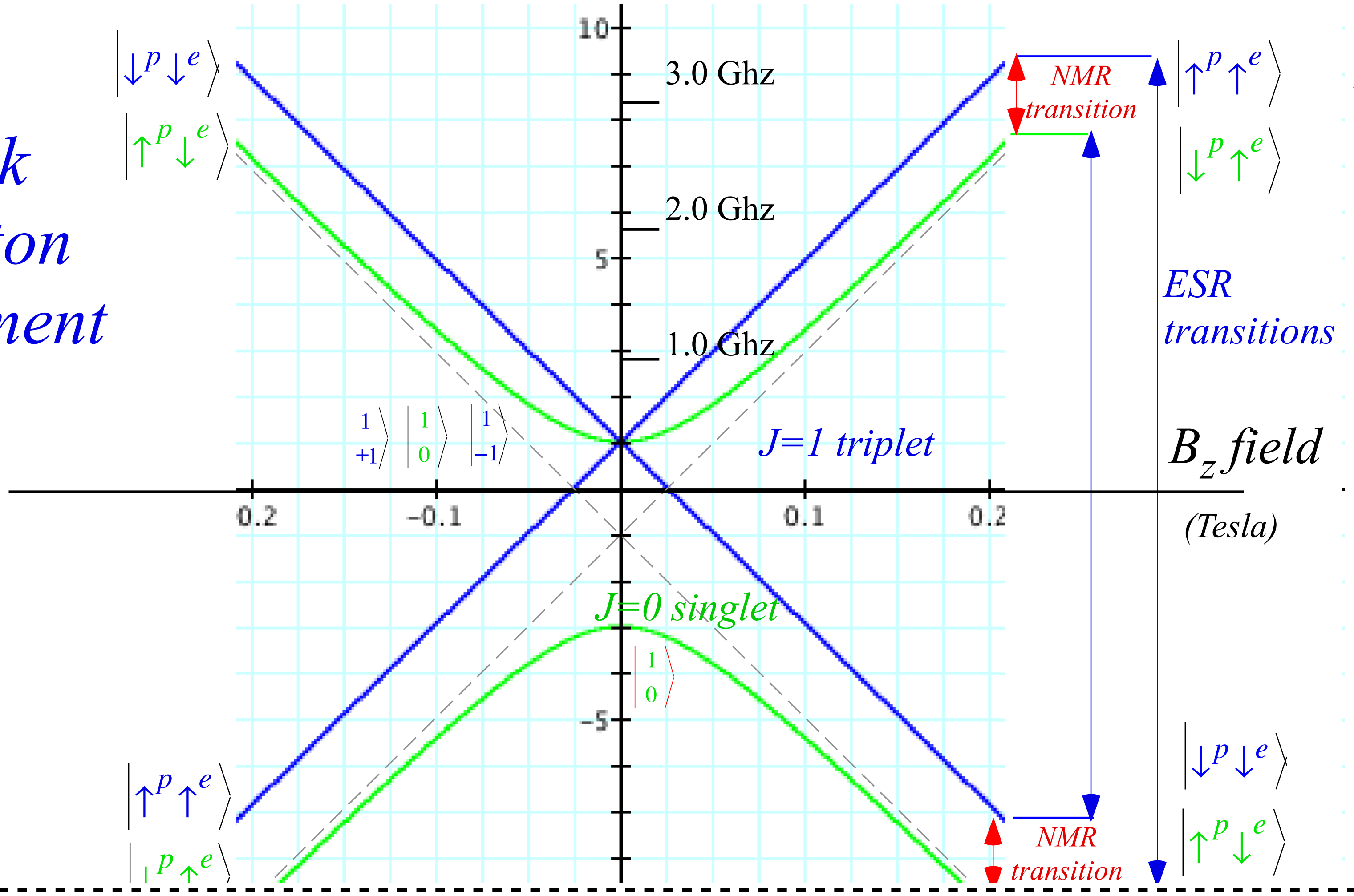
Tensor operators for spin-1 states: U(3) generalization of Pauli spinors

4th rank tensor example with exact splitting of d-orbital

6th rank tensor example with exact splitting of f-orbital

(a)
Weak
Proton
Moment

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



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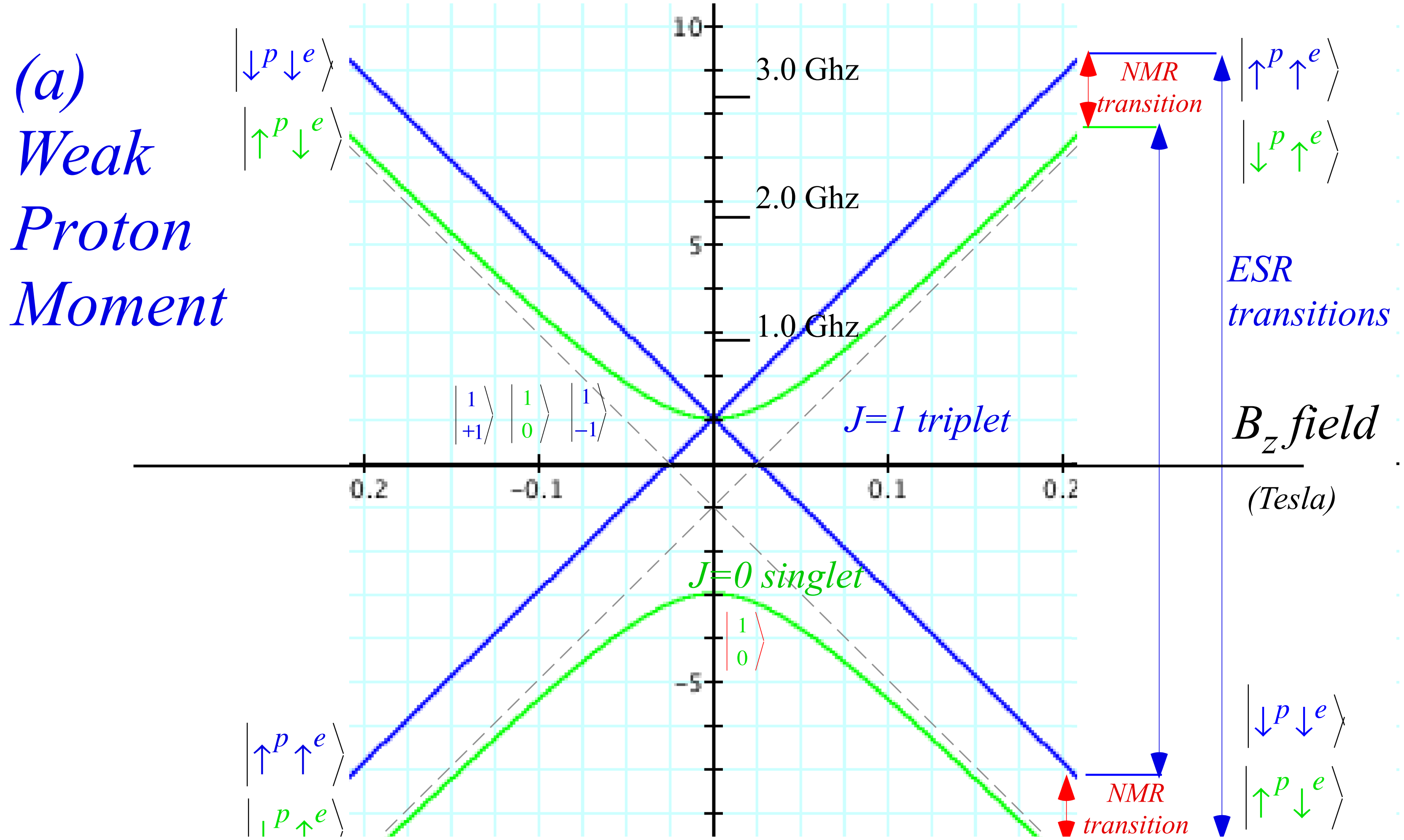
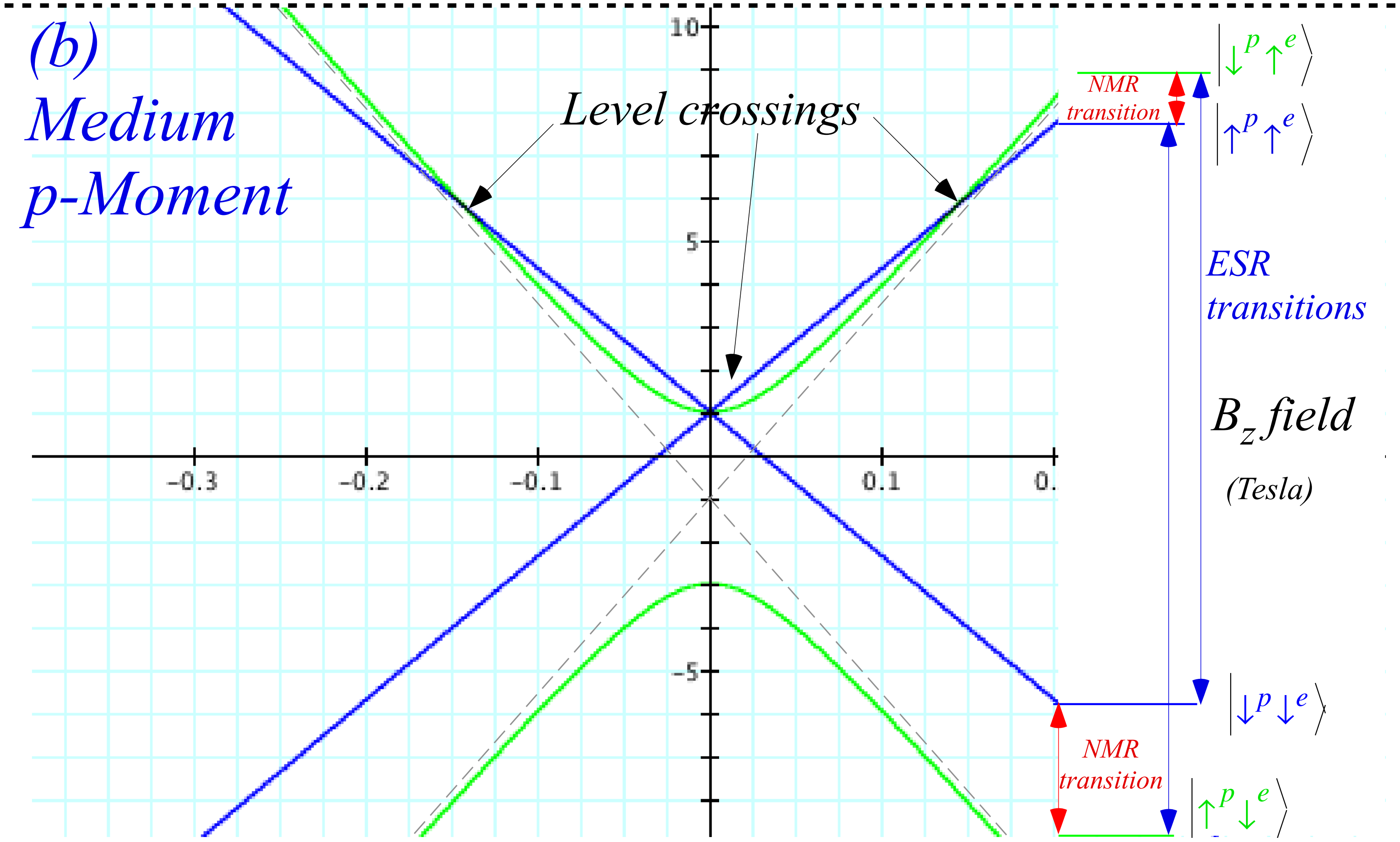
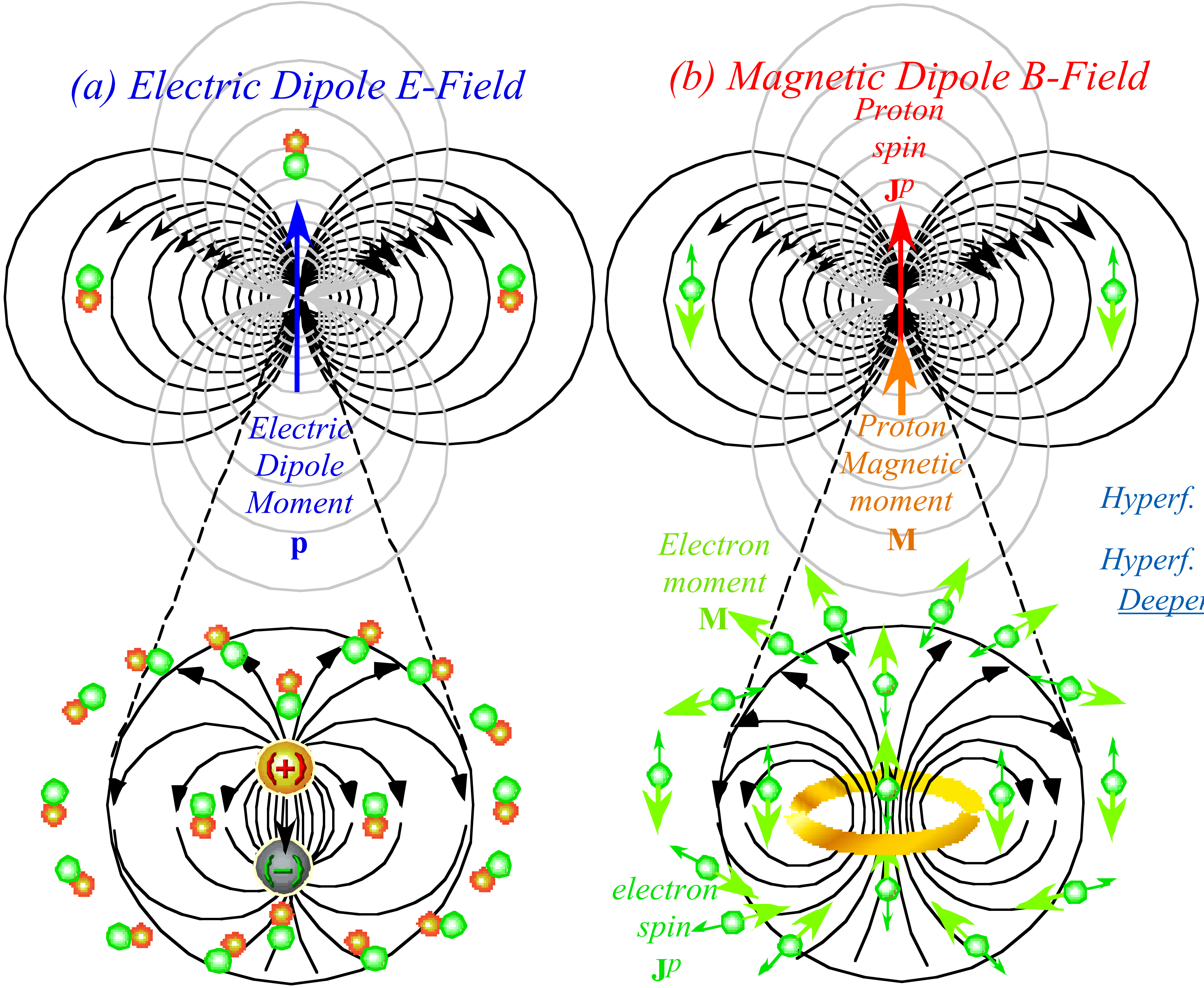




Anatomy of electric dipole vs magnetic dipole of Fermi-contact interaction + B-field



(a) Electric Dipole E-Field

(b) Magnetic Dipole B-Field

Hyperf. theory *Ch. 24 p48.*

Hyperf. theory Ch. 24 p48.

Deeper theory ends p53

$$H_{e-p-spin} = \frac{\mu_0 \left|g_e \mu_e g_p \mu_p\right|}{4\pi}\left[\frac{8\pi}{3}\delta(\mathbf{0})\mathbf{J}^e \bullet \mathbf{J}^p + \frac{\mathbf{L}^e \bullet \mathbf{J}^p}{r^3} - \frac{\mathbf{J}^e \bullet \mathbf{J}^p}{r^3} + \frac{3\left(\mathbf{J}^e \bullet \mathbf{r}\right)\left(\mathbf{J}^p \bullet \mathbf{r}\right)}{r^5}\right]$$

AMOP reference links on page 2

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Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$$\left|C^{1\ \ 1\ \ L}_{m_1 m_2 M}\right\rangle = \begin{array}{|cc|ccccc|ccc|c|} \hline & & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 0 \\ 1\quad\otimes & 1 & 2 & 1 & 0 & -1 & -2 & 1 & 0 & -1 & 0 \\ \hline 1 & 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\ 1 & -1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\ 0 & 1 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \sqrt{\frac{2}{3}} & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{3}} \\ 0 & -1 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot \\ -1 & 1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\ -1 & 0 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot \\ -1 & -1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \hline \end{array} \cdot\cdot$$

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$\left|C^{1\;\;1\;\;L}_{m_1 m_2 M}\right\rangle =$

		2	2	2	2	2	1	1	1	0
1 ⊗	1	2	1	0	−1	−2	1	0	−1	0
1	1	1	·	·	·	·	·	·	·	·
1	0	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·
1	−1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
0	1	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	·	·
0	0	·	·	$\sqrt{\frac{2}{3}}$	·	·	·	·	·	$-\frac{1}{\sqrt{3}}$
0	−1	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·
−1	1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
−1	0	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·
−1	−1	·	·	·	·	1	·	·	·	·

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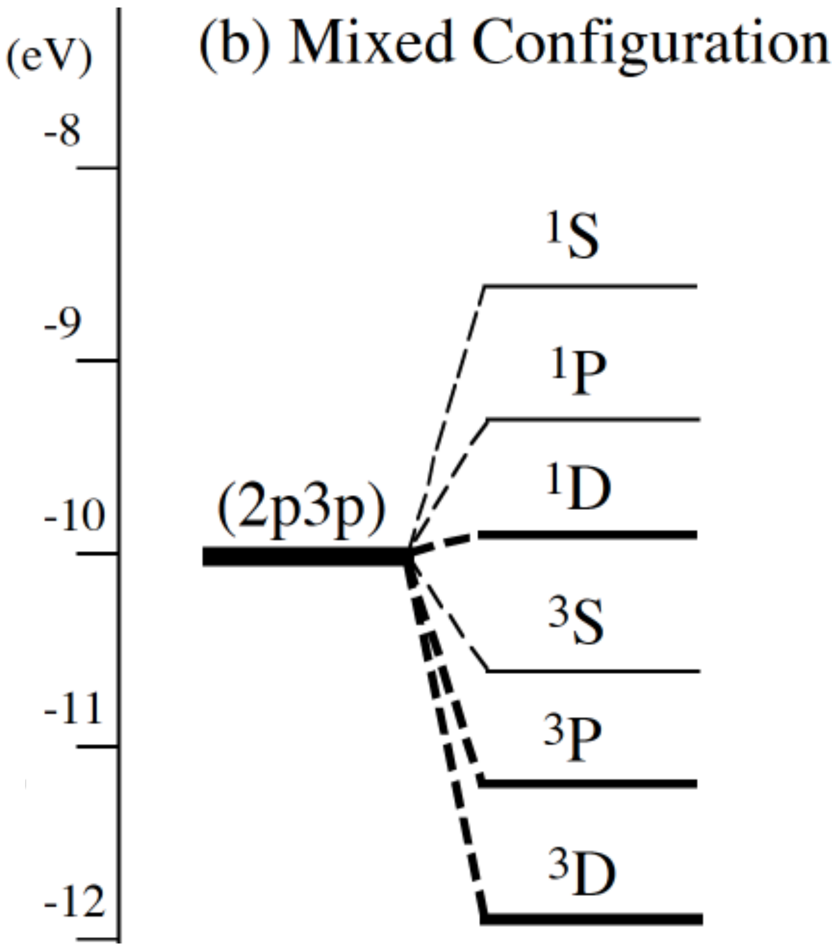

Intro 2p3p coupling
Unit 8 Ch. 24 p17.

Figure 24.1.3 *Atomic* $^{2S+1}$L *multiplet levels for two (l = 1)* p *electrons.*

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$\left|C^{1\ 1\ L}_{m_1\ m_2\ M}\right\rangle =$

		2	2	2	2	2	1	1	1	0
1 ⊗	1	2	1	0	−1	−2	1	0	−1	0
1	1	1	·	·	·	·	·	·	·	·
1	0	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·
1	−1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
0	1	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	·	·
0	0	·	·	$\sqrt{\frac{2}{3}}$	·	·	·	·	·	$-\frac{1}{\sqrt{3}}$
0	−1	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·
−1	1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
−1	0	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·
−1	−1	·	·	·	·	1	·	·	·	·

‥

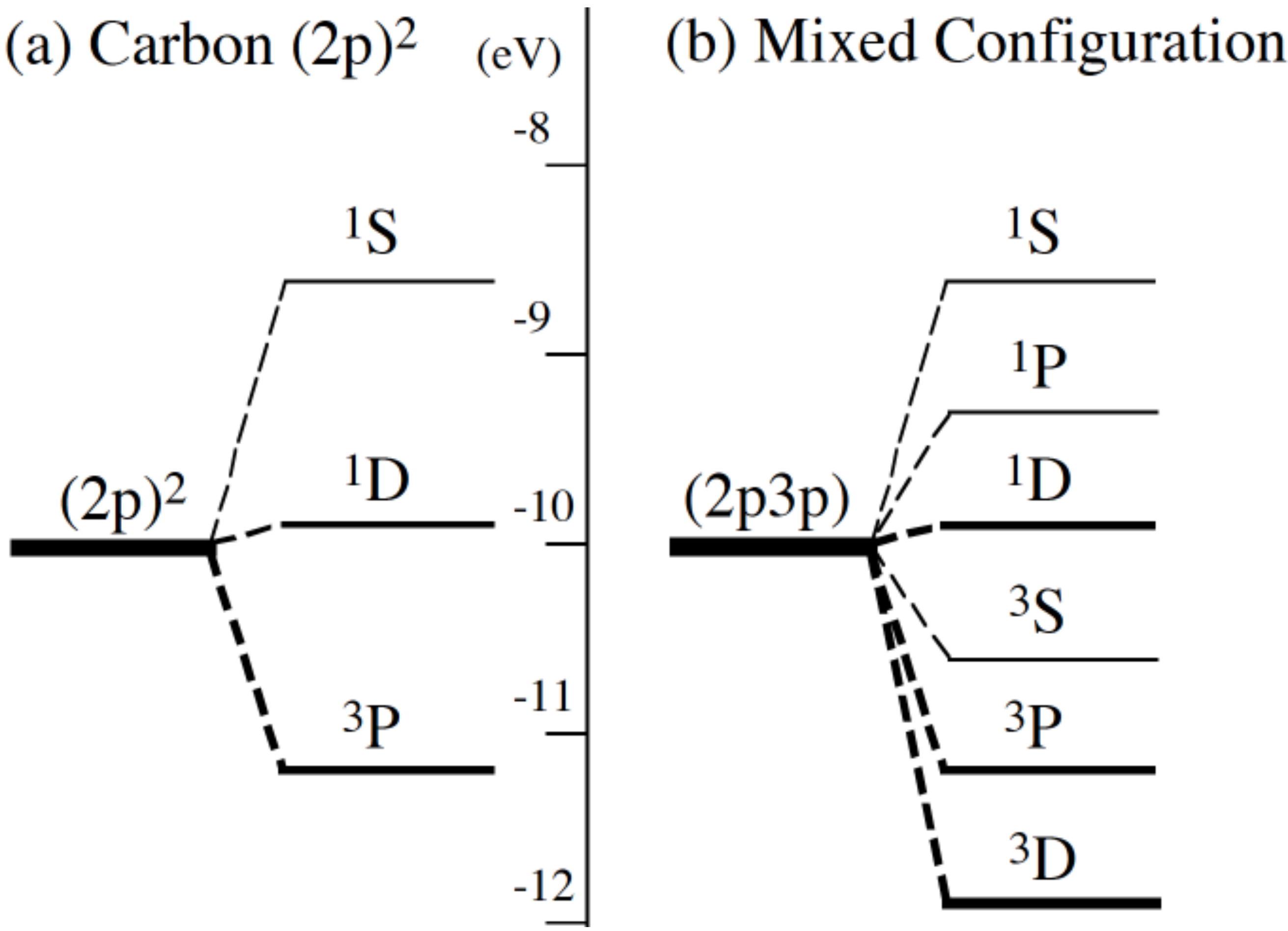

Figure 24.1.3 *Atomic* ${}^{2S+1}$L *multiplet levels for two (*l *= 1)* p *electrons.*

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$$\left|C^{1\ 1\ L}_{m_1\ m_2\ M}\right\rangle =$$

1 ⊗	1	2 2	2 1	2 0	2 −1	2 −2	1 1	1 0	1 −1	0 0
1	1	1	·	·	·	·	·	·	·	·
1	0	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·
1	−1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
0	1	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	·	·
0	0	·	·	$\sqrt{\frac{2}{3}}$	·	·	·	·	·	$-\frac{1}{\sqrt{3}}$
0	−1	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·
−1	1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
−1	0	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·
−1	−1	·	·	·	·	1	·	·	·	·

..

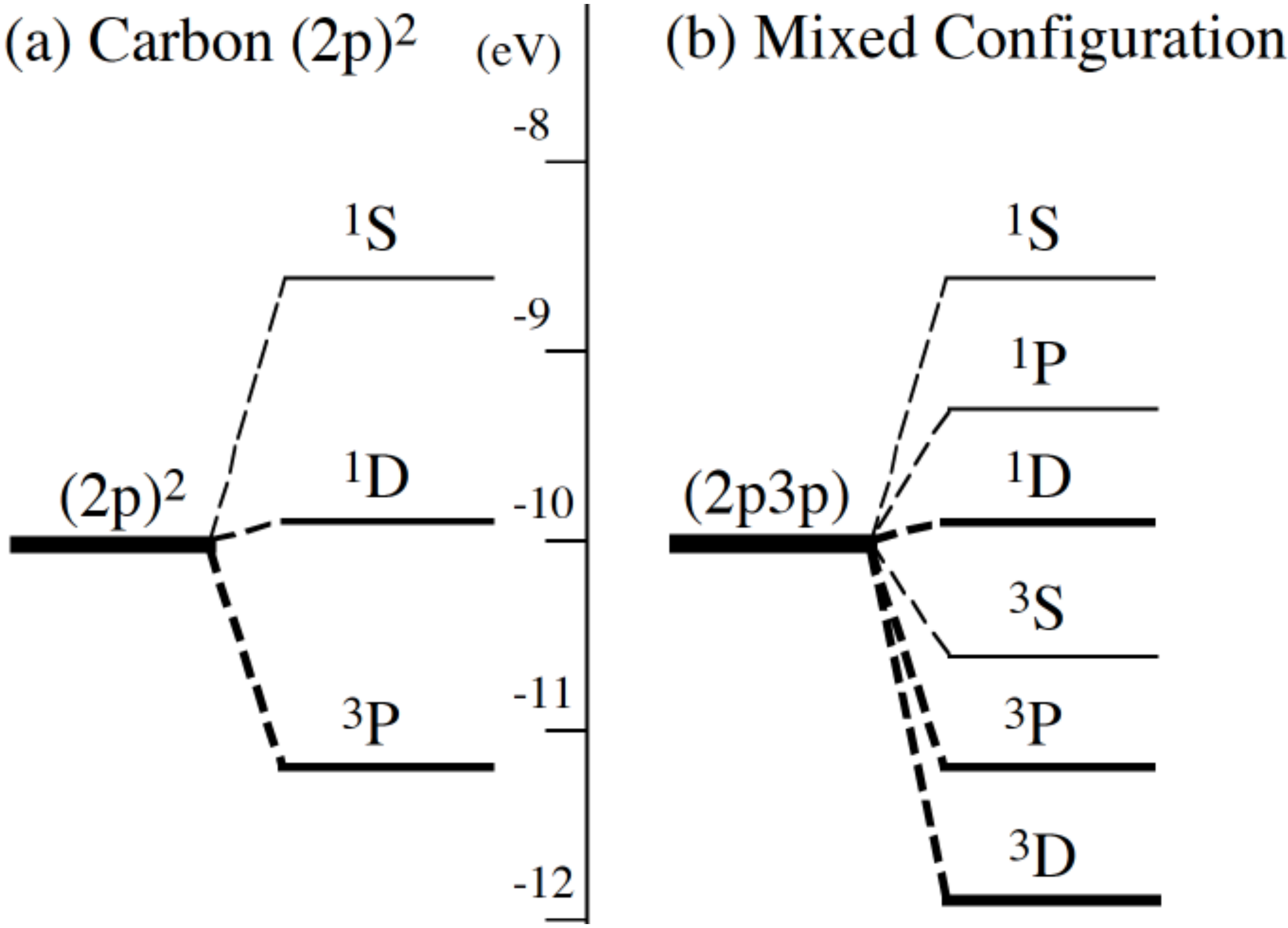


Figure 24.1.3 *Atomic* $^{2S+1}$L *multiplet levels for two (*l *= 1)* p *electrons.*

$\boxed{1\,|\,1}$

$\boxed{1\,|\,0}$ $\quad$ $\boxed{\begin{matrix}1\\0\end{matrix}}$

$\frac{1}{\sqrt{3}}\boxed{1\,|\,\bar{1}}+\frac{\sqrt{2}}{\sqrt{3}}\boxed{0\,|\,0}$ $\quad$ $\boxed{\begin{matrix}1\\\bar{1}\end{matrix}}$ $\quad$ $\frac{\sqrt{2}}{\sqrt{3}}\boxed{1\,|\,\bar{1}}-\frac{1}{\sqrt{3}}\boxed{0\,|\,0}$

$\boxed{0\,|\,\bar{1}}$ $\quad$ $\boxed{\begin{matrix}0\\\bar{1}\end{matrix}}$

$\boxed{\bar{1}\,|\,\bar{1}}$

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$$\left|C^{1\ 1\ L}_{m_1 m_2 M}\right\rangle = \begin{array}{cc|ccccc|ccc|c}
 & & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 0 \\
1\ \otimes & 1 & 2 & 1 & 0 & -1 & -2 & 1 & 0 & -1 & 0 \\
\hline
1 & 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
1 & 0 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\
1 & -1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\
0 & 1 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\
0 & 0 & \cdot & \cdot & \sqrt{\frac{2}{3}} & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{3}} \\
0 & -1 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot \\
-1 & 1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\
-1 & 0 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot \\
-1 & -1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot
\end{array} \ldots$$

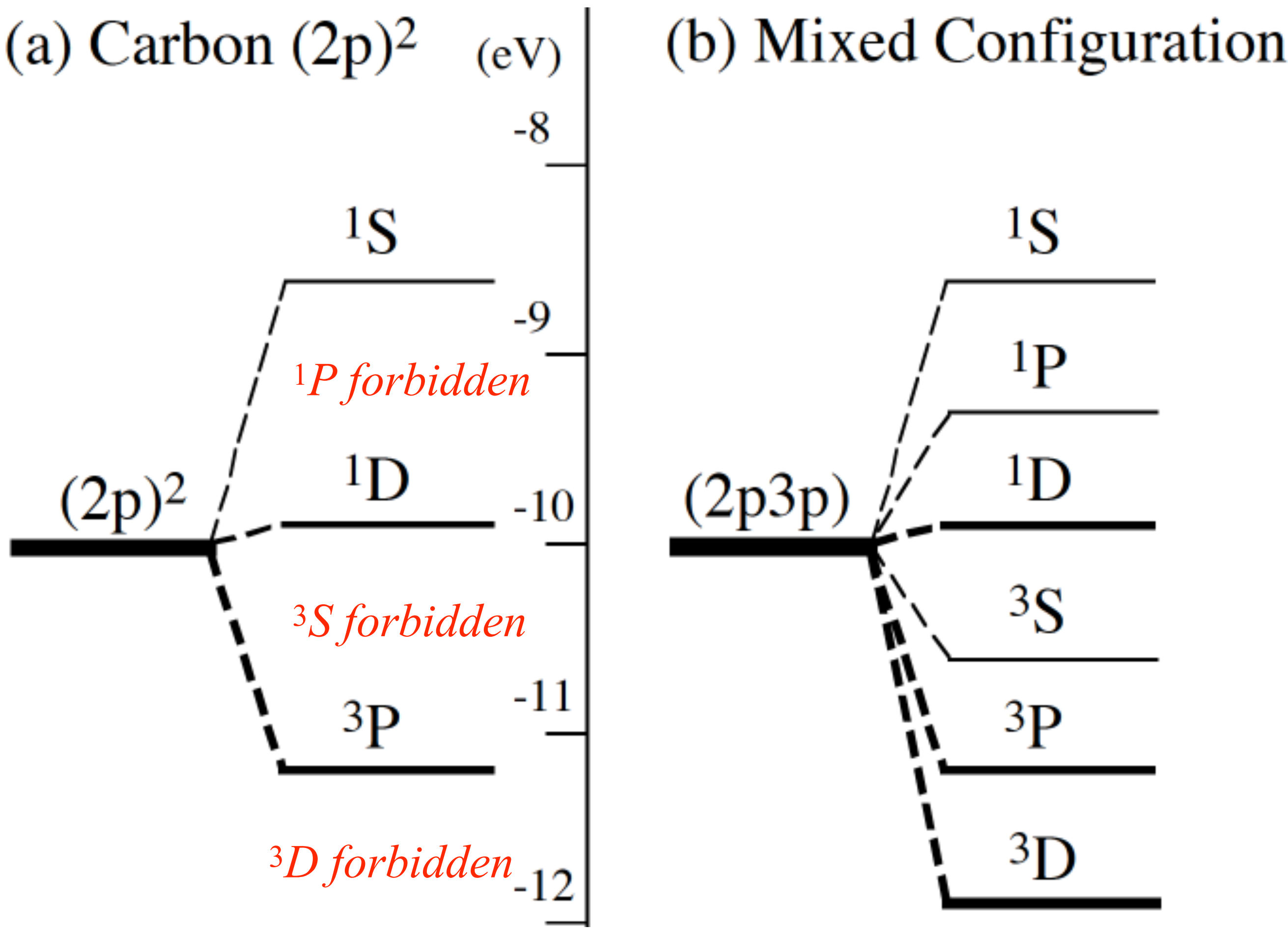
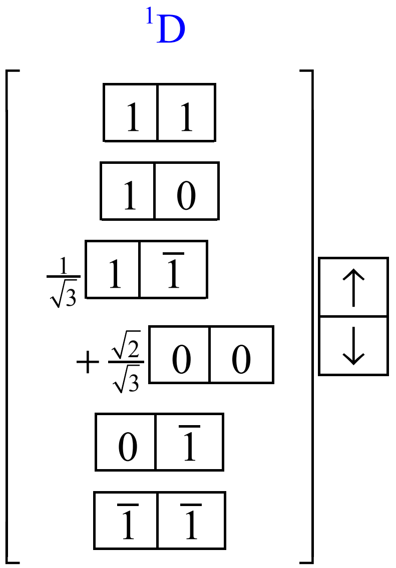


Figure 24.1.3 *Atomic* ^{2S+1}L *multiplet levels for two (l = 1)* p *electrons.*

Pauli-Fermi *selection rules*

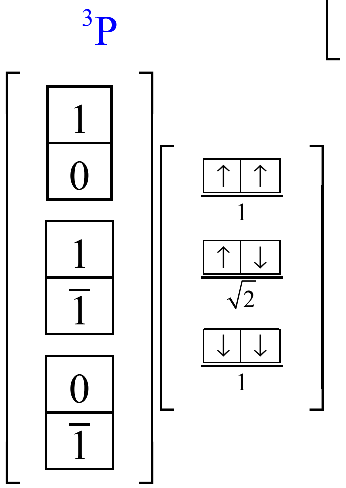
requires total anti-symmetry



Orbital. *Spin*

Symmetry*AntiSymmetry

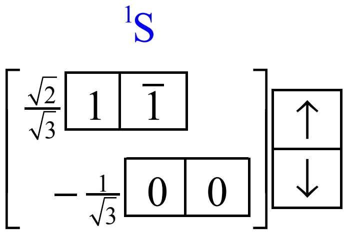
= Total Antisymmetry



Orbital. *Spin*

AntiSymmetry*Symmetry

= Total Antisymmetry



Orbital. *Spin*

Symmetry*AntiSymmetry

= Total Antisymmetry

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$$\left|C^{1\ \ 1\ \ L}_{m_1 m_2 M}\right\rangle = \begin{array}{cc|ccccc|ccc|c}
 & & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 0 \\
1 \otimes & 1 & 2 & 1 & 0 & -1 & -2 & 1 & 0 & -1 & 0 \\
\hline
1 & 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
1 & 0 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\
1 & -1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\
0 & 1 & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\
0 & 0 & \cdot & \cdot & \sqrt{\frac{2}{3}} & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{3}} \\
0 & -1 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot \\
-1 & 1 & \cdot & \cdot & \frac{1}{\sqrt{6}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{3}} \\
-1 & 0 & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot \\
-1 & -1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot
\end{array} \cdot\cdot$$

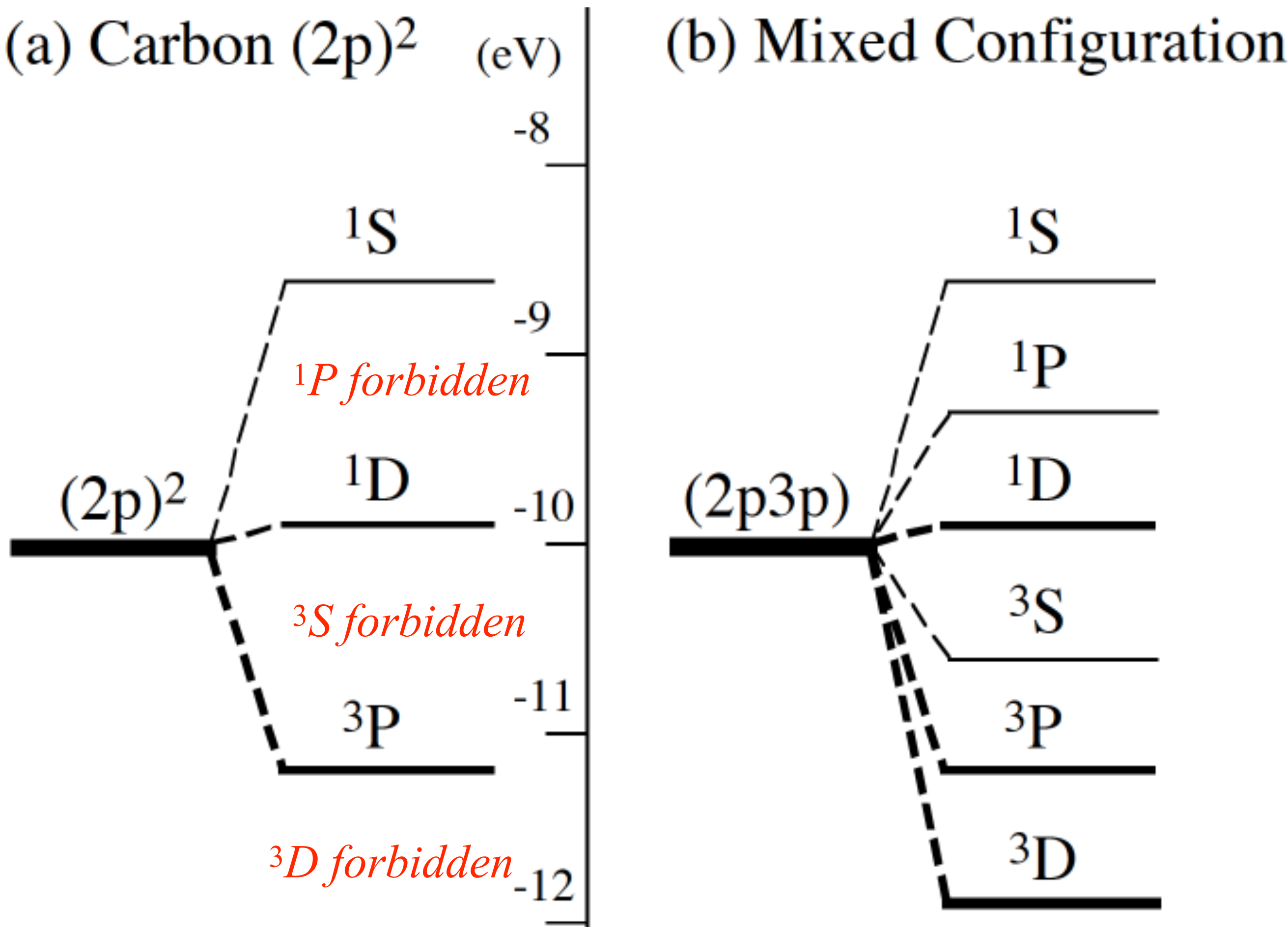
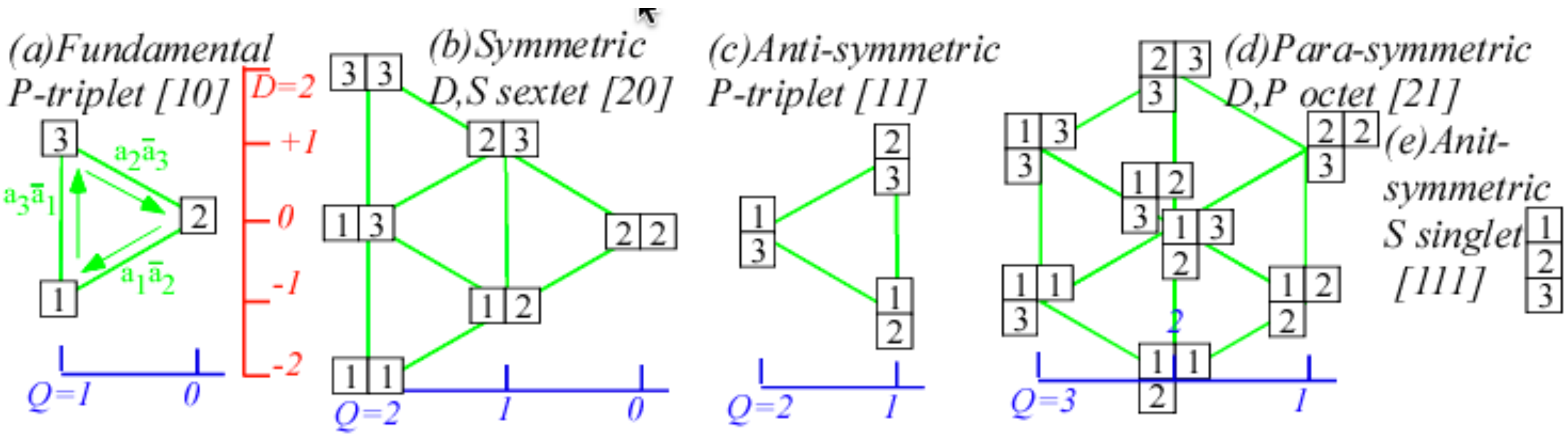


Figure 24.1.3 *Atomic* $^{2S+1}$L *multiplet levels for two (*l *= 1)* p *electrons.*

Pauli-Fermi *selection rules*
requires total anti-symmetry



AMOP
reference links
on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure
- *Kronecker product states and operators*
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  - *6th rank tensor example with exact splitting of f-orbital*

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$\left|C^{1\ 1\ L}_{m_1\ m_2\ M}\right\rangle=$

		2	2	2	2	2	1	1	1	0
1 ⊗	1	2	1	0	−1	−2	1	0	−1	0
1	1	1	·	·	·	·	·	·	·	·
1	0	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·
1	−1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
0	1	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	·	·
0	0	·	·	$\sqrt{\frac{2}{3}}$	·	·	·	·	·	$-\frac{1}{\sqrt{3}}$
0	−1	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·
−1	1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
−1	0	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·
−1	−1	·	·	·	·	1	·	·	·	·

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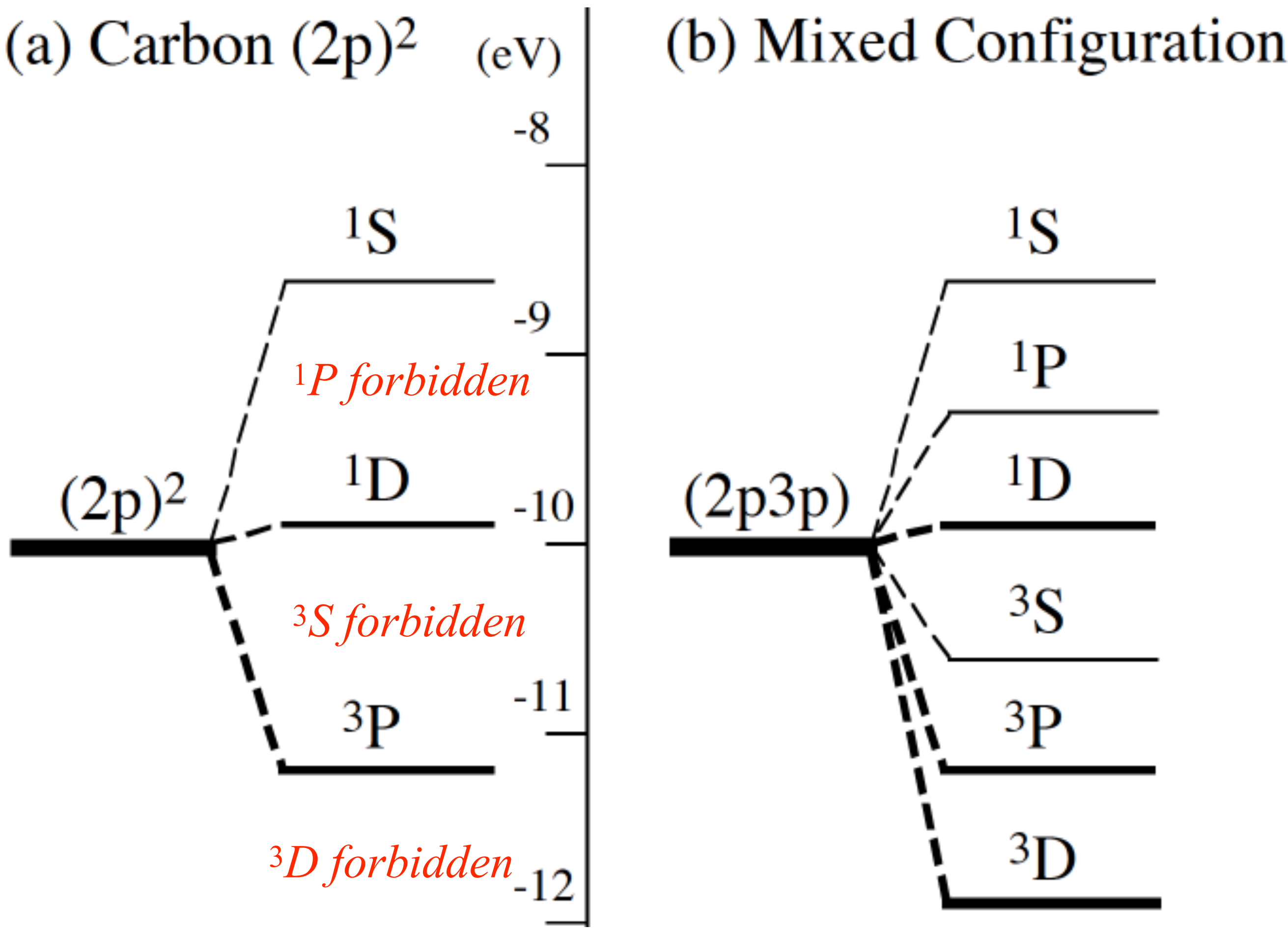

Figure 24.1.3 *Atomic* ^{2S+1}L *multiplet levels for two* (l = 1) p *electrons.*

General U(2) case

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

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} C^{j_1\ \ j_2\ \ j_3}_{m_1\ m_2\ m_3} \Big/ (2j_3+1)^{\frac{1}{2}}$$

Pauli-Fermi *selection rules*
requires total anti-symmetry

Wigner 3j vs. Clebsch-Gordon (CGC)

Higher-J product states

(J=1)⊗(J=1)=2⊕1⊕0 case

$\left| C^{1\ \ 1\ \ L}_{m_1\, m_2\, M} \right\rangle =$

		2	2	2	2	2	1	1	1	0
1 ⊗	1	2	1	0	−1	−2	1	0	−1	0
1	1	1	·	·	·	·	·	·	·	·
1	0	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·
1	−1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
0	1	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	·	·
0	0	·	·	$\sqrt{\frac{2}{3}}$	·	·	·	·	·	$-\frac{1}{\sqrt{3}}$
0	−1	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$\frac{1}{\sqrt{2}}$	·
−1	1	·	·	$\frac{1}{\sqrt{6}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·	$\frac{1}{\sqrt{3}}$
−1	0	·	·	·	$\frac{1}{\sqrt{2}}$	·	·	·	$-\frac{1}{\sqrt{2}}$	·
−1	−1	·	·	·	·	1	·	·	·	·

..

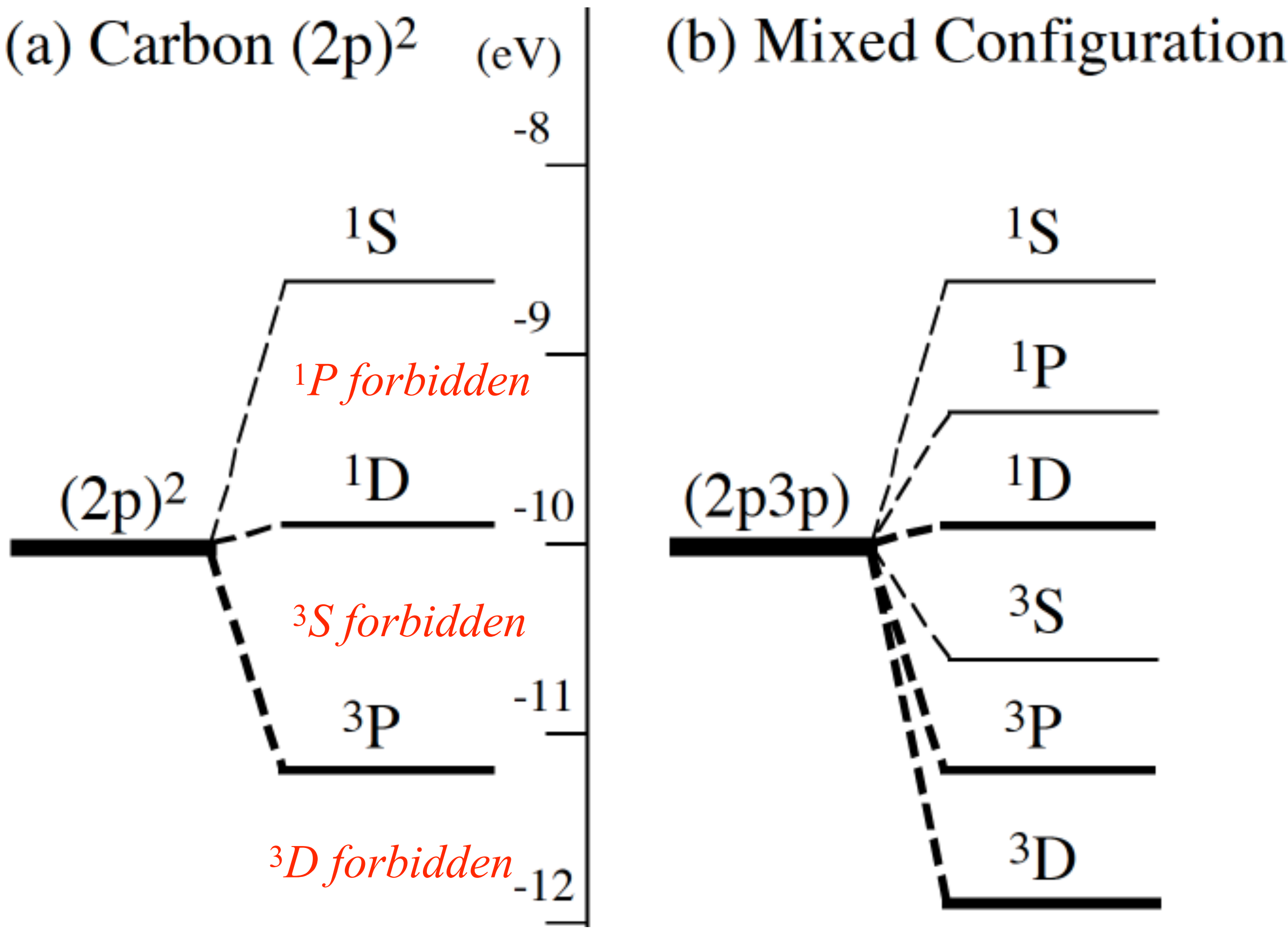

Figure 24.1.3 *Atomic* $^{2S+1}$L *multiplet levels for two (*l *= 1)* p *electrons.*

General U(2) case

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

Pauli-Fermi *selection rules*
requires total anti-symmetry

Wigner 3j vs. Clebsch-Gordon (CGC)

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} C^{j_1\ j_2\ j_3}_{m_1\ m_2\ m_3} \Big/ (2j_3+1)^{\frac{1}{2}}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-n_3} \sqrt{\frac{(j_1+j_2-j_3)!(j_1-j_2+j_3)(-j_1+j_2+j_3)}{(j_1+j_2+j_3+1)!}}$$

$$\sum_k \frac{(-1)^k}{k!} \frac{\sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j_3+m_3)!(j_3-m_3)!}}{(j_1-m_1-k)!(j_2-m_2-k)!(j_1+j_2-j_3-k)!(j_3-j_2-m_1+k)!(j_3-j_1-m_2+k)!}$$

AMOP reference links on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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U(2)~O(3)⊃O_h Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for O(3)⊃O_h symmetry breaking

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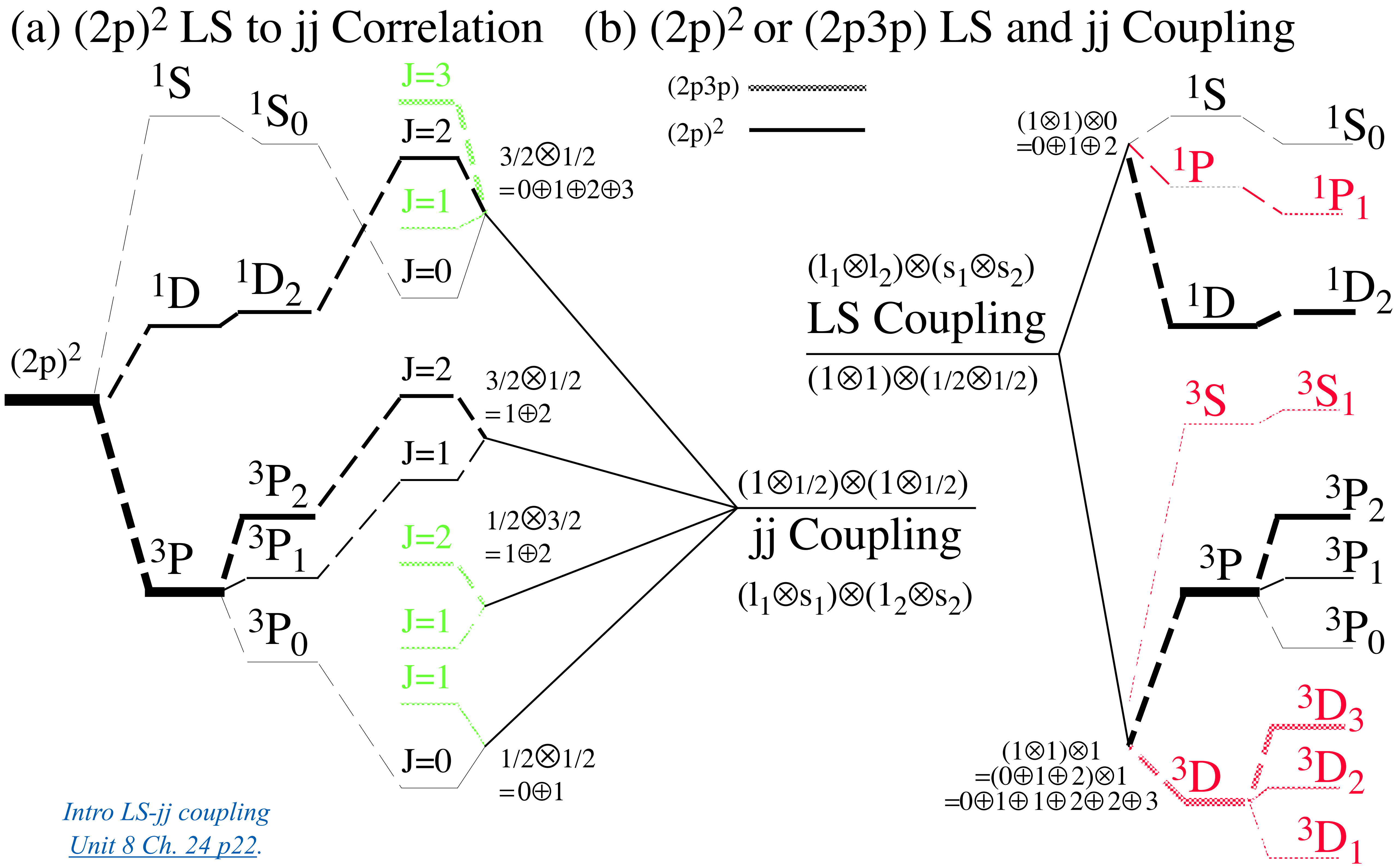 (a) $(2p)^2$ LS to jj Correlation (b) $(2p)^2$ or $(2p3p)$ LS and jj Coupling

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

Figure 24.1.4 *Fine-structure $n\ell_j$ levels for atomic hydrogen. Hyperfine splitting is not shown.*

AMOP reference links on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

U(2)~O(3)⊃O_h Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for O(3)⊃O_h symmetry breaking

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➡ *Higher-J product states:* $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$ *case*

- *Effect of Pauli-Fermi-Dirac symmetry*
- *General U(2) Clebsch-Gordan-Wigner-3j coupling coefficient formula*
    - *LS to jj Level corralations*
- ➡ *Angular momentum uncertainty cones related to 3j coefficients*

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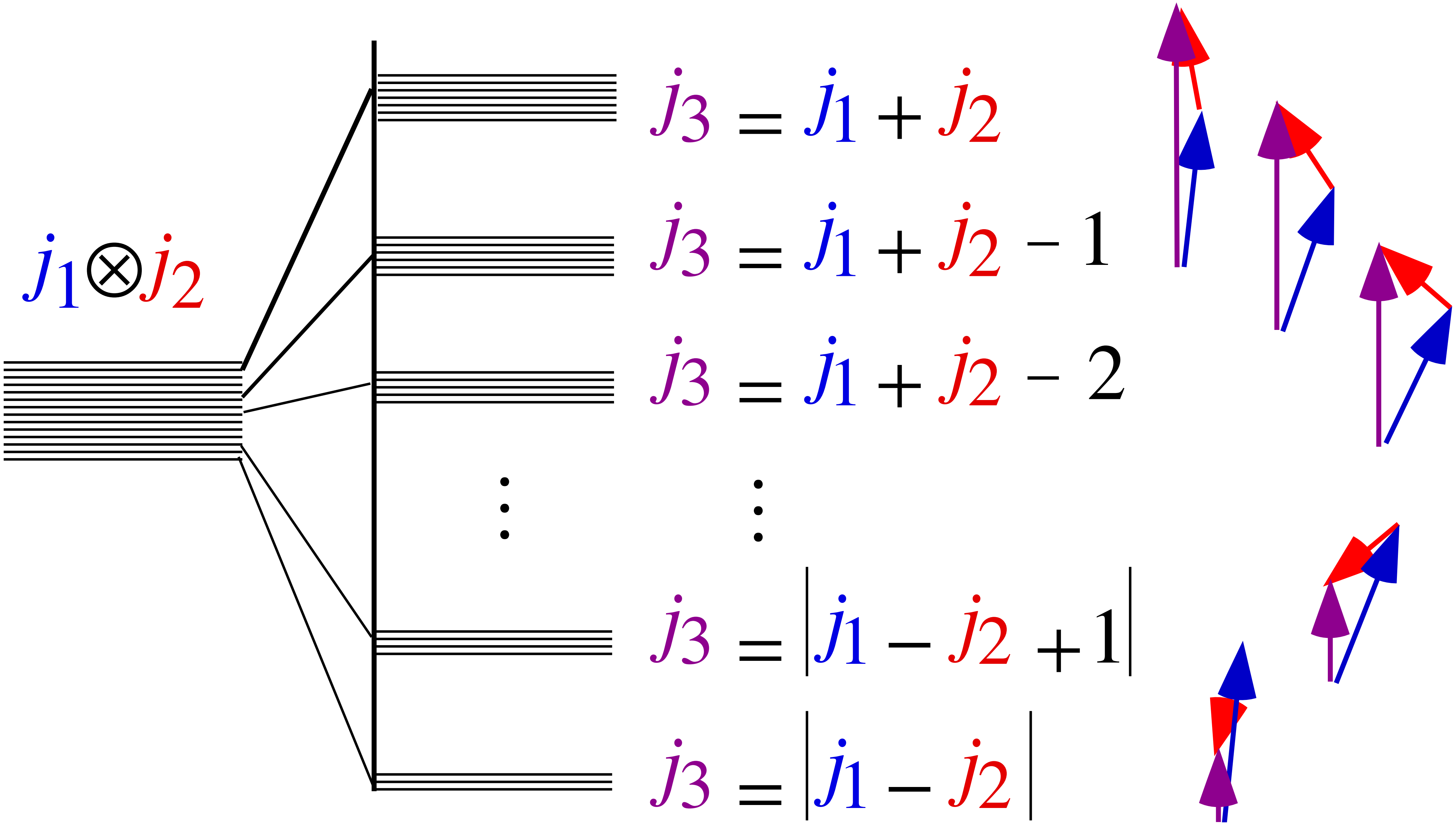
    - *6th rank tensor example with exact splitting of f-orbital*

Higher-J product states

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



$j_1 \otimes j_2$

$j_3 = j_1 + j_2$

$j_3 = j_1 + j_2 - 1$

$j_3 = j_1 + j_2 - 2$

$\vdots \qquad \vdots$

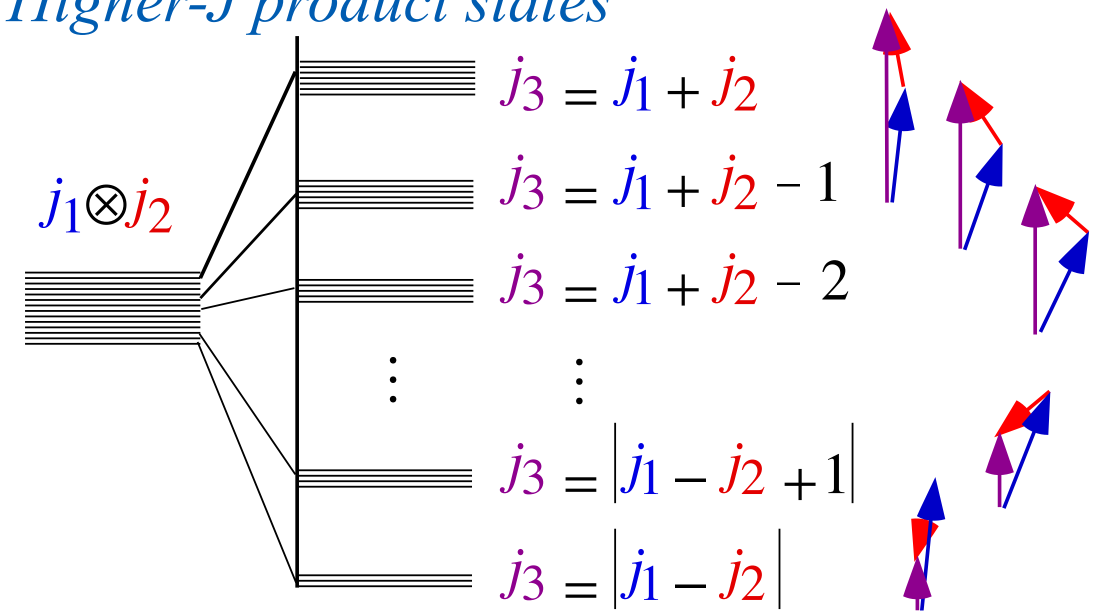
$j_3 = \left| j_1 - j_2 + 1 \right|$

$j_3 = \left| j_1 - j_2 \right|$

Figure 24.1.6 Level-splitting and vector-addition picture of angular-momentum coupling.

Higher-J product states

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



$j_1 \otimes j_2$

$j_3 = j_1 + j_2$

$j_3 = j_1 + j_2 - 1$

$j_3 = j_1 + j_2 - 2$

$\vdots \qquad \vdots$

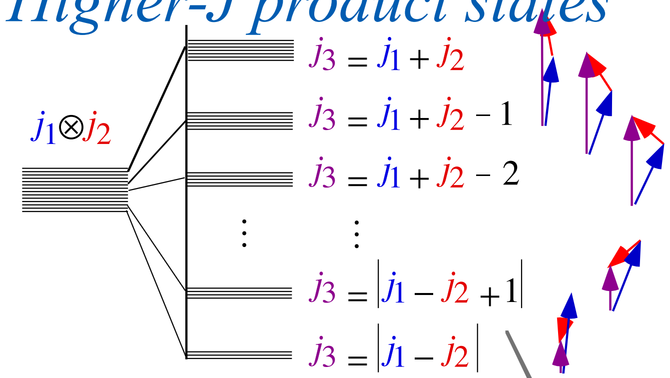
$j_3 = \left| j_1 - j_2 + 1 \right|$

$j_3 = \left| j_1 - j_2 \right|$

Figure 24.1.6 Level-splitting and vector-addition picture of angular-momentum coupling.

Higher-J product states

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



$j_3 = j_1 + j_2$

$j_3 = j_1 + j_2 - 1$

$j_3 = j_1 + j_2 - 2$

⋮ ⋮

$j_3 = |j_1 - j_2 + 1|$

$j_3 = |j_1 - j_2|$

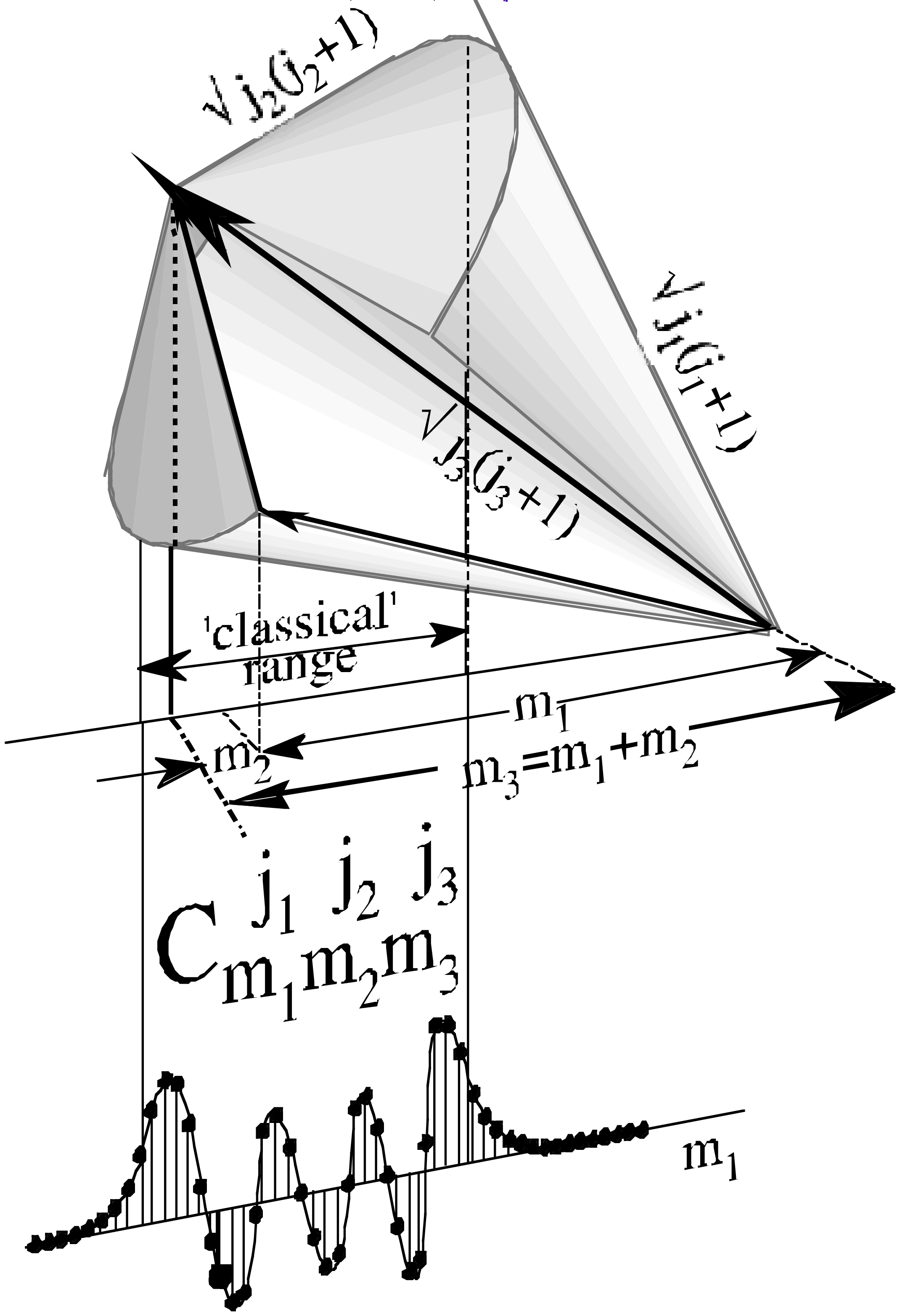
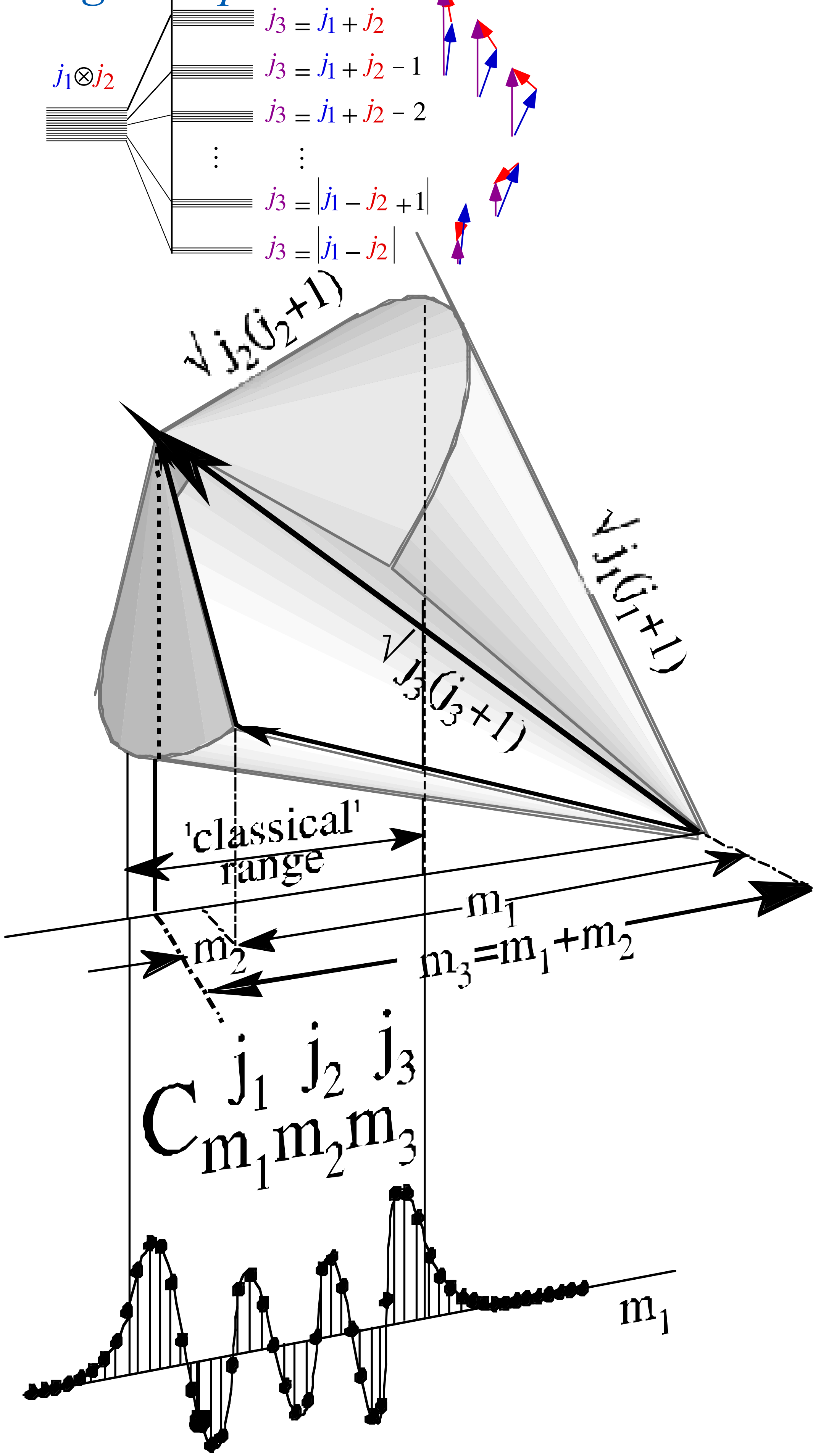


Figure 24.1.7 *Angular-momentum cone picture of Clebsch-Gordan coupling amplitudes.*

Higher-J product states

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



$C^{j_1\ j_2\ j_3}_{m_1 m_2 m_3}$

Figure 24.1.7 *Angular-momentum cone picture of Clebsch-Gordan coupling amplitudes.*

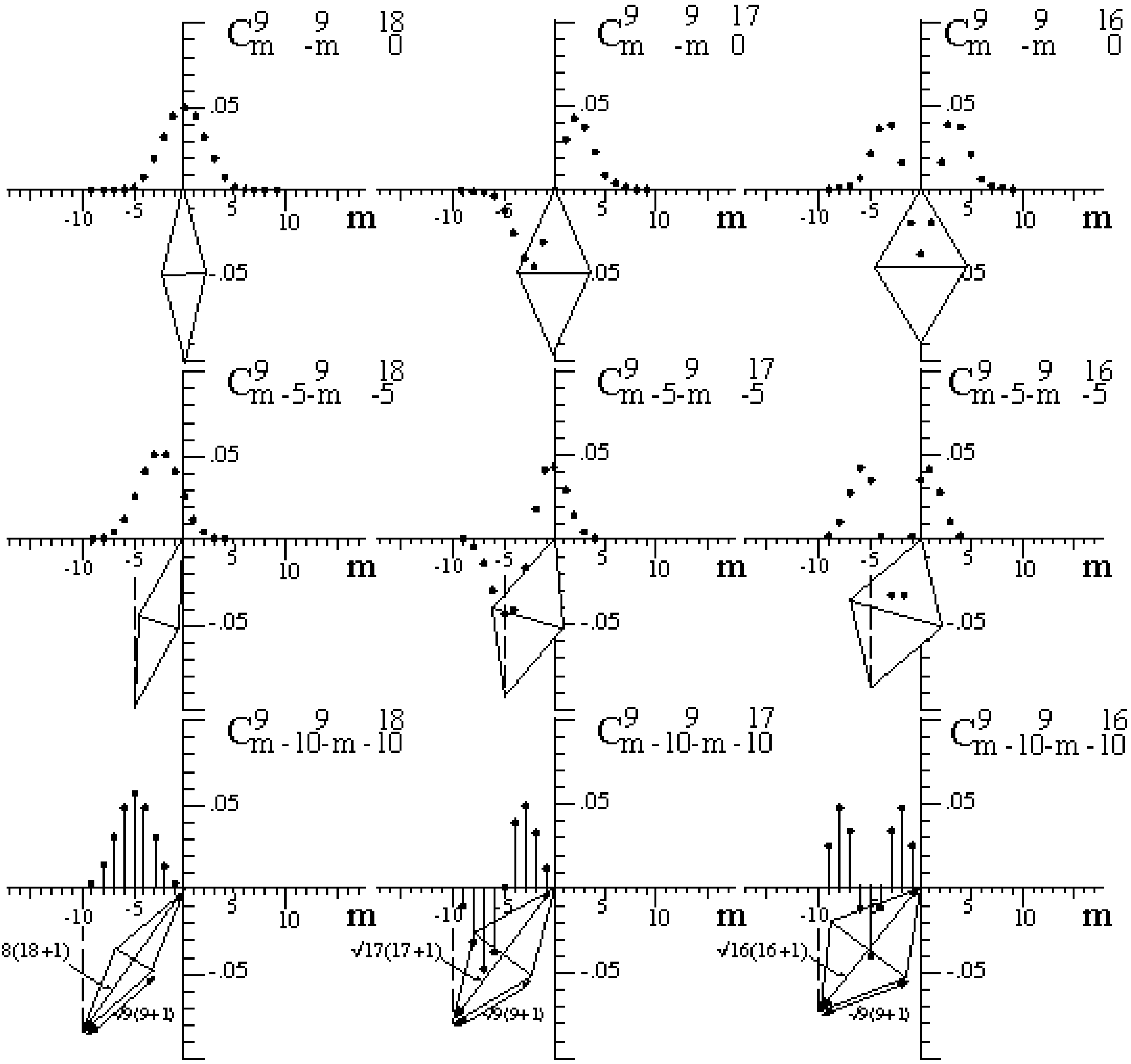
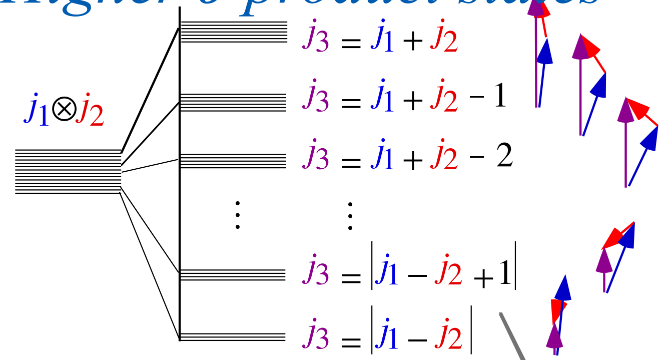
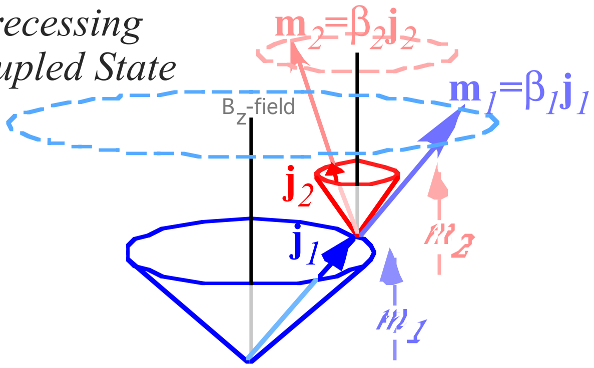
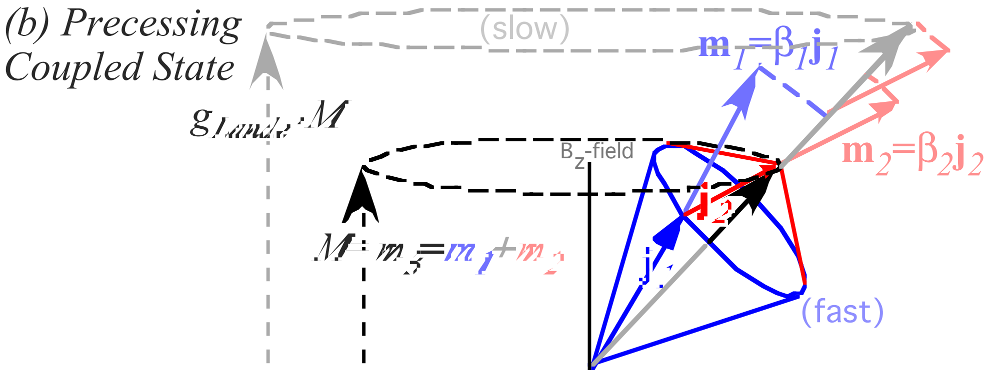


Figure 24.1.8 *Clebsch-Gordan coefficients plotted next to their angular-momentum cones.*

Higher-J product states







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

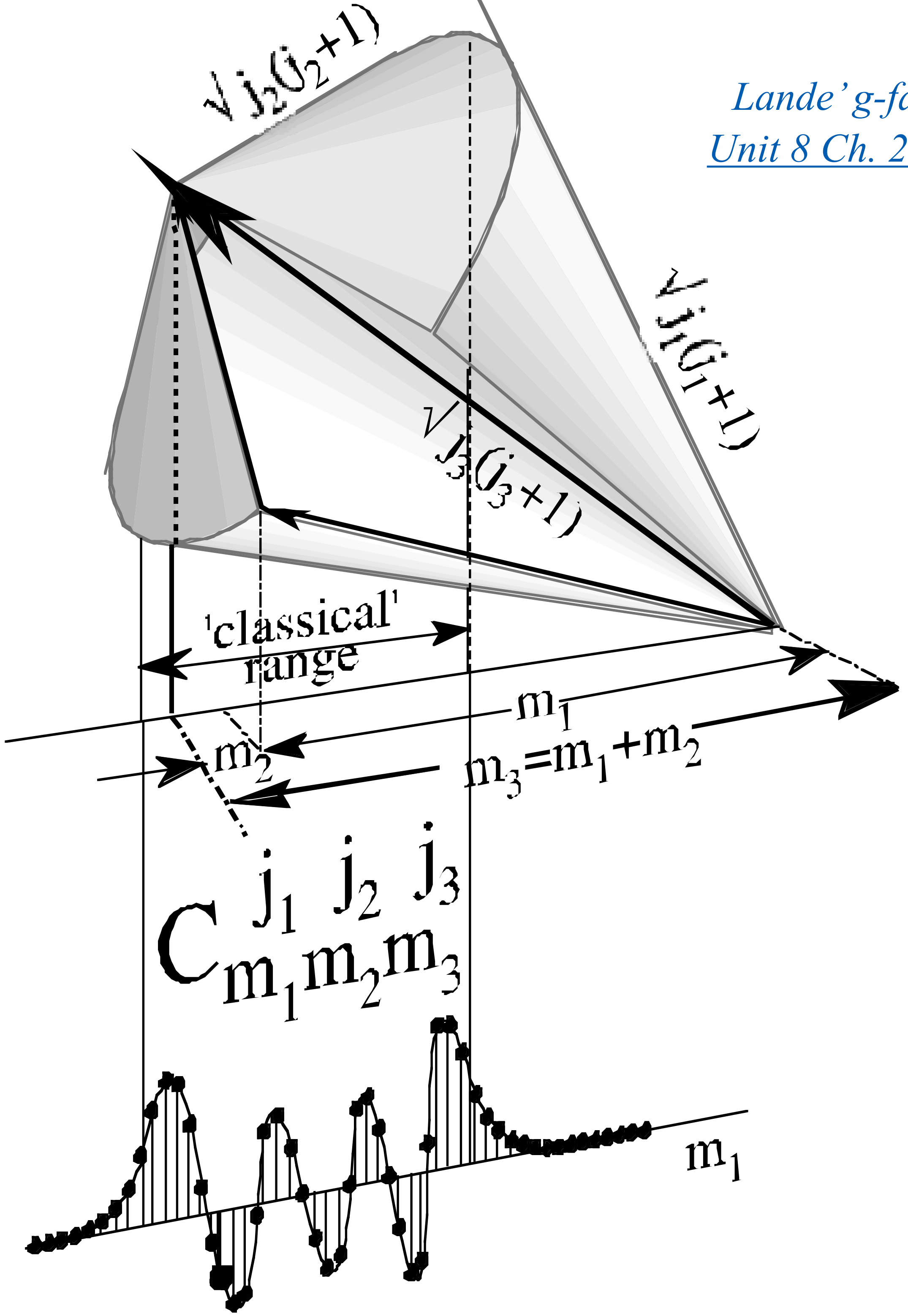


Figure 24.1.7 *Angular-momentum cone picture of Clebsch-Gordan coupling amplitudes.*

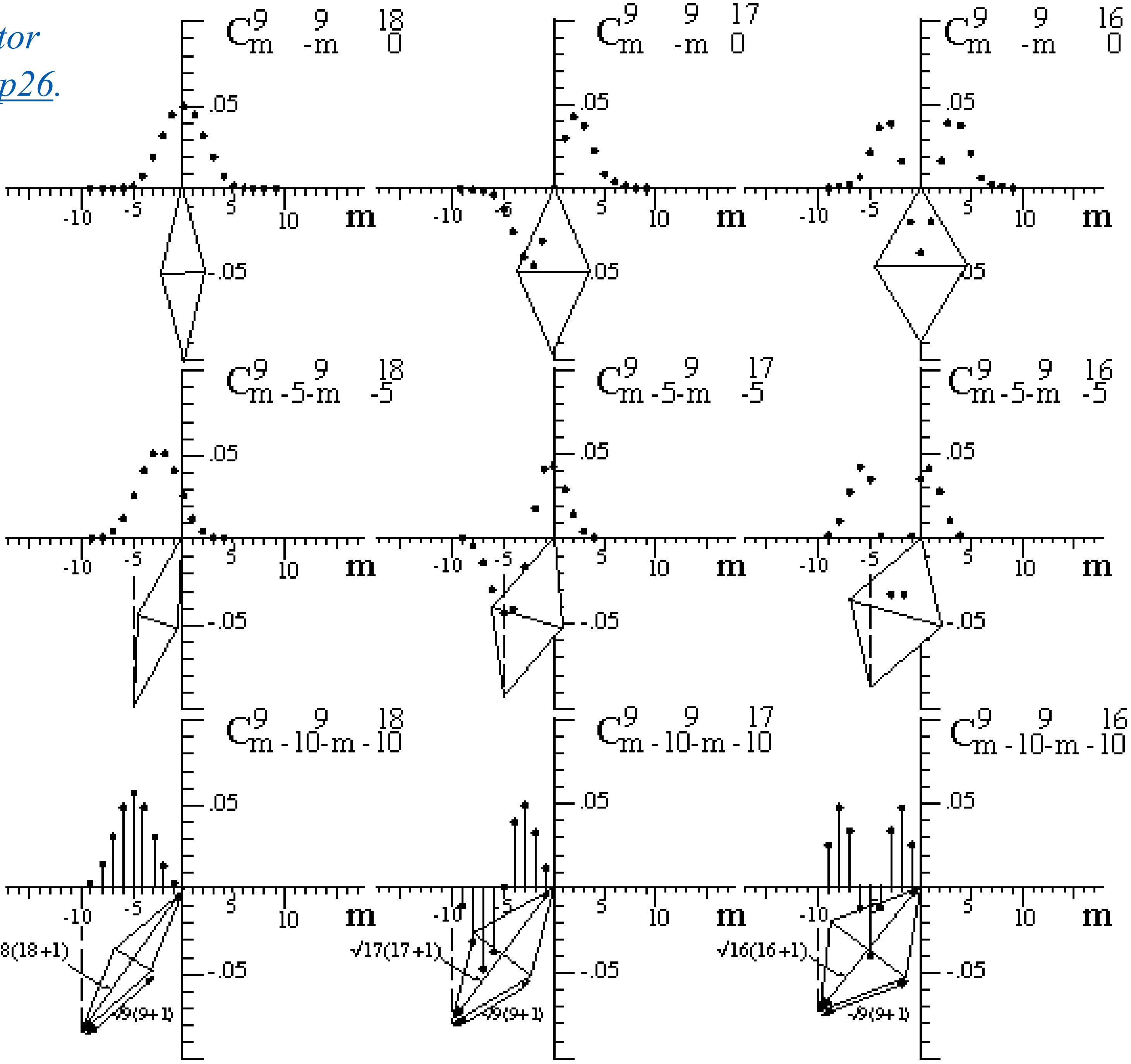
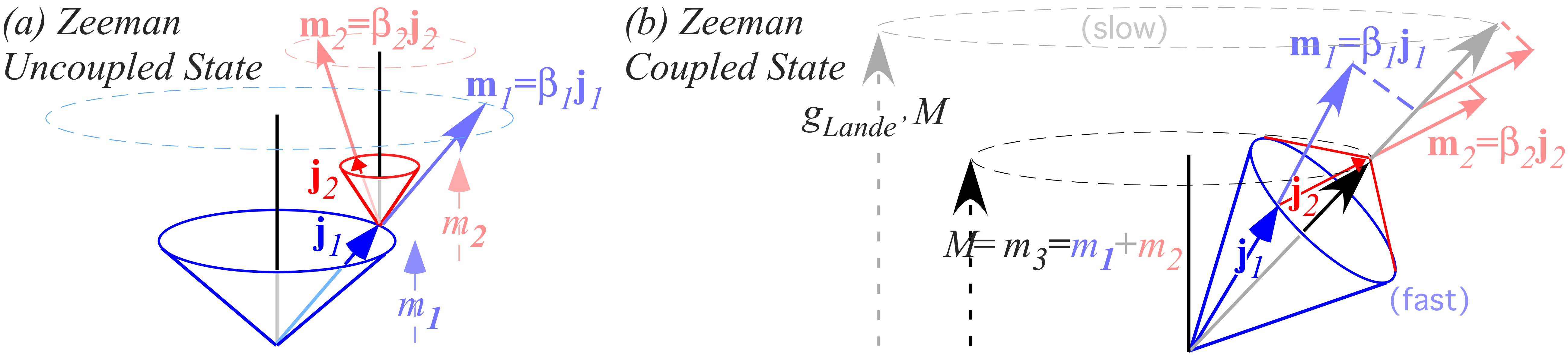


Figure 24.1.8 *Clebsch-Gordan coefficients plotted next to their angular-momentum cones.*

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

The Lande g-factor (Atomic LS-coupled gyro-magnetic factor)

$$g_{Lande'} = \frac{3J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} \quad \text{where: } \langle m_{TOTAL} B_z \rangle = g_{Lande'} \mu_{Bohr} m_3 B_z$$



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

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3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

- Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure
    - *Kronecker product states and operators*
    - *Spin-spin interaction reduces symmetry* $U(2)^{proton}\times U(2)^{electron}$ *to* $U(2)^{e+p}$
        - *Elementary ½ × ½ Clebsch-Gordan coefficients*
    - *Hydrogen hyperfine levels: Fermi-contact interaction, Racah's trick for energy eigenvalues*
        - *B-field gives avoided crossing*
- *Higher-J product states:* $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$ *case*
    - *Effect of Pauli-Fermi-Dirac symmetry*
    - *General U(2) Clebsch-Gordan-Wigner-3j coupling coefficient formula*
        - *LS to jj Level corralations*
    - *Angular momentum uncertainty cones related to 3j coefficients*
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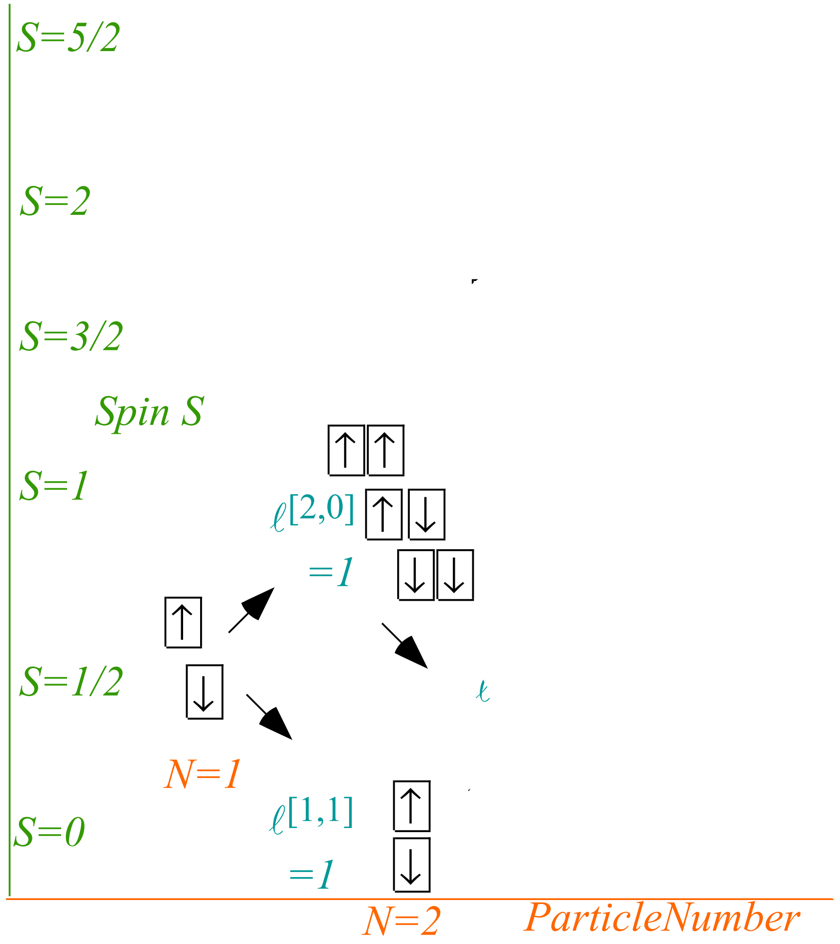
    - *Intro to U(2) Young Tableaus*
    - *Intro to U(3) and higher Young Tableaus and Lab-Bod or Particle-State summitry*
- *U(2) and U(3) tensor expansion of H operator*
    - *Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors*
    - *Tensor operators for spin-1 states: U(3) generalization of Pauli spinors*
        - *4th rank tensor example with exact splitting of d-orbital*
        - *6th rank tensor example with exact splitting of f-orbital*

Multi-spin $(1/2)^N$ product states

$$\left(\frac{1}{2}\otimes\frac{1}{2}\right)\otimes\frac{1}{2} :$$

Multi-spin $(1/2)^N$ product states

$$(d^{\frac{1}{2}} \otimes d^{\frac{1}{2}}) = d^0 + d^1$$

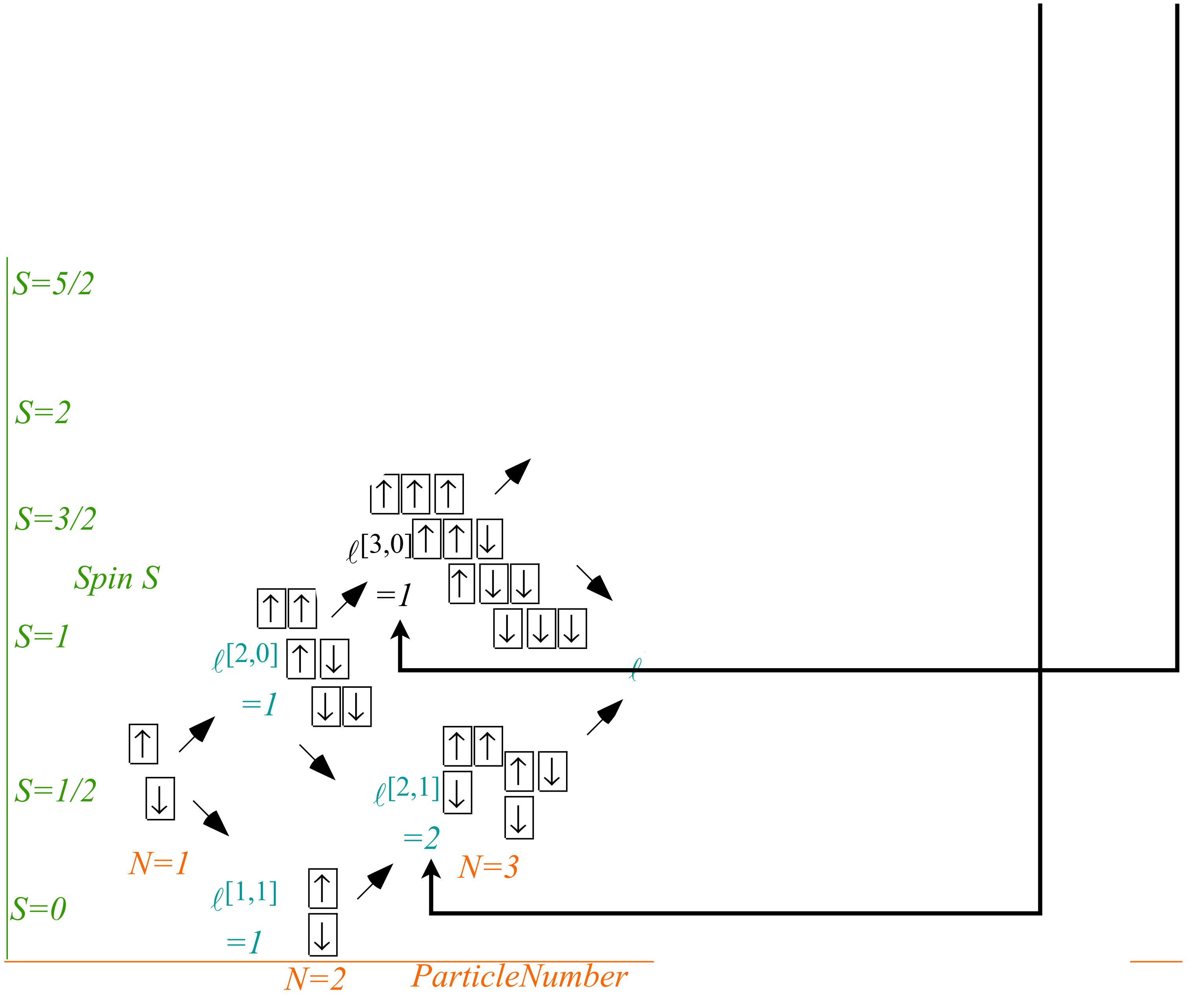


Multi-spin (1/2)^N product states

$$(d^{\frac{1}{2}}\otimes d^{\frac{1}{2}}) = d^0 + d^1$$

$$(d^{\frac{1}{2}}\otimes d^{\frac{1}{2}})\otimes d^{\frac{1}{2}} = (d^0 + d^1)\otimes d^{\frac{1}{2}} = d^0\otimes d^{\frac{1}{2}} + d^1\otimes d^{\frac{1}{2}}$$

$$= d^{\frac{1}{2}} + d^{\frac{1}{2}} + d^{\frac{3}{2}} = 2d^{\frac{1}{2}} + 1d^{\frac{3}{2}}$$



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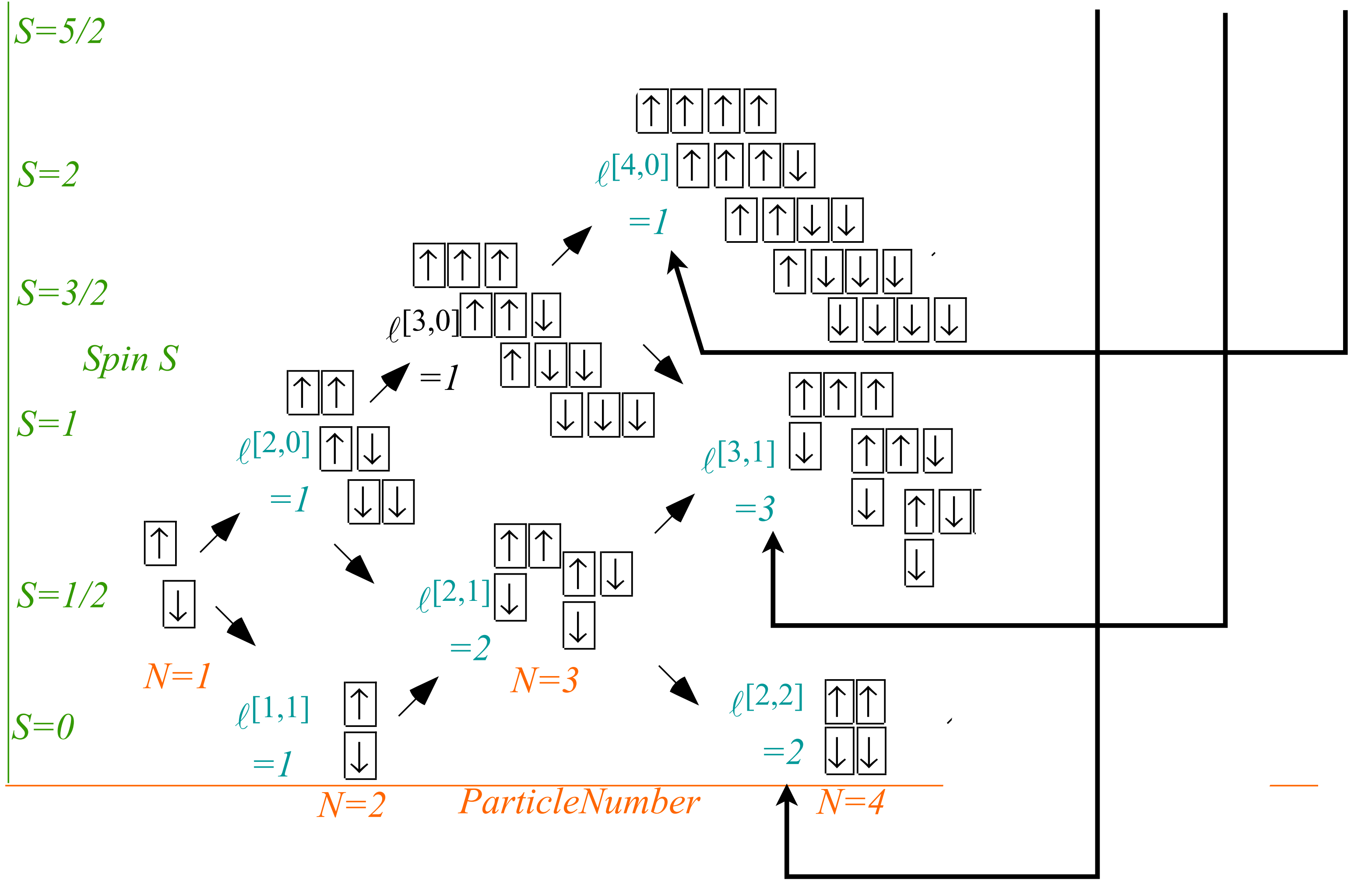
$$= \quad d^{\frac{1}{2}} + \qquad d^{\frac{1}{2}} + d^{\frac{3}{2}} = 2d^{\frac{1}{2}} + \ d^{\frac{3}{2}}$$

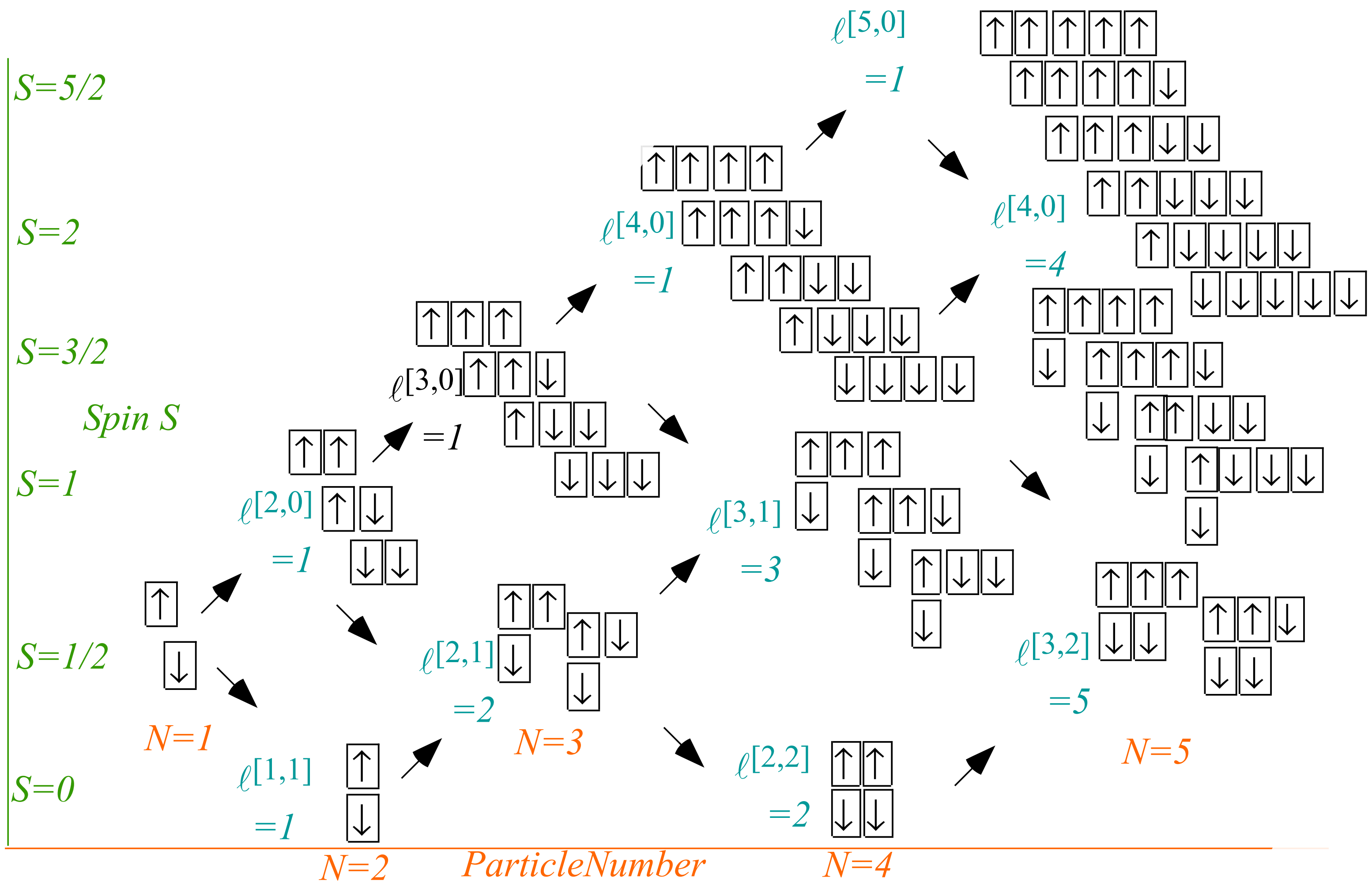
$$(d^{\frac{1}{2}}\otimes d^{\frac{1}{2}})\otimes(d^{\frac{1}{2}}\otimes d^{\frac{1}{2}}) = (2d^{\frac{1}{2}} + \ d^{\frac{3}{2}})\otimes d^{\frac{1}{2}}$$

$$(d^0 + d^1)\otimes(d^0 + d^1) = d^0 + 2d^0\otimes d^1 + d^1\otimes d^1$$

$$= d^0 \quad + 2d^1 \qquad + d^0 \ + d^1 \ + d^2 \ = \ 2d^0 + 3d^1 + 1d^2$$



Multi-spin $(1/2)^N$ product states



Multi-spin $(1/2)^N$ product states

$$\left|\begin{array}{cccccc}\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\downarrow}\\\boxed{\downarrow}&\boxed{\downarrow}&&&&\end{array}\quad\begin{array}{c}S=2\\M_S=1\end{array}\right\rangle = C^{5/2\ 1/2\ 2}_{1/2\ 1/2\ 1}\left|\begin{array}{cccccc}\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\downarrow}&\boxed{\downarrow}\\\boxed{\downarrow}&\boxed{\cdot\cdot}&&&&\end{array}\quad\begin{array}{c}5/2\\1/2\end{array}\right\rangle\left|\boxed{\uparrow}^{1/2}_{1/2}\right\rangle + C^{5/2\ 1/2\ 2}_{3/2\ -1/2\ 1}\left|\begin{array}{cccccc}\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\downarrow}\\\boxed{\downarrow}&\boxed{\cdot\cdot}&&&&\end{array}\quad\begin{array}{c}5/2\\1/2\end{array}\right\rangle\left|\boxed{\downarrow}^{1/2}_{-1/2}\right\rangle$$

$$+C^{3/2\ 1/2\ 2}_{1/2\ 1/2\ 1}\left|\begin{array}{cccccc}\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\downarrow}&\boxed{\cdot\cdot}\\\boxed{\downarrow}&\boxed{\downarrow}&&&&\end{array}\quad\begin{array}{c}3/2\\1/2\end{array}\right\rangle\left|\boxed{\uparrow}^{1/2}_{1/2}\right\rangle + C^{3/2\ 1/2\ 2}_{3/2\ -1/2\ 1}\left|\begin{array}{cccccc}\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\uparrow}&\boxed{\cdot\cdot}\\\boxed{\downarrow}&\boxed{\downarrow}&&&&\end{array}\quad\begin{array}{c}3/2\\1/2\end{array}\right\rangle\left|\boxed{\downarrow}^{1/2}_{-1/2}\right\rangle$$

$$\left(\begin{array}{cc}C^{j\ \ 1/2\ \ j+1/2}_{m\ 1/2\ \ m+1/2}=\sqrt{\dfrac{j+m+1}{2j+1}} & C^{j\ \ \ \ 1/2\ \ j+1/2}_{m+1\ -1/2\ \ m+1/2}=\sqrt{\dfrac{j-m}{2j+1}}\\ C^{j+1\ 1/2\ \ j+1/2}_{m\ \ \ \ 1/2\ \ m+1/2}=-\sqrt{\dfrac{j-m+1}{2j+3}} & C^{j+1\ \ 1/2\ \ j+1/2}_{m+1\ -1/2\ \ m+1/2}=\sqrt{\dfrac{j+m+2}{2j+3}}\end{array}\right)\quad \text{example:}\quad\left(\begin{array}{cc}C^{3/2\ 1/2\ 2}_{1/2\ \ 1/2\ 1}=\sqrt{\dfrac{2}{3}} & C^{3/2\ 1/2\ 2}_{1/2\ \ 1/2\ 1}=\sqrt{\dfrac{1}{3}}\\ C^{5/2\ 1/2\ 2}_{1/2\ \ 1/2\ 1}=-\sqrt{\dfrac{1}{3}} & C^{5/2\ 1/2\ 2}_{1/2\ \ 1/2\ 1}=\sqrt{\dfrac{2}{3}}\end{array}\right)$$

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

Intro 3,4-particle Young Tableaus
GrpThLect29 p42.

Young Tableau Magic Formulae
GrpThLect29 p46-48.

Multi-spin $(1/2)^N$ product states

$$2^N = \sum_{S}^{N/2} \ell^{[S]} \ell^{[\mu_1,\mu_2]}$$

$$= \sum_{S}^{N/2} (2S+1) \ell^{\left[\frac{N+2S}{2},\frac{N-2S}{2}\right]}$$

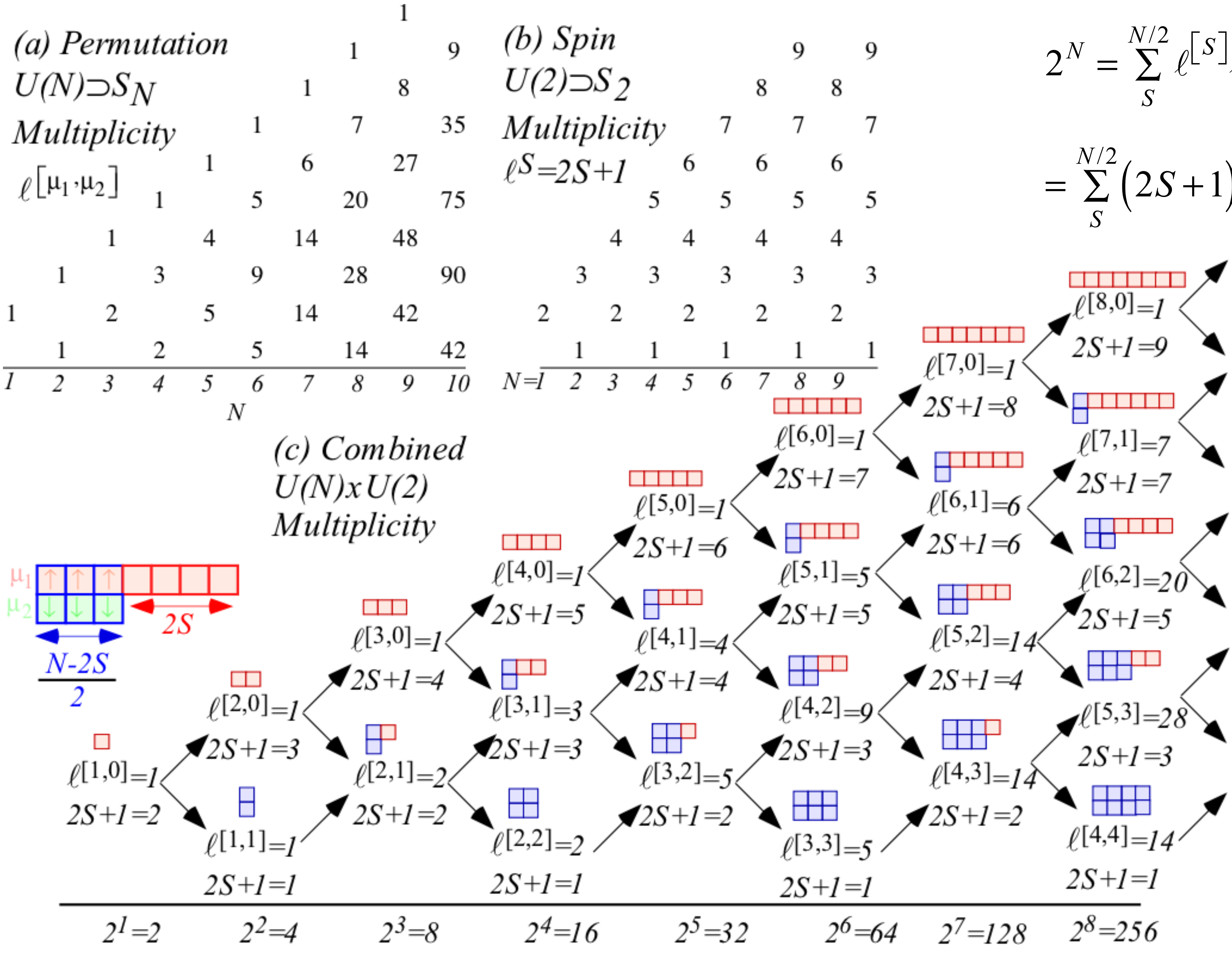
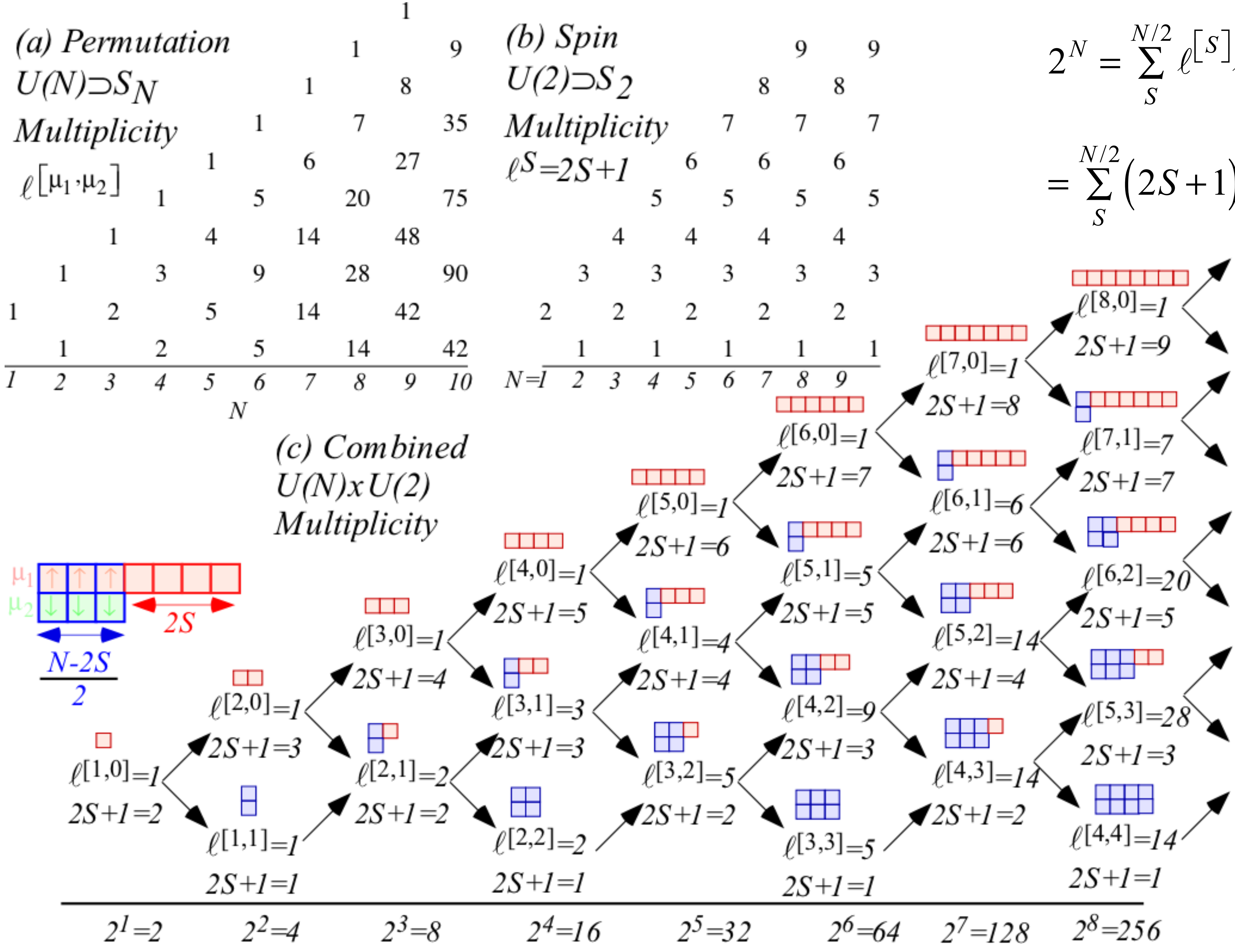


Fig. 23.3.2 *Spin-1/2 and U(2) Tableau branching diagrams*

Young Tableau Magic Formulae
GrpThLect29 p46-48.

Multi-spin $(1/2)^N$ product states



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$$=\sum_S^{N/2}(2S+1)\ell^{\left[\frac{N+2S}{2},\frac{N-2S}{2}\right]}$$

Tableau dimension formulae

U(2) dimension
$\ell^j=2j+1$

2	3	4	5
1	2	3	4

5	4	3	2
4	3	2	1

S_N
dimension $\ell^{[\mu]}$

~~8~~·~~7·6·5·4·3~~·2·1

~~5~~	~~4~~	~~3~~	~~2~~
4	~~3~~	2	1

Young Tableau Magic Formulae
GrpThLect29 p46-48.

Multi-spin $(1/2)^N$ product states

$$2^N = \sum_S^{N/2} \ell^{[S]}\ell^{[\mu_1,\mu_2]}$$

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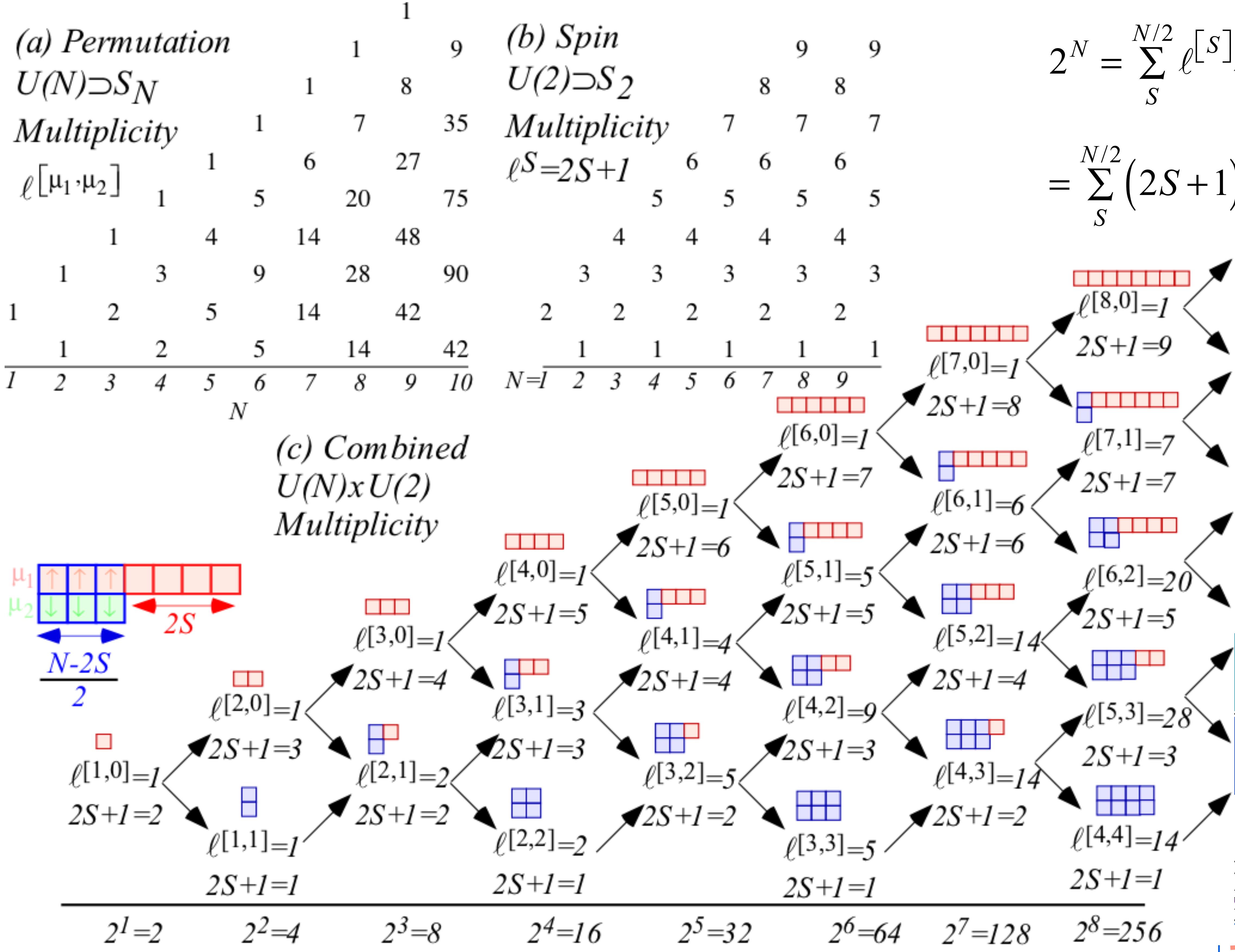
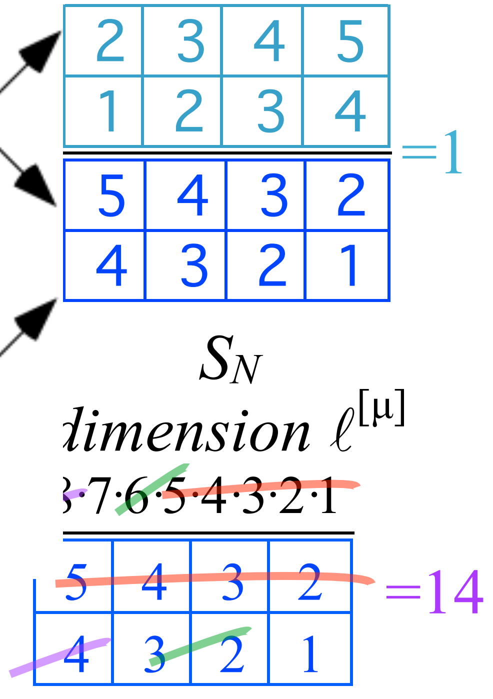


Tableau dimension formulae

U(2) dimension $\ell^j=2j+1$



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GrpThLect29 p46-48.

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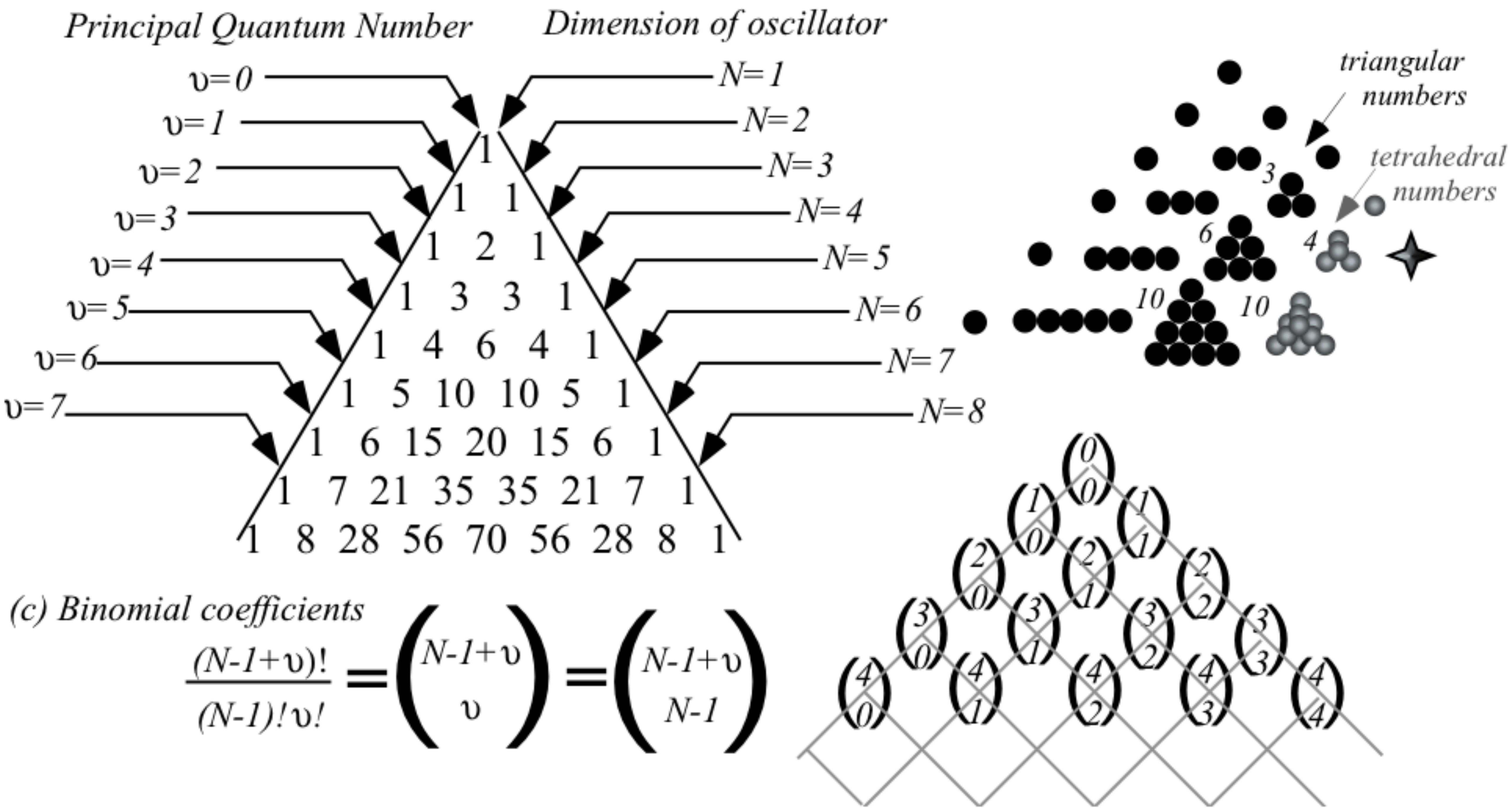
6th rank tensor example with exact splitting of f-orbital

Introducing U(N)

(a) N-D Oscillator Degeneracy ℓ of quamtum level υ

(b) Stacking numbers



(c) Binomial coefficients

$$\frac{(N\text{-}1+\upsilon)!}{(N\text{-}1)!\,\upsilon!}=\binom{N\text{-}1+\upsilon}{\upsilon}=\binom{N\text{-}1+\upsilon}{N\text{-}1}$$

Introducing U(3)

(b) N-particle 3-level states ...or spin-1 states

$\boxed{1} = |1\ 0\ 0\rangle = a_1^\dagger\ |0\ 0\ 0\rangle$

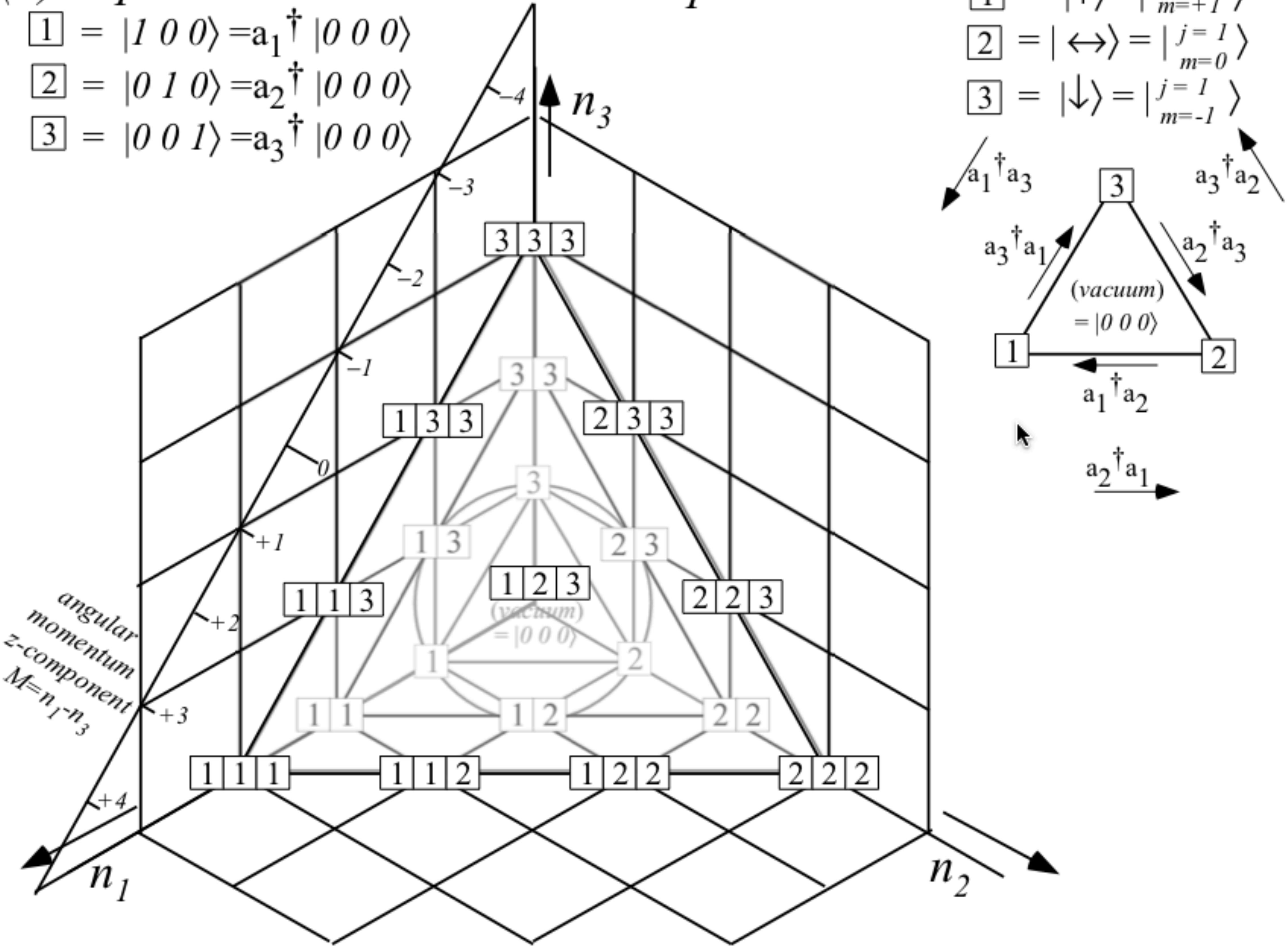
$\boxed{2} = |0\ 1\ 0\rangle = a_2^\dagger\ |0\ 0\ 0\rangle$

$\boxed{3} = |0\ 0\ 1\rangle = a_3^\dagger\ |0\ 0\ 0\rangle$

$\boxed{1} = |\uparrow\rangle = \left|{}^{j=1}_{m=+1}\right\rangle$

$\boxed{2} = |\leftrightarrow\rangle = \left|{}^{j=1}_{m=0}\right\rangle$

$\boxed{3} = |\downarrow\rangle = \left|{}^{j=1}_{m=-1}\right\rangle$



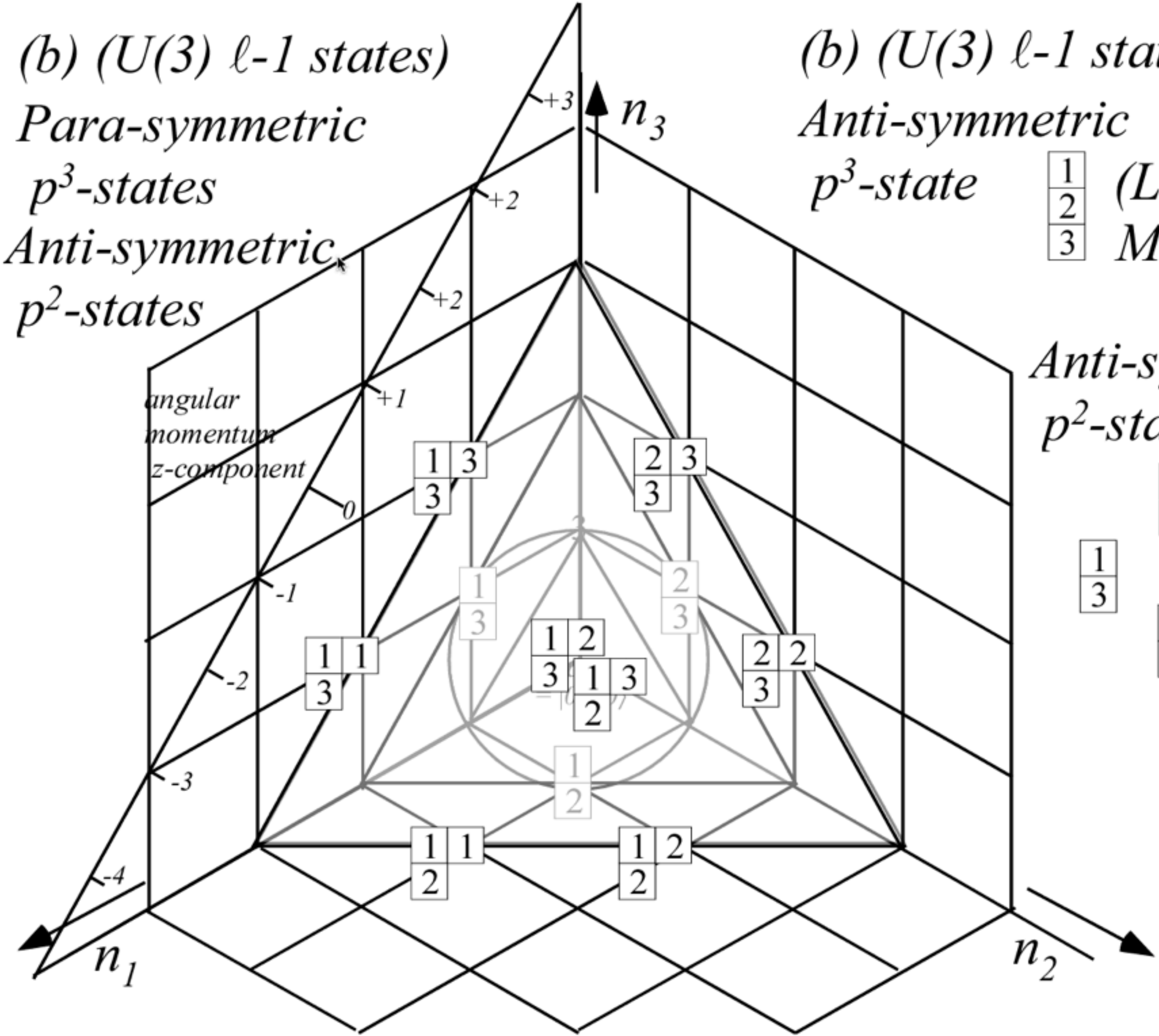
(b) (U(3) ℓ-1 states)

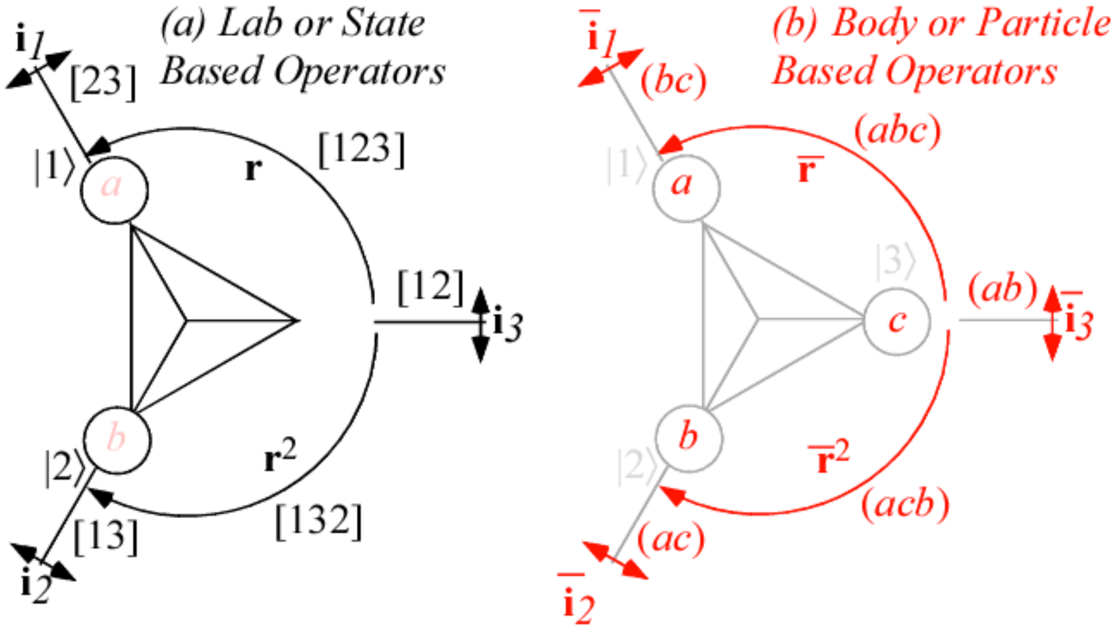
Para-symmetric
p^3-states
Anti-symmetric
p^2-states

(b) (U(3) ℓ-1 states)

Anti-symmetric
p^3-state (L=0)
M=0

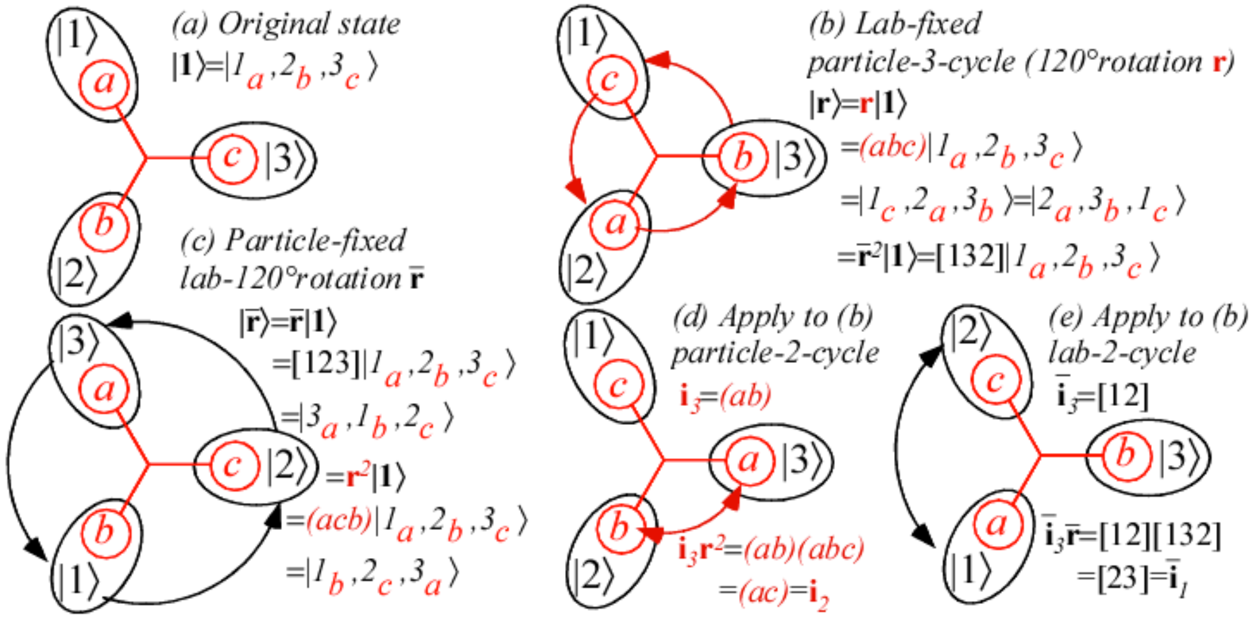
Anti-symmetric
p^2-states (L= 1
M=+1
M= 0
M=-1

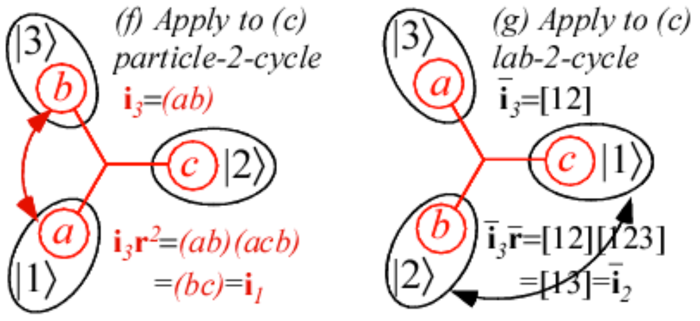


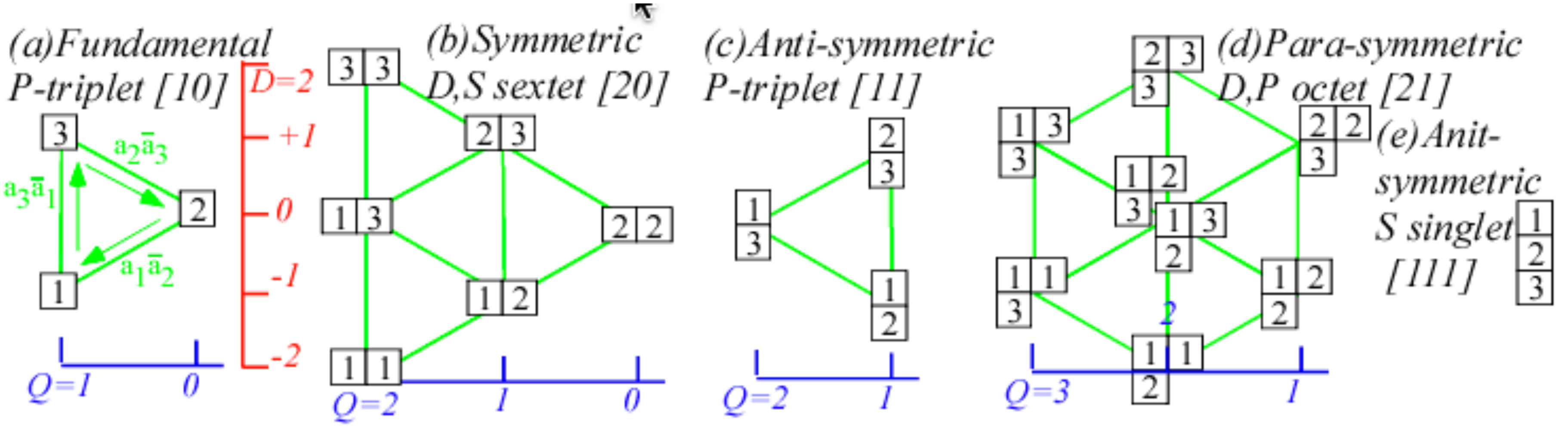


Intro 3-particle coupling.
Unit 8 Ch. 25 p28.

Intro 3,4-particle Young Tableaus
GrpThLect29 p42.







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  - *6th rank tensor example with exact splitting of f-orbital*

2^k-pole expansion of an N-by-N matrix **H**

2-by-2 case:

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

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

$$= \frac{A+D}{2}\,\mathbf{T}_0 + (B-iC)\underset{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}{\mathbf{T}_1} + (B+iC)\underset{\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}{\mathbf{T}_{-1}} + \frac{A-D}{2}\,\mathbf{T}_0$$

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

$$\mathbf{u}^1_{+1}=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \mathbf{u}^1_{0}=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \mathbf{u}^1_{-1}=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

rank-1
(vector)

$$\mathbf{u}^0_{0}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{\sqrt{2}}$$

rank-0
(scalar)

3-by-3 case:

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

Irrep Tensor building
Unit 8 Ch. 25 p5.

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

$$\mathbf{u}^2_{+2}=\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \mathbf{u}^2_{+1}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \mathbf{u}^2_{0}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}\frac{1}{\sqrt{6}} \quad \mathbf{u}^2_{-1}=\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \mathbf{u}^2_{-2}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

rank-2
(tensor)

$$\mathbf{u}^1_{+1}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \mathbf{u}^1_{0}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \mathbf{u}^1_{-1}=\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}$$

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*

Wigner-Clebsch-Gordan expressions for Tensor $\left\langle \mathbf{T}^k_q \right\rangle$

$$\left\langle {J' \atop M'} \middle| \mathbf{T}^k_q \middle| {J \atop M} \right\rangle = \begin{pmatrix} J' & k & J \\ M' & q & -M \end{pmatrix}(J'\|k\|J) = C^{k\,J\;J'}_{q\,M\,M'}\left\langle J'\|k\|J \right\rangle$$

Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors

CG-Products of spin-$^1/_2$ **ket-bras** $\left\{\left|\begin{matrix}1/2\\ m_1\end{matrix}\right\rangle, \left\langle\begin{matrix}1/2\\ m_2\end{matrix}\right|\right\}$ give scalar/vector operators analogous to: **ket-kets**

$$T_q^k = \sum_{m_1} C^{1/2\ 1/2\ k}_{m_1\ \ m_2\ \ q} \left|\begin{matrix}1/2\\ m_1\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ -m_2\end{matrix}\right| (-1)^{\frac{1}{2}-m_2}$$

analogous to:

$$\left|\begin{matrix}J & (1/2\otimes 1/2)\\ M & \end{matrix}\right\rangle = \sum_{m_1,m_2} C^{1/2\ 1/2\ J}_{m_1\ \ m_2\ \ M} \left|\begin{matrix}1/2\\ m_1\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ m_2\end{matrix}\right\rangle$$

$$T^1_{-1} = \begin{pmatrix} 0 & 0\\ -1 & 0\end{pmatrix} = -\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ 1/2\end{matrix}\right|,$$

$$T^1_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 0\\ 0 & 1\end{pmatrix} = -\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ 1/2\end{matrix}\right| - \left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ -1/2\end{matrix}\right|\right],$$

$$T^1_1 = \begin{pmatrix} 0 & 1\\ 0 & 0\end{pmatrix} = \left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ -1/2\end{matrix}\right|,$$

analogous to:

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ 1\end{matrix}\right\rangle = \left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ 0\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle + \frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ -1\end{matrix}\right\rangle = \left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle$$

$$T^0_0 = -\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0\\ 0 & 1\end{pmatrix} = -\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ 1/2\end{matrix}\right| + \left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\ -1/2\end{matrix}\right|\right].$$

analogous to:

$$\left|\begin{matrix}0(1/2\otimes 1/2)\\ 0\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle + \frac{-1}{\sqrt{2}}\left|\begin{matrix}1/2\\ -1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ 1/2\end{matrix}\right\rangle$$

1st three operators are a *vector* set with following Cartesian combinations:

$$T_x \equiv -\frac{T^1_{-1} - T^1_1}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1\\ 1 & 0\end{pmatrix} \equiv \frac{1}{\sqrt{2}}\sigma_x \equiv \sqrt{2}J_x$$

$$T_y \equiv -i\frac{T^1_{-1} + T^1_1}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i\\ i & 0\end{pmatrix} \equiv \frac{1}{\sqrt{2}}\sigma_y \equiv \sqrt{2}J_y$$

$$T_z \equiv -T^1_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix} \equiv \frac{1}{\sqrt{2}}\sigma_z \equiv \sqrt{2}J_z$$

(Some old friends!)

$$\sigma_X \to \begin{pmatrix} 0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_Y \to \begin{pmatrix} 0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_Z \to \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix},$$

Spherical vs. Cartesian operators

$$T^1_{-1} = J_-/2 = \left(J_x - iJ_y\right)/\sqrt{2}, \qquad T^1_0 = J_z/\sqrt{2}, \qquad T^1_{-1} = J_+/2 = \left(J_x + iJ_y\right)/2.$$

Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors

CG-Products of spin-$^1/_2$ **ket-bras** $\left\{\left|\begin{matrix}1/2\\m_1\end{matrix}\right\rangle,\left\langle\begin{matrix}1/2\\m_2\end{matrix}\right|\right\}$ give scalar/vector operators analogous to: **ket-kets**

$$T^k_q=\sum_{m_1}C^{1/2\ 1/2\ k}_{m_1\ \ m_2\ \ q}\left|\begin{matrix}1/2\\m_1\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-m_2\end{matrix}\right|(-1)^{\frac{1}{2}-m_2}$$

analogous to:

$$\left|\begin{matrix}J & (1/2\otimes 1/2)\\M & \end{matrix}\right\rangle=\sum_{m_1,m_2}C^{1/2\ 1/2\ J}_{m_1\ \ m_2\ \ M}\left|\begin{matrix}1/2\\m_1\end{matrix}\right\rangle\left|\begin{matrix}1/2\\m_2\end{matrix}\right\rangle$$

$$T^1_{-1}=\begin{pmatrix}0&0\\-1&0\end{pmatrix}=-\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|,\quad T^1_0=\frac{1}{\sqrt{2}}\begin{pmatrix}-1&0\\0&1\end{pmatrix}=-\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|-\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|\right],\quad T^1_1=\begin{pmatrix}0&1\\0&0\end{pmatrix}=\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|,$$

analogous to:

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\1\end{matrix}\right\rangle=\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\0\end{matrix}\right\rangle=\frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle+\frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\-1\end{matrix}\right\rangle=\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle$$

$$T^0_0=-\frac{1}{\sqrt{2}}\begin{pmatrix}1&0\\0&1\end{pmatrix}=-\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|+\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|\right].$$

analogous to:

$$\left|\begin{matrix}0(1/2\otimes 1/2)\\0\end{matrix}\right\rangle=\frac{1}{\sqrt{2}}\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle+\frac{-1}{\sqrt{2}}\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

1st three operators are a *vector* set with following Cartesian combinations:

$$R(0\beta 0)\qquad T^1_0\qquad R^\dagger(0\beta 0)\qquad = \qquad T'_0$$

$$\downarrow\qquad\downarrow\qquad\downarrow\qquad\downarrow$$

$$\begin{pmatrix}\cos\frac{\beta}{2}&-\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2}&\cos\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}-1/\sqrt{2}&0\\0&1/\sqrt{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\beta}{2}&\sin\frac{\beta}{2}\\ -\sin\frac{\beta}{2}&\cos\frac{\beta}{2}\end{pmatrix}=-\frac{1}{\sqrt{2}}\begin{pmatrix}\cos\beta&\sin\beta\\ \sin\beta&-\cos\beta\end{pmatrix}$$

$$=D^1_{10}(0\beta 0)T^1_1\qquad +D^1_{00}(0\beta 0)T^1_0\qquad +D^1_{-10}(0\beta 0)T^1_{-1}$$

$$\downarrow\qquad\downarrow\qquad\downarrow$$

$$=\frac{-\sin\beta}{\sqrt{2}}\begin{pmatrix}0&1\\0&0\end{pmatrix}+\cos\beta\begin{pmatrix}-1/\sqrt{2}&0\\0&1/\sqrt{2}\end{pmatrix}+\frac{\sin\beta}{\sqrt{2}}\begin{pmatrix}0&0\\-1&0\end{pmatrix}$$

Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors

CG-Products of spin-$^1/_2$ **ket-bras** $\left\{\left|\begin{smallmatrix}1/2\\ m_1\end{smallmatrix}\right\rangle,\left\langle\begin{smallmatrix}1/2\\ m_2\end{smallmatrix}\right|\right\}$ give scalar/vector operators analogous to: **ket-kets**

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analogous to:

$$\left|\begin{matrix}J\ (1/2\otimes 1/2)\\ M\end{matrix}\right\rangle=\sum_{m_1,m_2}C^{1/2\ 1/2\ J}_{m_1\ m_2\ M}\left|\begin{matrix}1/2\\ m_1\end{matrix}\right\rangle\left|\begin{matrix}1/2\\ m_2\end{matrix}\right\rangle$$

$$T^1_{-1}=\begin{pmatrix}0&0\\-1&0\end{pmatrix}=-\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|,\qquad T^1_0=\frac{1}{\sqrt2}\begin{pmatrix}-1&0\\0&1\end{pmatrix}=-\frac{1}{\sqrt2}\left[\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|-\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|\right],\qquad T^1_1=\begin{pmatrix}0&1\\0&0\end{pmatrix}=\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|,$$

analogous to:

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ 1\end{matrix}\right\rangle=\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ 0\end{matrix}\right\rangle=\frac{1}{\sqrt2}\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle+\frac{1}{\sqrt2}\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

$$\left|\begin{matrix}1(1/2\otimes 1/2)\\ -1\end{matrix}\right\rangle=\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle$$

$$T^0_0=-\frac{1}{\sqrt2}\begin{pmatrix}1&0\\0&1\end{pmatrix}=-\frac{1}{\sqrt2}\left[\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\1/2\end{matrix}\right|+\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left\langle\begin{matrix}1/2\\-1/2\end{matrix}\right|\right].$$

analogous to:

$$\left|\begin{matrix}0(1/2\otimes 1/2)\\ 0\end{matrix}\right\rangle=\frac{1}{\sqrt2}\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle-\frac{1}{\sqrt2}\left|\begin{matrix}1/2\\-1/2\end{matrix}\right\rangle\left|\begin{matrix}1/2\\1/2\end{matrix}\right\rangle$$

1st three operators are a *vector* set with following Cartesian combinations:

$$\begin{matrix}R(0\beta0) & T^1_0 & R^\dagger(0\beta0) & = & T'_0\\ \downarrow & \downarrow & \downarrow & & \downarrow\end{matrix}$$

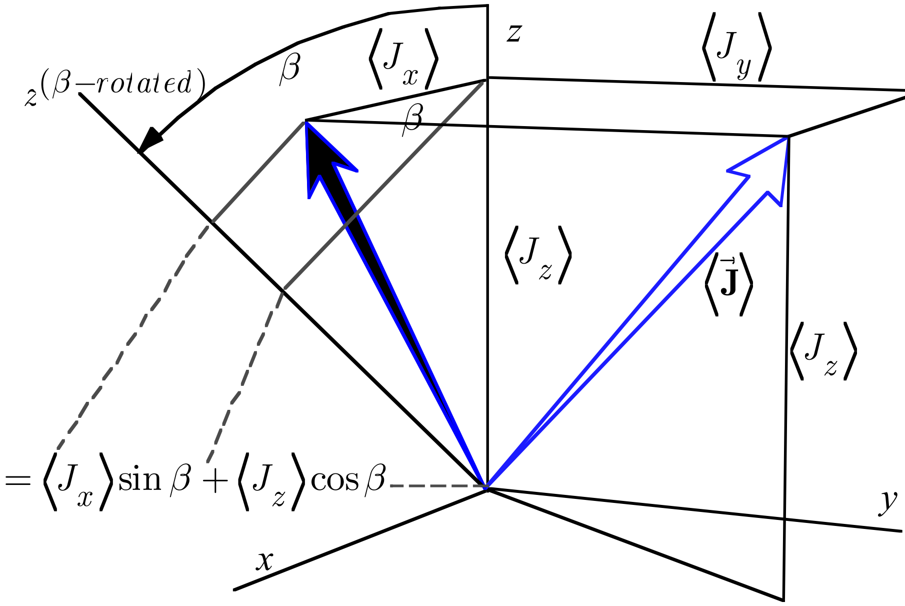
$$\begin{pmatrix}\cos\frac{\beta}{2}&-\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2}&\cos\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}-1/\sqrt2&0\\0&1/\sqrt2\end{pmatrix}\begin{pmatrix}\cos\frac{\beta}{2}&\sin\frac{\beta}{2}\\ -\sin\frac{\beta}{2}&\cos\frac{\beta}{2}\end{pmatrix}=-\frac{1}{\sqrt2}\begin{pmatrix}\cos\beta&\sin\beta\\ \sin\beta&-\cos\beta\end{pmatrix}$$

$$=D^1_{10}(0\beta0)T^1_1+D^1_{00}(0\beta0)T^1_0+D^1_{-10}(0\beta0)T^1_{-1}$$

$$\downarrow\qquad\qquad\downarrow\qquad\qquad\downarrow$$

$$=\frac{-\sin\beta}{\sqrt2}\begin{pmatrix}0&1\\0&0\end{pmatrix}+\cos\beta\begin{pmatrix}-1/\sqrt2&0\\0&1/\sqrt2\end{pmatrix}+\frac{\sin\beta}{\sqrt2}\begin{pmatrix}0&0\\-1&0\end{pmatrix}$$

So do expectation values:



$$\langle J_z(\beta-rotated)\rangle=\langle J_x\rangle\sin\beta+\langle J_z\rangle\cos\beta$$

AMOP reference links on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure

- *Kronecker product states and operators*
- *Spin-spin interaction reduces symmetry $U(2)^{proton}\times U(2)^{electron}$ to $U(2)^{e+p}$*
  - *Elementary ½ × ½ Clebsch-Gordan coefficients*
- *Hydrogen hyperfine levels: Fermi-contact interaction, Racah's trick for energy eigenvalues*
  - *B-field gives avoided crossing*

Higher-J product states: $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$ case

- *Effect of Pauli-Fermi-Dirac symmetry*
- *General U(2) Clebsch-Gordan-Wigner-3j coupling coefficient formula*
  - *LS to jj Level corralations*
- *Angular momentum uncertainty cones related to 3j coefficients*

Multi-spin $(1/2)^N$ product states Magic squares

- *Intro to U(2) Young Tableaus*
- *Intro to U(3) and higher Young Tableaus and Lab-Bod or Particle-State summitry*

U(2) and U(3) tensor expansion of H operator

- *Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors*
- *Tensor operators for spin-1 states: U(3) generalization of Pauli spinors*
  - *4th rank tensor example with exact splitting of d-orbital*
  - *6th rank tensor example with exact splitting of f-orbital*

Tensor operators for spin-1 states: U(1) generalization of Pauli spinors

CGC definition:

$$\mathbf{v}^k_q = \sum_{m,m'} C^{j\ \ j\ \ \ k}_{m\ -m'\ q}(-1)^{j-m'}\left|\begin{matrix}j\\m\end{matrix}\right\rangle\left\langle\begin{matrix}j\\m'\end{matrix}\right| = (-1)^{2j}\,T^k_q .$$

Wigner 3jm definition:

$$\mathbf{v}^k_q = \sum_{m,m'} (-1)^{j-m}\sqrt{2k+1}\begin{pmatrix}k & j & j\\ q & m' & -m\end{pmatrix}\left|\begin{matrix}j\\m\end{matrix}\right\rangle\left\langle\begin{matrix}j\\m'\end{matrix}\right|$$

k=2

Quadrupole tensor T[2] *row*

$$T^2_{-2} = \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right|, \quad T^2_{-1} = \frac{\left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| - \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right|}{\sqrt{2}}, \quad T^2_{0} = \frac{\left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| - 2\left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| + \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right|}{\sqrt{6}}, \quad T^2_{1} = \frac{-\left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| + \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right|}{\sqrt{2}}, \quad T^2_{2} = \left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right|$$

$$\rightarrow\begin{pmatrix}0&0&0\\0&0&0\\1&0&0\end{pmatrix} \quad \rightarrow\begin{pmatrix}0&0&0\\1/\sqrt{2}&0&0\\0&-1/\sqrt{2}&0\end{pmatrix} \quad \rightarrow\begin{pmatrix}1/\sqrt{6}&0&0\\0&-2/\sqrt{6}&0\\0&0&1/\sqrt{6}\end{pmatrix} \quad \rightarrow\begin{pmatrix}0&-1/\sqrt{2}&0\\0&0&1/\sqrt{2}\\0&0&0\end{pmatrix} \quad \rightarrow\begin{pmatrix}0&0&1\\0&0&0\\0&0&0\end{pmatrix}$$

k=1

Dipole vector T[1] *row*

$$T^1_{-1} = \frac{\left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| + \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right|}{\sqrt{2}}, \quad T^1_{0} = \frac{\left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| - \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right|}{\sqrt{2}}, \quad T^1_{1} = \frac{-\left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| - \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right|}{\sqrt{2}}$$

$$\rightarrow\begin{pmatrix}0&0&0\\1/\sqrt{2}&0&0\\0&1/\sqrt{2}&0\end{pmatrix} \quad \rightarrow\begin{pmatrix}1/\sqrt{2}&0&0\\0&0&0\\0&0&-1/\sqrt{2}\end{pmatrix} \quad \rightarrow\begin{pmatrix}0&-1/\sqrt{2}&0\\0&0&-1/\sqrt{2}\\0&0&0\end{pmatrix}$$

k=0

Monopole scalar T[0] *invariant*

$$T^0_{0} = \frac{\left|\begin{smallmatrix}1\\1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\1\end{smallmatrix}\right| + \left|\begin{smallmatrix}1\\0\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\0\end{smallmatrix}\right| + \left|\begin{smallmatrix}1\\-1\end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix}1\\-1\end{smallmatrix}\right|}{\sqrt{3}}$$

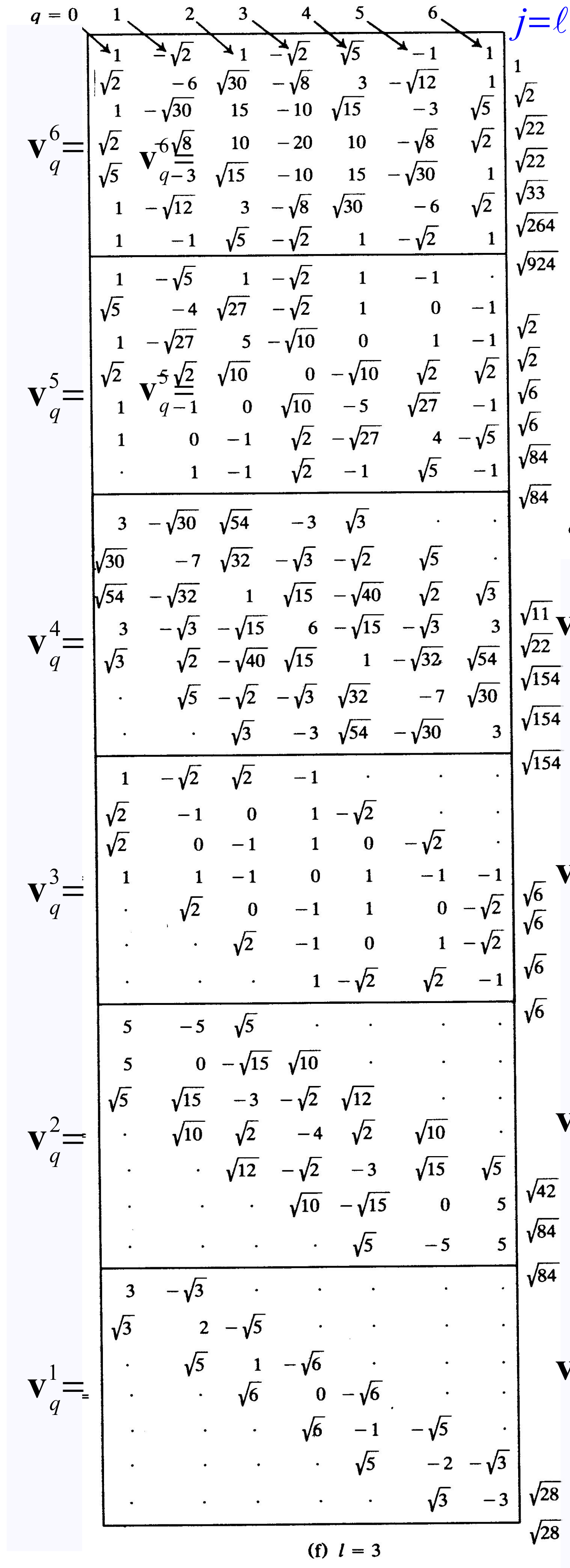
$$\rightarrow\begin{pmatrix}1/\sqrt{3}&0&0\\0&1/\sqrt{3}&0\\0&0&1/\sqrt{3}\end{pmatrix}$$

Irrep Tensor building
Unit 8 Ch. 25 p5.

Tensor operators for spin-j states:
U(2*j*+1) *generalization of Pauli spinors*

$$\mathbf{v}^{k}_{q}=\sum_{m,m'}(-1)^{j-m}\sqrt{2k+1}\begin{pmatrix}k & j & j\\ q & m' & -m\end{pmatrix}\left|\begin{matrix}j\\ m\end{matrix}\right\rangle\left\langle\begin{matrix}j\\ m'\end{matrix}\right|$$

Tables for j=1 (p-shell), j=2 (d-shell), j=3 (f-shell),...



$j=\ell=3$

$q=0$ 1 2 3 4 5 6

$$\mathbf{v}^{6}_{q}=\begin{array}{ccccccc}1 & -\sqrt{2} & 1 & -\sqrt{2} & \sqrt{5} & -1 & 1\\ \sqrt{2} & -6 & \sqrt{30} & -\sqrt{8} & 3 & -\sqrt{12} & 1\\ 1 & -\sqrt{30} & 15 & -10 & \sqrt{15} & -3 & \sqrt{5}\\ \sqrt{2} & -\sqrt{8} & 10 & -20 & 10 & -\sqrt{8} & \sqrt{2}\\ \sqrt{5} & -3 & \sqrt{15} & -10 & 15 & -\sqrt{30} & 1\\ 1 & -\sqrt{12} & 3 & -\sqrt{8} & \sqrt{30} & -6 & \sqrt{2}\\ 1 & -1 & \sqrt{5} & -\sqrt{2} & 1 & -\sqrt{2} & 1\end{array}$$

1, $\sqrt{2}$, $\sqrt{22}$, $\sqrt{22}$, $\sqrt{33}$, $\sqrt{264}$, $\sqrt{924}$

$$\mathbf{v}^{5}_{q}=\begin{array}{ccccccc}1 & -\sqrt{5} & 1 & -\sqrt{2} & 1 & -1 & \cdot\\ \sqrt{5} & -4 & \sqrt{27} & -\sqrt{2} & 1 & 0 & -1\\ 1 & -\sqrt{27} & 5 & -\sqrt{10} & 0 & 1 & -1\\ \sqrt{2} & -\sqrt{2} & \sqrt{10} & 0 & -\sqrt{10} & \sqrt{2} & \sqrt{2}\\ 1 & -1 & 0 & \sqrt{10} & -5 & \sqrt{27} & -1\\ 1 & 0 & -1 & \sqrt{2} & -\sqrt{27} & 4 & -\sqrt{5}\\ \cdot & 1 & -1 & \sqrt{2} & -1 & \sqrt{5} & -1\end{array}$$

$\sqrt{2}$, $\sqrt{2}$, $\sqrt{6}$, $\sqrt{6}$, $\sqrt{84}$, $\sqrt{84}$

$$\mathbf{v}^{4}_{q}=\begin{array}{ccccccc}3 & -\sqrt{30} & \sqrt{54} & -3 & \sqrt{3} & \cdot & \cdot\\ \sqrt{30} & -7 & \sqrt{32} & -\sqrt{3} & -\sqrt{2} & \sqrt{5} & \cdot\\ \sqrt{54} & -\sqrt{32} & 1 & \sqrt{15} & -\sqrt{40} & \sqrt{2} & \sqrt{3}\\ 3 & -\sqrt{3} & -\sqrt{15} & 6 & -\sqrt{15} & -\sqrt{3} & 3\\ \sqrt{3} & \sqrt{2} & -\sqrt{40} & \sqrt{15} & 1 & -\sqrt{32} & \sqrt{54}\\ \cdot & \sqrt{5} & -\sqrt{2} & -\sqrt{3} & \sqrt{32} & -7 & \sqrt{30}\\ \cdot & \cdot & \sqrt{3} & -3 & \sqrt{54} & -\sqrt{30} & 3\end{array}$$

$\sqrt{11}$, $\sqrt{22}$, $\sqrt{154}$, $\sqrt{154}$, $\sqrt{154}$

$$\mathbf{v}^{3}_{q}=\begin{array}{ccccccc}1 & -\sqrt{2} & \sqrt{2} & -1 & \cdot & \cdot & \cdot\\ \sqrt{2} & -1 & 0 & 1 & -\sqrt{2} & \cdot & \cdot\\ \sqrt{2} & 0 & -1 & 1 & 0 & -\sqrt{2} & \cdot\\ 1 & 1 & -1 & 0 & 1 & -1 & -1\\ \cdot & \sqrt{2} & 0 & -1 & 1 & 0 & -\sqrt{2}\\ \cdot & \cdot & \sqrt{2} & -1 & 0 & 1 & -\sqrt{2}\\ \cdot & \cdot & \cdot & 1 & -\sqrt{2} & \sqrt{2} & -1\end{array}$$

$\sqrt{6}$, $\sqrt{6}$, $\sqrt{6}$, $\sqrt{6}$

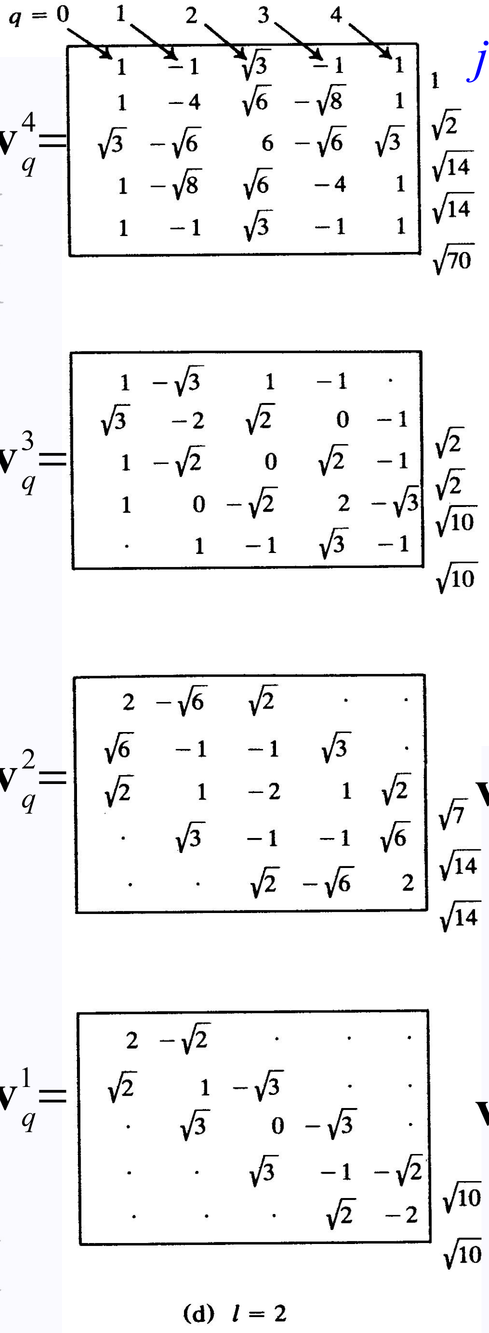
$$\mathbf{v}^{2}_{q}=\begin{array}{ccccccc}5 & -5 & \sqrt{5} & \cdot & \cdot & \cdot & \cdot\\ 5 & 0 & -\sqrt{15} & \sqrt{10} & \cdot & \cdot & \cdot\\ \sqrt{5} & \sqrt{15} & -3 & -\sqrt{2} & \sqrt{12} & \cdot & \cdot\\ \cdot & \sqrt{10} & \sqrt{2} & -4 & \sqrt{2} & \sqrt{10} & \cdot\\ \cdot & \cdot & \sqrt{12} & -\sqrt{2} & -3 & \sqrt{15} & \sqrt{5}\\ \cdot & \cdot & \cdot & \sqrt{10} & -\sqrt{15} & 0 & 5\\ \cdot & \cdot & \cdot & \cdot & \sqrt{5} & -5 & 5\end{array}$$

$\sqrt{42}$, $\sqrt{84}$, $\sqrt{84}$

$$\mathbf{v}^{1}_{q}=\begin{array}{ccccccc}3 & -\sqrt{3} & \cdot & \cdot & \cdot & \cdot & \cdot\\ \sqrt{3} & 2 & -\sqrt{5} & \cdot & \cdot & \cdot & \cdot\\ \cdot & \sqrt{5} & 1 & -\sqrt{6} & \cdot & \cdot & \cdot\\ \cdot & \cdot & \sqrt{6} & 0 & -\sqrt{6} & \cdot & \cdot\\ \cdot & \cdot & \cdot & \sqrt{6} & -1 & -\sqrt{5} & \cdot\\ \cdot & \cdot & \cdot & \cdot & \sqrt{5} & -2 & -\sqrt{3}\\ \cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{3} & -3\end{array}$$

$\sqrt{28}$, $\sqrt{28}$

(f) $l=3$



$j=\ell=2$

$q=0$ 1 2 3 4

$$\mathbf{v}^{4}_{q}=\begin{array}{ccccc}1 & -1 & \sqrt{3} & -1 & 1\\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1\\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3}\\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1\\ 1 & -1 & \sqrt{3} & -1 & 1\end{array}$$

1, $\sqrt{2}$, $\sqrt{14}$, $\sqrt{14}$, $\sqrt{70}$

$$\mathbf{v}^{3}_{q}=\begin{array}{ccccc}1 & -\sqrt{3} & 1 & -1 & \cdot\\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1\\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1\\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3}\\ \cdot & 1 & -1 & \sqrt{3} & -1\end{array}$$

$\sqrt{2}$, $\sqrt{2}$, $\sqrt{10}$, $\sqrt{10}$

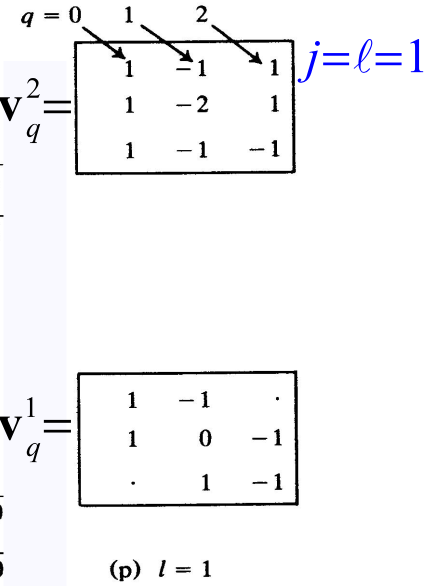
$$\mathbf{v}^{2}_{q}=\begin{array}{ccccc}2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot\\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot\\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2}\\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6}\\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2\end{array}$$

$\sqrt{7}$, $\sqrt{14}$, $\sqrt{14}$

$$\mathbf{v}^{1}_{q}=\begin{array}{ccccc}2 & -\sqrt{2} & \cdot & \cdot & \cdot\\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot\\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot\\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2}\\ \cdot & \cdot & \cdot & \sqrt{2} & -2\end{array}$$

$\sqrt{10}$, $\sqrt{10}$

(d) $l=2$



$j=\ell=1$

$q=0$ 1 2

$$\mathbf{v}^{2}_{q}=\begin{array}{ccc}1 & -1 & 1\\ 1 & -2 & 1\\ 1 & -1 & -1\end{array}$$

$$\mathbf{v}^{1}_{q}=\begin{array}{ccc}1 & -1 & \cdot\\ 1 & 0 & -1\\ \cdot & 1 & -1\end{array}$$

(p) $l=1$

Irrep Tensor Tables
Unit 8 Ch. 25 p12.

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

Tensor operators $\mathbf{v}^k_q$ *for spin-j states:*
U(2*j*+1) *generalization of Pauli spinors*

$$\mathbf{v}^k_q = \sum_{m,m'} (-1)^{j-m}\sqrt{2k+1}\begin{pmatrix} k & j & j \\ q & m' & -m \end{pmatrix} \left| \begin{matrix} j \\ m \end{matrix} \right\rangle\!\left\langle \begin{matrix} j \\ m' \end{matrix} \right|$$

Tables for $j=1$ (*p-shell*), $j=2$ (*d-shell*), $j=3$ (*f-shell*),... *and* $j=\frac{1}{2}, j=\frac{3}{2}, j=\frac{5}{2}$ ....

$j=\ell=3$

$$\mathbf{v}^6_q=\begin{array}{ccccccc|c}
q=0 & 1 & 2 & 3 & 4 & 5 & 6 & \\
\hline
1 & -\sqrt{2} & 1 & -\sqrt{2} & \sqrt{5} & -1 & 1 & 1\\
\sqrt{2} & -6 & \sqrt{30} & -\sqrt{8} & 3 & -\sqrt{12} & 1 & \sqrt{2}\\
1 & -\sqrt{30} & 15 & -10 & \sqrt{15} & -3 & \sqrt{5} & \sqrt{22}\\
\sqrt{2} & -\sqrt{8} & 10 & -20 & 10 & -\sqrt{8} & \sqrt{2} & \sqrt{22}\\
\sqrt{5} & -3 & \sqrt{15} & -10 & 15 & -\sqrt{30} & 1 & \sqrt{33}\\
1 & -\sqrt{12} & 3 & -\sqrt{8} & \sqrt{30} & -6 & \sqrt{2} & \sqrt{264}\\
1 & -1 & \sqrt{5} & -\sqrt{2} & 1 & -\sqrt{2} & 1 & \sqrt{924}
\end{array}$$

$$\mathbf{v}^5_q=\begin{array}{ccccccc|c}
1 & -\sqrt{5} & 1 & -\sqrt{2} & 1 & -1 & \cdot & \\
\sqrt{5} & -4 & \sqrt{27} & -\sqrt{2} & 1 & 0 & -1 & \sqrt{2}\\
1 & -\sqrt{27} & 5 & -\sqrt{10} & 0 & 1 & -1 & \sqrt{2}\\
\sqrt{2} & -\sqrt{2} & \sqrt{10} & 0 & -\sqrt{10} & \sqrt{2} & \sqrt{2} & \sqrt{6}\\
1 & -1 & 0 & \sqrt{10} & -5 & \sqrt{27} & -1 & \sqrt{6}\\
1 & 0 & -1 & \sqrt{2} & -\sqrt{27} & 4 & -\sqrt{5} & \sqrt{84}\\
\cdot & 1 & -1 & \sqrt{2} & -1 & \sqrt{5} & -1 & \sqrt{84}
\end{array}$$

$$\mathbf{v}^4_q=\begin{array}{ccccccc|c}
3 & -\sqrt{30} & \sqrt{54} & -3 & \sqrt{3} & \cdot & \cdot & \\
\sqrt{30} & -7 & \sqrt{32} & -\sqrt{3} & -\sqrt{2} & \sqrt{5} & \cdot & \\
\sqrt{54} & -\sqrt{32} & 1 & \sqrt{15} & -\sqrt{40} & \sqrt{2} & \sqrt{3} & \sqrt{11}\\
3 & -\sqrt{3} & -\sqrt{15} & 6 & -\sqrt{15} & -\sqrt{3} & 3 & \sqrt{22}\\
\sqrt{3} & \sqrt{2} & -\sqrt{40} & \sqrt{15} & 1 & -\sqrt{32} & \sqrt{54} & \sqrt{154}\\
\cdot & \sqrt{5} & -\sqrt{2} & -\sqrt{3} & \sqrt{32} & -7 & \sqrt{30} & \sqrt{154}\\
\cdot & \cdot & \sqrt{3} & -3 & \sqrt{54} & -\sqrt{30} & 3 & \sqrt{154}
\end{array}$$

$$\mathbf{v}^3_q=\begin{array}{ccccccc|c}
1 & -\sqrt{2} & \sqrt{2} & -1 & \cdot & \cdot & \cdot & \\
\sqrt{2} & -1 & 0 & 1 & -\sqrt{2} & \cdot & \cdot & \\
\sqrt{2} & 0 & -1 & 1 & 0 & -\sqrt{2} & \cdot & \\
1 & 1 & -1 & 0 & 1 & -1 & -1 & \sqrt{6}\\
\cdot & \sqrt{2} & 0 & -1 & 1 & 0 & -\sqrt{2} & \sqrt{6}\\
\cdot & \cdot & \sqrt{2} & -1 & 0 & 1 & -\sqrt{2} & \sqrt{6}\\
\cdot & \cdot & \cdot & 1 & -\sqrt{2} & \sqrt{2} & -1 & \sqrt{6}
\end{array}$$

$$\mathbf{v}^2_q=\begin{array}{ccccccc|c}
5 & -5 & \sqrt{5} & \cdot & \cdot & \cdot & \cdot & \\
5 & 0 & -\sqrt{15} & \sqrt{10} & \cdot & \cdot & \cdot & \\
\sqrt{5} & \sqrt{15} & -3 & -\sqrt{2} & \sqrt{12} & \cdot & \cdot & \\
\cdot & \sqrt{10} & \sqrt{2} & -4 & \sqrt{2} & \sqrt{10} & \cdot & \\
\cdot & \cdot & \sqrt{12} & -\sqrt{2} & -3 & \sqrt{15} & \sqrt{5} & \sqrt{42}\\
\cdot & \cdot & \cdot & \sqrt{10} & -\sqrt{15} & 0 & 5 & \sqrt{84}\\
\cdot & \cdot & \cdot & \cdot & \sqrt{5} & -5 & 5 & \sqrt{84}
\end{array}$$

$$\mathbf{v}^1_q=\begin{array}{ccccccc|c}
3 & -\sqrt{3} & \cdot & \cdot & \cdot & \cdot & \cdot & \\
\sqrt{3} & 2 & -\sqrt{5} & \cdot & \cdot & \cdot & \cdot & \\
\cdot & \sqrt{5} & 1 & -\sqrt{6} & \cdot & \cdot & \cdot & \\
\cdot & \cdot & \sqrt{6} & 0 & -\sqrt{6} & \cdot & \cdot & \\
\cdot & \cdot & \cdot & \sqrt{6} & -1 & -\sqrt{5} & \cdot & \\
\cdot & \cdot & \cdot & \cdot & \sqrt{5} & -2 & -\sqrt{3} & \sqrt{28}\\
\cdot & \cdot & \cdot & \cdot & \cdot & \sqrt{3} & -3 & \sqrt{28}
\end{array}$$

(f) $l = 3$

$j=\ell=2$

$$\mathbf{v}^4_q=\begin{array}{ccccc|c}
q=0 & 1 & 2 & 3 & 4 & \\
\hline
1 & -1 & \sqrt{3} & -1 & 1 & 1\\
1 & -4 & \sqrt{6} & -\sqrt{8} & 1 & \sqrt{2}\\
\sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} & \sqrt{14}\\
1 & -\sqrt{8} & \sqrt{6} & -4 & 1 & \sqrt{14}\\
1 & -1 & \sqrt{3} & -1 & 1 & \sqrt{70}
\end{array}$$

$$\mathbf{v}^3_q=\begin{array}{ccccc|c}
1 & -\sqrt{3} & 1 & -1 & \cdot & \\
\sqrt{3} & -2 & \sqrt{2} & 0 & -1 & \sqrt{2}\\
1 & -\sqrt{2} & 0 & \sqrt{2} & -1 & \sqrt{2}\\
1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} & \sqrt{10}\\
\cdot & 1 & -1 & \sqrt{3} & -1 & \sqrt{10}
\end{array}$$

$$\mathbf{v}^2_q=\begin{array}{ccccc|c}
2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot & \\
\sqrt{6} & -1 & -1 & \sqrt{3} & \cdot & \\
\sqrt{2} & 1 & -2 & 1 & \sqrt{2} & \sqrt{7}\\
\cdot & \sqrt{3} & -1 & -1 & \sqrt{6} & \sqrt{14}\\
\cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 & \sqrt{14}
\end{array}$$

$$\mathbf{v}^1_q=\begin{array}{ccccc|c}
2 & -\sqrt{2} & \cdot & \cdot & \cdot & \\
\sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot & \\
\cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot & \\
\cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} & \sqrt{10}\\
\cdot & \cdot & \cdot & \sqrt{2} & -2 & \sqrt{10}
\end{array}$$

(d) $l = 2$

$j=\ell=1$

$$\mathbf{v}^2_q=\begin{array}{ccc}
q=0 & 1 & 2\\
\hline
1 & -1 & 1\\
1 & -2 & 1\\
1 & -1 & -1
\end{array}$$

$$\mathbf{v}^1_q=\begin{array}{ccc}
1 & -1 & \cdot\\
1 & 0 & -1\\
\cdot & 1 & -1
\end{array}$$

(p) $l = 1$

(a) $j = \frac{1}{2}$

$$\mathbf{v}^1_q=\begin{array}{cc|c}
 & 1 & \\
\hline
1 & -1 & 1\\
1 & -1 & \sqrt{2}
\end{array}$$

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

(b) $j = \frac{3}{2}$

$$\mathbf{v}^1_q=\begin{array}{cccc|c}
q=0 & 1 & 2 & 3 & \\
\hline
3 & -\sqrt{3} & \cdot & \cdot & \\
\sqrt{3} & 1 & -2 & \cdot & \\
\cdot & 2 & -1 & -\sqrt{3} & \sqrt{10}\\
\cdot & \cdot & \sqrt{3} & -3 & \sqrt{20}
\end{array}$$

$$\mathbf{v}^2_q=\begin{array}{cccc|c}
1 & -1 & 1 & \cdot & \\
1 & -1 & 0 & 1 & \sqrt{2}\\
1 & 0 & -1 & 1 & \sqrt{2}\\
\cdot & 1 & -1 & 1 & \sqrt{4}
\end{array}$$

$$\mathbf{v}^3_q=\begin{array}{cccc|c}
1 & -1 & 1 & -1 & 1\\
1 & -3 & \sqrt{3} & -1 & \sqrt{2}\\
1 & -\sqrt{3} & 3 & -1 & \sqrt{5}\\
1 & -1 & 1 & -1 & \sqrt{20}
\end{array}$$

$j=\frac{3}{2}$

(c) $j = \frac{5}{2}$

$$\mathbf{v}^1_q=\begin{array}{cccccc|c}
q=0 & 1 & 2 & 3 & 4 & 5 & \\
\hline
5 & -\sqrt{5} & \cdot & \cdot & \cdot & \cdot & \\
\sqrt{5} & 3 & -\sqrt{8} & \cdot & \cdot & \cdot & \\
\cdot & \sqrt{8} & 1 & -3 & \cdot & \cdot & \\
\cdot & \cdot & 3 & -1 & -\sqrt{8} & \cdot & \\
\cdot & \cdot & \cdot & \sqrt{8} & -3 & -\sqrt{5} & \sqrt{35}\\
\cdot & \cdot & \cdot & \cdot & \sqrt{5} & -5 & \sqrt{70}
\end{array}$$

$$\mathbf{v}^2_q=\begin{array}{cccccc|c}
5 & -\sqrt{5} & \sqrt{5} & \cdot & \cdot & \cdot & \\
\sqrt{5} & -1 & -\sqrt{2} & 3 & \cdot & \cdot & \\
\sqrt{5} & \sqrt{2} & -4 & 0 & 3 & \cdot & \\
\cdot & 3 & 0 & -4 & \sqrt{2} & \sqrt{5} & \sqrt{28}\\
\cdot & \cdot & 3 & -\sqrt{2} & -1 & \sqrt{5} & \sqrt{14}\\
\cdot & \cdot & \cdot & \sqrt{5} & -\sqrt{5} & 5 & \sqrt{84}
\end{array}$$

$$\mathbf{v}^3_q=\begin{array}{cccccc|c}
5 & -\sqrt{10} & \sqrt{5} & -\sqrt{5} & \cdot & \cdot & \\
\sqrt{10} & -7 & 1 & 1 & -\sqrt{8} & \cdot & \\
\sqrt{5} & -1 & -4 & \sqrt{8} & -1 & -\sqrt{5} & \sqrt{18}\\
\sqrt{5} & 1 & -\sqrt{8} & 4 & 1 & -\sqrt{5} & \sqrt{12}\\
\cdot & \sqrt{8} & -1 & -1 & 7 & -\sqrt{10} & \sqrt{30}\\
\cdot & \cdot & \sqrt{5} & -\sqrt{5} & \sqrt{10} & -5 & \sqrt{180}
\end{array}$$

$$\mathbf{v}^4_q=\begin{array}{cccccc|c}
1 & -\sqrt{2} & 3 & -1 & 1 & \cdot & \\
\sqrt{2} & -3 & \sqrt{5} & -\sqrt{5} & 0 & 1 & \sqrt{2}\\
3 & -\sqrt{5} & 2 & 0 & -\sqrt{5} & 1 & \sqrt{2}\\
1 & -\sqrt{5} & 0 & 2 & -\sqrt{5} & 3 & \sqrt{28}\\
1 & 0 & -\sqrt{5} & \sqrt{5} & -3 & \sqrt{2} & \sqrt{14}\\
\cdot & 1 & -1 & 3 & -\sqrt{2} & 1 & \sqrt{28}
\end{array}$$

$$\mathbf{v}^5_q=\begin{array}{cccccc|c}
1 & -1 & 1 & -\sqrt{2} & 1 & -1 & 1\\
1 & -5 & \sqrt{10} & -\sqrt{5} & \sqrt{5} & -1 & \sqrt{2}\\
1 & -\sqrt{10} & 10 & -\sqrt{20} & \sqrt{5} & -\sqrt{2} & \sqrt{9}\\
\sqrt{2} & -\sqrt{5} & \sqrt{20} & -10 & \sqrt{10} & -1 & \sqrt{12}\\
1 & -\sqrt{5} & \sqrt{5} & -\sqrt{10} & 5 & -1 & \sqrt{42}\\
1 & -1 & \sqrt{2} & -1 & 1 & -1 & \sqrt{252}
\end{array}$$

$j=\frac{5}{2}$

Octahedral 4th-rank A_{1g} tensor operator $\mathrm{T}^{[4]}$*: Application to splitting* d*-orbital (l=j=2)*

$$\mathbf{T}^{[4]}(A_{1g}) = D\left[x^4+y^4+z^4-\tfrac{3}{4}r^4\right] = D\left[\frac{2}{\sqrt{70}}\left(X_4^4+X_{-4}^4\right)+\tfrac{2}{5}X_0^4\right]$$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = D\left\langle \frac{2}{\sqrt{70}}\left(\mathbf{v}_4^4+\mathbf{v}_{-4}^4\right)+\tfrac{2}{5}\mathbf{v}_0^4\right\rangle_{j=2}\frac{\sqrt{5}}{3}\left\langle 2\left\|\mathrm{v}^4\right\|2\right\rangle.$$

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

j=ℓ=2

$$\mathbf{v}_q^4 = \begin{array}{ccccc} q=0 & 1 & 2 & 3 & 4 \\ \hline 1 & -1 & \sqrt{3} & -1 & 1 \\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1 \\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} \\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1 \\ 1 & -1 & \sqrt{3} & -1 & 1 \end{array} \quad \begin{array}{c} 1 \\ \sqrt{2} \\ \sqrt{14} \\ \sqrt{14} \\ \sqrt{70} \end{array}$$

$$\mathbf{v}_q^3 = \begin{array}{|ccccc|} \hline 1 & -\sqrt{3} & 1 & -1 & \cdot \\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1 \\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1 \\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} \\ \cdot & 1 & -1 & \sqrt{3} & -1 \\ \hline \end{array} \quad \begin{array}{c} \sqrt{2} \\ \sqrt{2} \\ \sqrt{10} \\ \sqrt{10} \end{array}$$

$$\mathbf{v}_q^2 = \begin{array}{|ccccc|} \hline 2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot \\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot \\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2} \\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6} \\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 \\ \hline \end{array} \quad \begin{array}{c} \sqrt{7} \\ \sqrt{14} \\ \sqrt{14} \end{array}$$

$$\mathbf{v}_q^1 = \begin{array}{|ccccc|} \hline 2 & -\sqrt{2} & \cdot & \cdot & \cdot \\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot \\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot \\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} \\ \cdot & \cdot & \cdot & \sqrt{2} & -2 \\ \hline \end{array} \quad \begin{array}{c} \sqrt{10} \\ \sqrt{10} \end{array}$$

(d) $l = 2$

j=ℓ=1

$$\mathbf{v}_q^2 = \begin{array}{ccc} q=0 & 1 & 2 \\ \hline 1 & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & -1 \end{array}$$

$$\mathbf{v}_q^1 = \begin{array}{|ccc|} \hline 1 & -1 & \cdot \\ 1 & 0 & -1 \\ \cdot & 1 & -1 \\ \hline \end{array}$$

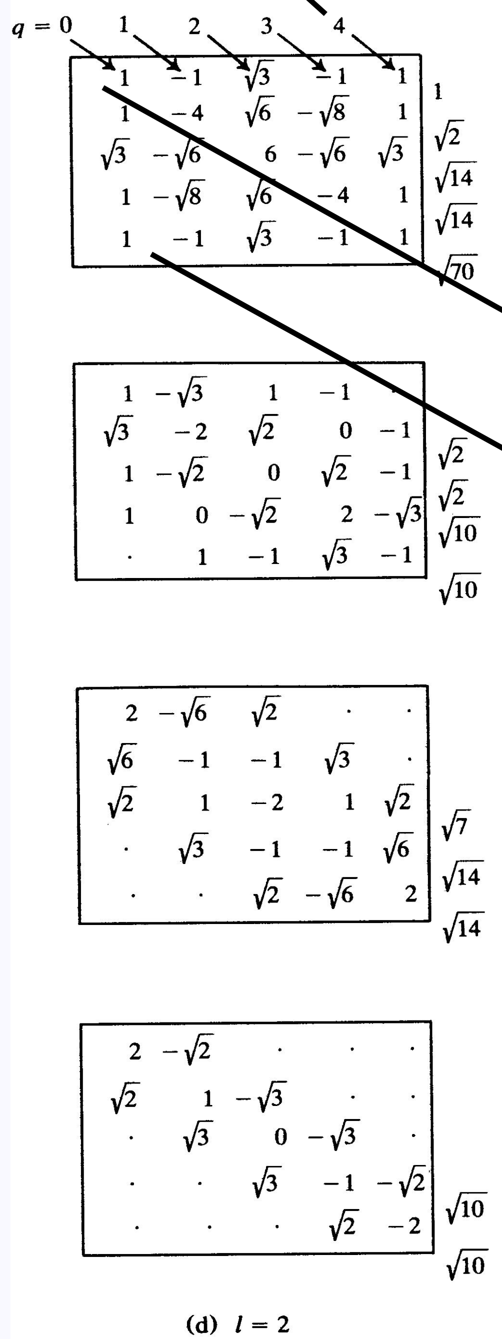
(p) $l = 1$

$_g$ *tensor operator* T$^{[4]}$*: Application to splitting* d*-orbital (l=j=2)*

$$^4 + z^4 - \tfrac{3}{4} r^4 \Big] = D\left[\frac{2}{\sqrt{70}}\left(X_4^4 + X_{-4}^4\right) + \tfrac{2}{5} X_0^4\right]$$

$$\mathbf{\Gamma}^{[4]}(A_{1g})\rangle_{j=2} = D\left\langle \frac{2}{\sqrt{70}}\left(\mathbf{v}_4^4 + \mathbf{v}_{-4}^4\right) + \tfrac{2}{5}\mathbf{v}_0^4\right\rangle_{j=2} \frac{\sqrt{5}}{3}\langle 2\|\mathrm{v}^4\|2\rangle.$$

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



$$\begin{array}{ccccc} q=0 & 1 & 2 & 3 & 4 \end{array}$$

$$\boxed{\begin{array}{ccccc} 1 & -1 & \sqrt{3} & -1 & 1 \\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1 \\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} \\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1 \\ 1 & -1 & \sqrt{3} & -1 & 1 \end{array}} \begin{array}{c} 1 \\ \sqrt{2} \\ \sqrt{14} \\ \sqrt{14} \\ \sqrt{70} \end{array}$$

$$\boxed{\begin{array}{ccccc} 1 & -\sqrt{3} & 1 & -1 & \cdot \\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1 \\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1 \\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} \\ \cdot & 1 & -1 & \sqrt{3} & -1 \end{array}} \begin{array}{c} \sqrt{2} \\ \sqrt{2} \\ \sqrt{10} \\ \sqrt{10} \end{array}$$

$$\boxed{\begin{array}{ccccc} 2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot \\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot \\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2} \\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6} \\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 \end{array}} \begin{array}{c} \sqrt{7} \\ \sqrt{14} \\ \sqrt{14} \end{array}$$

$$\boxed{\begin{array}{ccccc} 2 & -\sqrt{2} & \cdot & \cdot & \cdot \\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot \\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot \\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} \\ \cdot & \cdot & \cdot & \sqrt{2} & -2 \end{array}} \begin{array}{c} \sqrt{10} \\ \sqrt{10} \end{array}$$

(d) $l = 2$

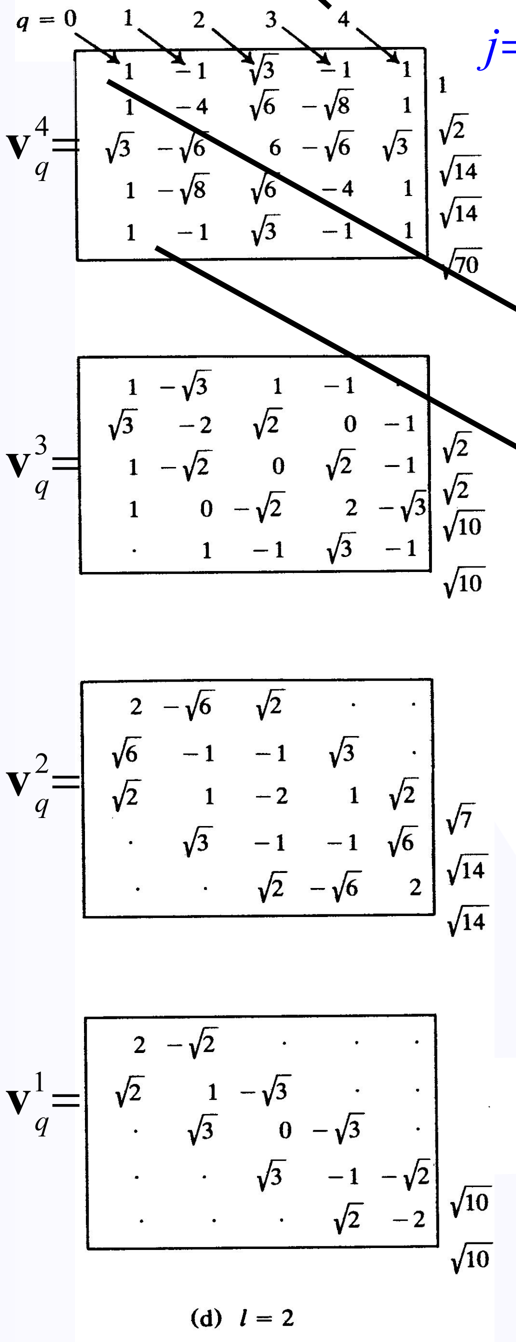
$$\mathbf{\Gamma}^{[4]}(A_{1g})\rangle_{j=2} = \frac{D}{\sqrt{70}} \begin{pmatrix} \frac{2}{5} & \cdot & \cdot & \cdot & 2 \\ \cdot & -\frac{8}{5} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{12}{5} & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\frac{8}{5} & \cdot \\ 2 & \cdot & \cdot & \cdot & \frac{2}{5} \end{pmatrix} \frac{\sqrt{5}}{3}\langle 2\|\mathrm{v}^4\|2\rangle$$

Octahedral 4th-rank A_{1g} tensor operator $\mathrm{T}^{[4]}$*: Application to splitting* d*-orbital* (l=j=2)

$$\mathbf{T}^{[4]}(A_{1g}) = D\left[x^4+y^4+z^4-\tfrac{3}{4}r^4\right] = D\left[\frac{2}{\sqrt{70}}\left(X_4^4+X_{-4}^4\right)+\tfrac{2}{5}X_0^4\right]$$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = D\left\langle \frac{2}{\sqrt{70}}\left(\mathbf{v}_4^4+\mathbf{v}_{-4}^4\right)+\tfrac{2}{5}\mathbf{v}_0^4\right\rangle_{j=2}\frac{\sqrt{5}}{3}\left\langle 2\middle\|\mathrm{v}^4\middle\|2\right\rangle.$$

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



j=ℓ=2

$$\mathbf{v}_q^4 = \begin{array}{ccccc} q=0 & 1 & 2 & 3 & 4 \\ 1 & -1 & \sqrt{3} & -1 & 1 \\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1 \\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} \\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1 \\ 1 & -1 & \sqrt{3} & -1 & 1 \end{array} \quad \begin{array}{c} 1 \\ \sqrt{2} \\ \sqrt{14} \\ \sqrt{14} \\ \sqrt{70} \end{array}$$

$$\mathbf{v}_q^3 = \begin{array}{ccccc} 1 & -\sqrt{3} & 1 & -1 & \cdot \\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1 \\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1 \\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} \\ \cdot & 1 & -1 & \sqrt{3} & -1 \end{array} \quad \begin{array}{c} \sqrt{2} \\ \sqrt{2} \\ \sqrt{10} \\ \sqrt{10} \end{array}$$

$$\mathbf{v}_q^2 = \begin{array}{ccccc} 2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot \\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot \\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2} \\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6} \\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 \end{array} \quad \begin{array}{c} \sqrt{7} \\ \sqrt{14} \\ \sqrt{14} \end{array}$$

$$\mathbf{v}_q^1 = \begin{array}{ccccc} 2 & -\sqrt{2} & \cdot & \cdot & \cdot \\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot \\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot \\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} \\ \cdot & \cdot & \cdot & \sqrt{2} & -2 \end{array} \quad \begin{array}{c} \sqrt{10} \\ \sqrt{10} \end{array}$$

(d) $l = 2$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = \frac{D}{\sqrt{70}}\begin{pmatrix} \frac{2}{5} & \cdot & \cdot & \cdot & 2 \\ \cdot & -\frac{8}{5} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{12}{5} & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\frac{8}{5} & \cdot \\ 2 & \cdot & \cdot & \cdot & \frac{2}{5} \end{pmatrix}\frac{\sqrt{5}}{3}\left\langle 2\middle\|\mathrm{v}^4\middle\|2\right\rangle$$

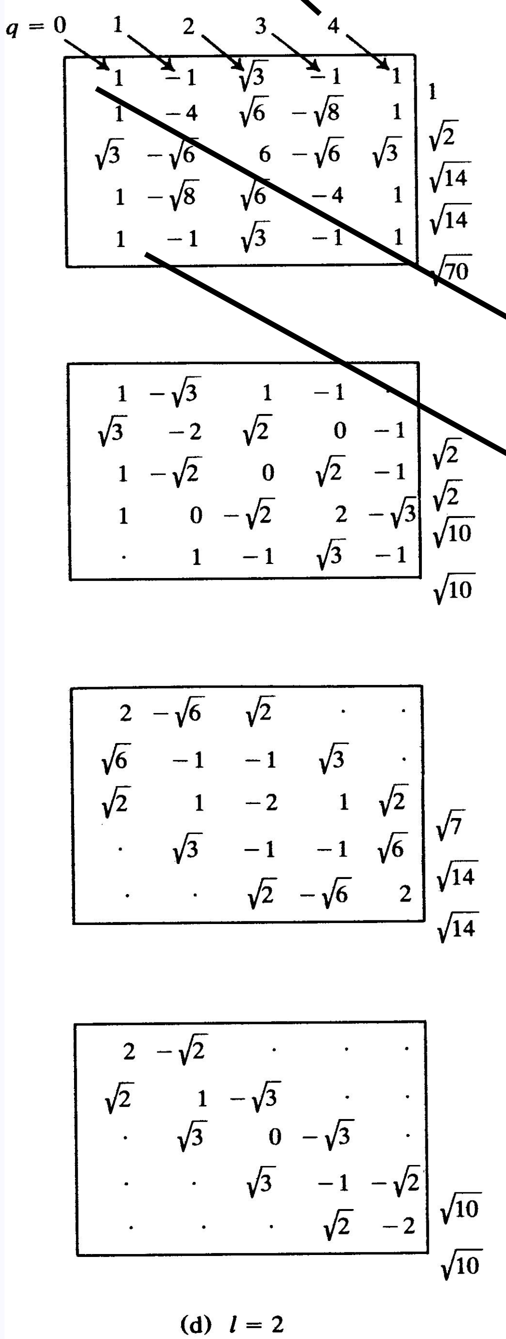
$$\left\langle \hat{\mathbf{T}}^{[4]}(A_{1g}^{j=2})\right\rangle = \begin{pmatrix} 2 & \cdot & \cdot & \cdot & 10 \\ \cdot & -8 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 12 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -8 & \cdot \\ 10 & \cdot & \cdot & \cdot & 2 \end{pmatrix}$$

Octahedral 4th-rank A_{1g} *tensor operator* T[4]*: Application to splitting* d*-orbital (l=j=2)*

$$\mathbf{T}^{[4]}(A_{1g}) = D\left[x^4+y^4+z^4-\tfrac{3}{4}r^4\right] = D\left[\frac{2}{\sqrt{70}}\left(X_4^4+X_{-4}^4\right)+\tfrac{2}{5}X_0^4\right]$$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = D\left\langle \frac{2}{\sqrt{70}}\left(\mathbf{v}_4^4+\mathbf{v}_{-4}^4\right)+\tfrac{2}{5}\mathbf{v}_0^4\right\rangle_{j=2} \frac{\sqrt{5}}{3}\left\langle 2\middle\|\mathrm{v}^4\middle\|2\right\rangle.$$

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



$q = 0 \quad 1 \quad 2 \quad 3 \quad 4$

$$\begin{array}{|ccccc|l}
1 & -1 & \sqrt{3} & -1 & 1 & 1\\
1 & -4 & \sqrt{6} & -\sqrt{8} & 1 & \sqrt{2}\\
\sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} & \sqrt{14}\\
1 & -\sqrt{8} & \sqrt{6} & -4 & 1 & \sqrt{14}\\
1 & -1 & \sqrt{3} & -1 & 1 & \sqrt{70}
\end{array}$$

$$\begin{array}{|ccccc|l}
1 & -\sqrt{3} & 1 & -1 & \cdot & \\
\sqrt{3} & -2 & \sqrt{2} & 0 & -1 & \sqrt{2}\\
1 & -\sqrt{2} & 0 & \sqrt{2} & -1 & \sqrt{2}\\
1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} & \sqrt{10}\\
\cdot & 1 & -1 & \sqrt{3} & -1 & \sqrt{10}
\end{array}$$

$$\begin{array}{|ccccc|l}
2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot & \\
\sqrt{6} & -1 & -1 & \sqrt{3} & \cdot & \\
\sqrt{2} & 1 & -2 & 1 & \sqrt{2} & \sqrt{7}\\
\cdot & \sqrt{3} & -1 & -1 & \sqrt{6} & \sqrt{14}\\
\cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 & \sqrt{14}
\end{array}$$

$$\begin{array}{|ccccc|l}
2 & -\sqrt{2} & \cdot & \cdot & \cdot & \\
\sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot & \\
\cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot & \\
\cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} & \sqrt{10}\\
\cdot & \cdot & \cdot & \sqrt{2} & -2 & \sqrt{10}
\end{array}$$

(d) $l = 2$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = \frac{D}{\sqrt{70}}\begin{pmatrix}
\frac{2}{5} & \cdot & \cdot & \cdot & 2\\
\cdot & -\frac{8}{5} & \cdot & \cdot & \cdot\\
\cdot & \cdot & \frac{12}{5} & \cdot & \cdot\\
\cdot & \cdot & \cdot & -\frac{8}{5} & \cdot\\
2 & \cdot & \cdot & \cdot & \frac{2}{5}
\end{pmatrix}\frac{\sqrt{5}}{3}\left\langle 2\middle\|\mathrm{v}^4\middle\|2\right\rangle$$

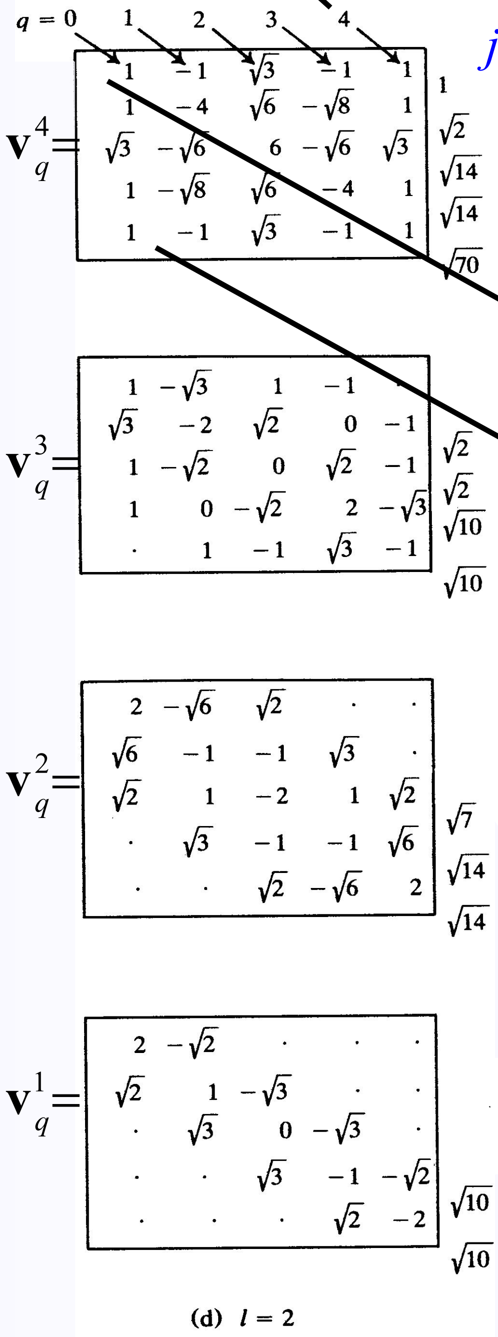
$$\left\langle \hat{\mathbf{T}}^{[4]}(A_{1g}^{j=2})\right\rangle = \begin{pmatrix}
2 & \cdot & \cdot & \cdot & 10\\
\cdot & -8 & \cdot & \cdot & \cdot\\
\cdot & \cdot & 12 & \cdot & \cdot\\
\cdot & \cdot & \cdot & -8 & \cdot\\
10 & \cdot & \cdot & \cdot & 2
\end{pmatrix} \sim \begin{pmatrix}
2 & 10 & \cdot & \cdot & \\
10 & 2 & \cdot & \cdot & \cdot\\
\cdot & \cdot & -8 & \cdot & \cdot\\
\cdot & \cdot & \cdot & 12 & \cdot\\
10 & \cdot & \cdot & \cdot & -8
\end{pmatrix}$$

Octahedral 4th-rank A_{1g} tensor operator $\mathrm{T}^{[4]}$*: Application to splitting* d*-orbital (l=j=2)*

$$\mathbf{T}^{[4]}(A_{1g}) = D\left[x^4+y^4+z^4-\tfrac{3}{4}r^4\right] = D\left[\frac{2}{\sqrt{70}}\left(X^4_4+X^4_{-4}\right)+\tfrac{2}{5}X^4_0\right]$$

$$\left\langle\mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = D\left\langle\frac{2}{\sqrt{70}}\left(\mathbf{v}^4_4+\mathbf{v}^4_{-4}\right)+\tfrac{2}{5}\mathbf{v}^4_0\right\rangle_{j=2}\frac{\sqrt{5}}{3}\left\langle 2\left\|\mathrm{v}^4\right\|2\right\rangle.$$

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



$j=\ell=2$

$$\mathbf{v}^4_q=\begin{array}{ccccc} q=0 & 1 & 2 & 3 & 4\\ \hline 1 & -1 & \sqrt{3} & -1 & 1\\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1\\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3}\\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1\\ 1 & -1 & \sqrt{3} & -1 & 1 \end{array}\quad\begin{array}{c}1\\ \sqrt{2}\\ \sqrt{14}\\ \sqrt{14}\\ \sqrt{70}\end{array}$$

$$\mathbf{v}^3_q=\begin{array}{ccccc} 1 & -\sqrt{3} & 1 & -1 & \cdot\\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1\\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1\\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3}\\ \cdot & 1 & -1 & \sqrt{3} & -1 \end{array}\quad\begin{array}{c}\sqrt{2}\\ \sqrt{2}\\ \sqrt{10}\\ \sqrt{10}\end{array}$$

$$\mathbf{v}^2_q=\begin{array}{ccccc} 2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot\\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot\\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2}\\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6}\\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 \end{array}\quad\begin{array}{c}\sqrt{7}\\ \sqrt{14}\\ \sqrt{14}\end{array}$$

$$\mathbf{v}^1_q=\begin{array}{ccccc} 2 & -\sqrt{2} & \cdot & \cdot & \cdot\\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot\\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot\\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2}\\ \cdot & \cdot & \cdot & \sqrt{2} & -2 \end{array}\quad\begin{array}{c}\sqrt{10}\\ \sqrt{10}\end{array}$$

(d) $l = 2$

$$\left\langle\mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = \frac{D}{\sqrt{70}}\begin{pmatrix} \frac{2}{5} & \cdot & \cdot & \cdot & 2\\ \cdot & -\frac{8}{5} & \cdot & \cdot & \cdot\\ \cdot & \cdot & \frac{12}{5} & \cdot & \cdot\\ \cdot & \cdot & \cdot & -\frac{8}{5} & \cdot\\ 2 & \cdot & \cdot & \cdot & \frac{2}{5} \end{pmatrix}\frac{\sqrt{5}}{3}\left\langle 2\left\|\mathrm{v}^4\right\|2\right\rangle$$

$$\left\langle\hat{\mathbf{T}}^{[4]}(A^{j=2}_{1g})\right\rangle = \begin{pmatrix} 2 & \cdot & \cdot & \cdot & 10\\ \cdot & -8 & \cdot & \cdot & \cdot\\ \cdot & \cdot & 12 & \cdot & \cdot\\ \cdot & \cdot & \cdot & -8 & \cdot\\ 10 & \cdot & \cdot & \cdot & 2 \end{pmatrix} \sim \begin{pmatrix} 2 & 10 & \cdot & \cdot & \\ 10 & 2 & \cdot & \cdot & \cdot\\ \cdot & \cdot & -8 & \cdot & \cdot\\ \cdot & \cdot & \cdot & 12 & \cdot\\ 10 & \cdot & \cdot & \cdot & -8 \end{pmatrix} \rightarrow \begin{pmatrix} 12 & \cdot & \cdot & \cdot & \\ \cdot & -8 & \cdot & \cdot & \cdot\\ \cdot & \cdot & -8 & \cdot & \cdot\\ \cdot & \cdot & \cdot & 12 & \cdot\\ 10 & \cdot & \cdot & \cdot & -8 \end{pmatrix}$$

Octahedral 4th-rank A_{1g} tensor operator $\mathbf{T}^{[4]}$*: Application to splitting* d*-orbital* (l=j=2)

$$\mathbf{T}^{[4]}(A_{1g}) = D\left[x^4 + y^4 + z^4 - \tfrac{3}{4}r^4\right] = D\left[\frac{2}{\sqrt{70}}\left(X^4_4 + X^4_{-4}\right) + \tfrac{2}{5}X^4_0\right]$$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = D\left\langle \frac{2}{\sqrt{70}}\left(\mathbf{v}^4_4 + \mathbf{v}^4_{-4}\right) + \tfrac{2}{5}\mathbf{v}^4_0\right\rangle_{j=2} \frac{\sqrt{5}}{3}\left\langle 2\left\|\mathrm{v}^4\right\|2\right\rangle.$$

j=ℓ=2

$$\begin{array}{c} q=0 \quad 1 \quad 2 \quad 3 \quad 4 \end{array}$$

$$\mathbf{v}^4_q = \begin{array}{|ccccc|c} 1 & -1 & \sqrt{3} & -1 & 1 & 1 \\ 1 & -4 & \sqrt{6} & -\sqrt{8} & 1 & \sqrt{2} \\ \sqrt{3} & -\sqrt{6} & 6 & -\sqrt{6} & \sqrt{3} & \sqrt{14} \\ 1 & -\sqrt{8} & \sqrt{6} & -4 & 1 & \sqrt{14} \\ 1 & -1 & \sqrt{3} & -1 & 1 & \sqrt{70} \end{array}$$

$$\mathbf{v}^3_q = \begin{array}{|ccccc|c} 1 & -\sqrt{3} & 1 & -1 & \cdot & \\ \sqrt{3} & -2 & \sqrt{2} & 0 & -1 & \sqrt{2} \\ 1 & -\sqrt{2} & 0 & \sqrt{2} & -1 & \sqrt{2} \\ 1 & 0 & -\sqrt{2} & 2 & -\sqrt{3} & \sqrt{10} \\ \cdot & 1 & -1 & \sqrt{3} & -1 & \sqrt{10} \end{array}$$

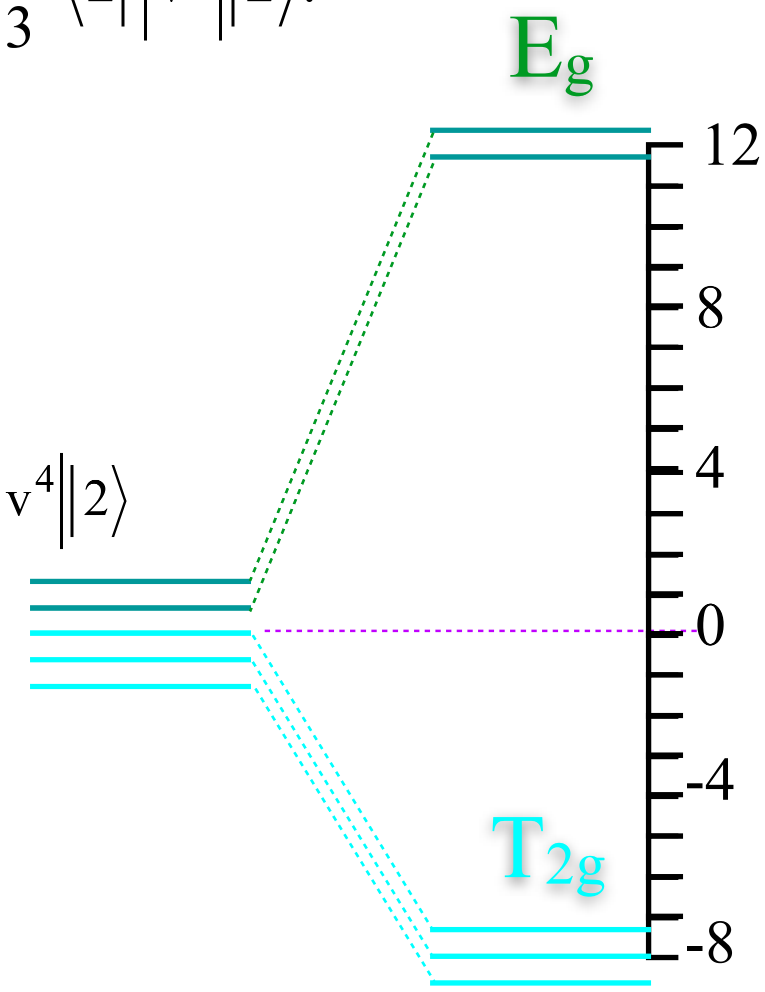
$$\mathbf{v}^2_q = \begin{array}{|ccccc|c} 2 & -\sqrt{6} & \sqrt{2} & \cdot & \cdot & \\ \sqrt{6} & -1 & -1 & \sqrt{3} & \cdot & \\ \sqrt{2} & 1 & -2 & 1 & \sqrt{2} & \sqrt{7} \\ \cdot & \sqrt{3} & -1 & -1 & \sqrt{6} & \sqrt{14} \\ \cdot & \cdot & \sqrt{2} & -\sqrt{6} & 2 & \sqrt{14} \end{array}$$

$$\mathbf{v}^1_q = \begin{array}{|ccccc|c} 2 & -\sqrt{2} & \cdot & \cdot & \cdot & \\ \sqrt{2} & 1 & -\sqrt{3} & \cdot & \cdot & \\ \cdot & \sqrt{3} & 0 & -\sqrt{3} & \cdot & \\ \cdot & \cdot & \sqrt{3} & -1 & -\sqrt{2} & \sqrt{10} \\ \cdot & \cdot & \cdot & \sqrt{2} & -2 & \sqrt{10} \end{array}$$

(d) $l = 2$

$$\left\langle \mathbf{T}^{[4]}(A_{1g})\right\rangle_{j=2} = \frac{D}{\sqrt{70}}\begin{pmatrix} \frac{2}{5} & \cdot & \cdot & \cdot & 2 \\ \cdot & -\frac{8}{5} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{12}{5} & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\frac{8}{5} & \cdot \\ 2 & \cdot & \cdot & \cdot & \frac{2}{5} \end{pmatrix} \frac{\sqrt{5}}{3}\left\langle 2\left\|\mathrm{v}^4\right\|2\right\rangle$$

$$\left\langle \hat{\mathbf{T}}^{[4]}(A^{j=2}_{1g})\right\rangle = \begin{pmatrix} 2 & \cdot & \cdot & \cdot & 10 \\ \cdot & -8 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 12 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -8 & \cdot \\ 10 & \cdot & \cdot & \cdot & 2 \end{pmatrix} \sim \begin{pmatrix} 2 & 10 & \cdot & \cdot & \\ 10 & 2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & -8 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 12 & \cdot \\ 10 & \cdot & \cdot & \cdot & -8 \end{pmatrix} \rightarrow \begin{pmatrix} 12 & \cdot & \cdot & \cdot & \\ \cdot & -8 & \cdot & \cdot & \cdot \\ \cdot & \cdot & -8 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 12 & \cdot \\ \cdot & \cdot & \cdot & \cdot & -8 \end{pmatrix}$$



AMOP reference links on page 2

3.26.18 class 18.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

$U(2)\sim O(3)\supset O_h$ Clebsch-Gordan irep product analysis, spin-orbit multiplets, and Wigner tensor matrices giving exact orbital splitting for $O(3)\supset O_h$ symmetry breaking

- Spin-spin $(1/2)^2$ product states: Hydrogen hyperfine structure
  - *Kronecker product states and operators*
  - *Spin-spin interaction reduces symmetry* $U(2)^{proton}\times U(2)^{electron}$ *to* $U(2)^{e+p}$
    - *Elementary ½ × ½ Clebsch-Gordan coefficients*
  - *Hydrogen hyperfine levels: Fermi-contact interaction, Racah's trick for energy eigenvalues*
    - *B-field gives avoided crossing*
- *Higher-J product states:* $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$ *case*
  - *Effect of Pauli-Fermi-Dirac symmetry*
  - *General U(2) Clebsch-Gordan-Wigner-3j coupling coefficient formula*
    - *LS to jj Level corralations*
  - *Angular momentum uncertainty cones related to 3j coefficients*
- *Multi-spin* $(1/2)^N$ *product states Magic squares*
  - *Intro to U(2) Young Tableaus*
  - *Intro to U(3) and higher Young Tableaus and Lab-Bod or Particle-State summitry*
- ➡ *U(2) and U(3) tensor expansion of H operator*
  - *Tensor operators for spin-1/2 states: Outer products give Hamilton-Pauli-spinors*
  - *Tensor operators for spin-1 states: U(3) generalization of Pauli spinors*
    - *4th rank tensor example with exact splitting of d-orbital*
    - ➡ *6th rank tensor example with exact splitting of f-orbital*

Octahedral 4th-rank A_{1g} tensor operator T[4]: *Application to splitting* f-*orbital* (*l*=*j*=3)

$$\left\langle V^{(4)}\right\rangle_{j=3} = D\left\langle 2\left(v_4^4+v_{-4}^4\right)/\sqrt{70}+\left(2/5\right)v_0^4\right\rangle\left(\sqrt{7}/3\right)\left\langle 3\right|\left|X^4\right|\left|3\right\rangle = D\begin{pmatrix} 3 & \cdot & \cdot & \cdot & \sqrt{15} & \cdot & \cdot \\ \cdot & -7 & \cdot & \cdot & \cdot & 5 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \sqrt{15} \\ \cdot & \cdot & \cdot & 6 & \cdot & \cdot & \cdot \\ \sqrt{15} & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & 5 & \cdot & \cdot & \cdot & -7 & \cdot \\ \cdot & \cdot & \sqrt{15} & \cdot & \cdot & \cdot & 3 \end{pmatrix}\left(2\sqrt{7}/15\sqrt{154}\right)\left\langle 3\right|\left|X^4\right|\left|3\right\rangle$$

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

T[4] *eigenfunction* f-*orbitals*

$$X^{A_{2u}} = xyz = -i\left(X_{-2}^3 - X_2^3\right)/\sqrt{30}.$$

$$\left|A_{2u}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{1u}} = \left(x^2-y^2\right)z = i\left(X_2^3 + X_{-2}^3\right)/\sqrt{2}$$

$$\left|\begin{matrix}T_{1u}\\3\end{matrix}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{2u}} = \left(x^2+y^2\right)z = -X_0^3/10.$$

$$\left|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = \left|\begin{matrix}3\\0\end{matrix}\right\rangle$$

Octahedral 4th-rank A_{1g} tensor operator T[4]*: Application to splitting* f*-orbital* (l=j=3)

$$\left\langle V^{(4)}\right\rangle_{j=3} = D\left\langle 2\left(v_4^4+v_{-4}^4\right)/\sqrt{70}+\left(2/5\right)v_0^4\right\rangle\left(\sqrt{7}/3\right)\langle 3\|X^4\|3\rangle = D\begin{pmatrix} 3 & \cdot & \cdot & \cdot & \sqrt{15} & \cdot & \cdot \\ \cdot & -7 & \cdot & \cdot & \cdot & 5 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \sqrt{15} \\ \cdot & \cdot & \cdot & 6 & \cdot & \cdot & \cdot \\ \sqrt{15} & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & 5 & \cdot & \cdot & \cdot & -7 & \cdot \\ \cdot & \cdot & \sqrt{15} & \cdot & \cdot & \cdot & 3 \end{pmatrix}\left(2\sqrt{7}/15\sqrt{154}\right)\langle 3\|X^4\|3\rangle$$

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

T[4] *eigenfunction* f*-orbitals*

$$X^{A_{2u}} = xyz = -i\left(X_{-2}^3 - X_2^3\right)/\sqrt{30}.$$

$$\left|A_{2u}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{1u}} = \left(x^2-y^2\right)z = i\left(X_2^3 + X_{-2}^3\right)/\sqrt{2}$$

$$\left|\begin{matrix}T_{1u}\\3\end{matrix}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{2u}} = \left(x^2+y^2\right)z = -X_0^3/10.$$

$$\left|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = \left|\begin{matrix}3\\0\end{matrix}\right\rangle$$

T[4] *eigenvalues*

$$\left\langle A_{2u}\right|V^{(4)}\left|A_{2u}\right\rangle = -12\delta^{(4)}$$

$$\left\langle\begin{matrix}T_{1u}\\3\end{matrix}\right|V^{(4)}\left|\begin{matrix}T_{1u}\\3\end{matrix}\right\rangle = -2\delta^{(4)}$$

$$\left\langle\begin{matrix}T_{2u}\\3\end{matrix}\right|V^{(4)}\left|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = 6\delta^{(4)}$$

Octahedral 4th-rank A_{1g} tensor operator $\mathrm{T}^{[4]}$*: Application to splitting* f*-orbital (l=j=3)*

$$\left\langle V^{(4)}\right\rangle_{j=3} = D\left\langle 2\left(v_4^4+v_{-4}^4\right)/\sqrt{70}+\left(2/5\right)v_0^4\right\rangle\left(\sqrt{7}/3\right)\langle 3\|X^4\|3\rangle = D\begin{pmatrix} 3 & \cdot & \cdot & \cdot & \sqrt{15} & \cdot & \cdot \\ \cdot & -7 & \cdot & \cdot & \cdot & 5 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \sqrt{15} \\ \cdot & \cdot & \cdot & 6 & \cdot & \cdot & \cdot \\ \sqrt{15} & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & 5 & \cdot & \cdot & \cdot & -7 & \cdot \\ \cdot & \cdot & \sqrt{15} & \cdot & \cdot & \cdot & 3 \end{pmatrix}\left(2\sqrt{7}/15\sqrt{154}\right)\langle 3\|X^4\|3\rangle$$

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

$\mathrm{T}^{[4]}$ *and* $\mathrm{T}^{[6]}$ *eigenfunction* f*-orbitals*

$$X^{A_{2u}} = xyz = -i\left(X_{-2}^3 - X_2^3\right)/\sqrt{30}.$$

$$\left|A_{2u}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{1u}} = \left(x^2-y^2\right)z = i\left(X_2^3 + X_{-2}^3\right)/\sqrt{2}$$

$$\left|\begin{matrix}T_{1u}\\3\end{matrix}\right\rangle = \left(\left|\begin{matrix}3\\2\end{matrix}\right\rangle - \left|\begin{matrix}3\\-2\end{matrix}\right\rangle\right)\Big/\sqrt{2}$$

$$X_3^{T_{2u}} = \left(x^2+y^2\right)z = -X_0^3/10.$$

$$\left|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = \left|\begin{matrix}3\\0\end{matrix}\right\rangle$$

$\mathrm{T}^{[4]}$ *eigenvalues*

$$\left\langle A_{2u}\middle|V^{(4)}\middle|A_{2u}\right\rangle = -12\delta^{(4)}$$

$$\left\langle\begin{matrix}T_{1u}\\3\end{matrix}\middle|V^{(4)}\middle|\begin{matrix}T_{1u}\\3\end{matrix}\right\rangle = -2\delta^{(4)}$$

$$\left\langle\begin{matrix}T_{2u}\\3\end{matrix}\middle|V^{(4)}\middle|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = 6\delta^{(4)}$$

Octahedral 6th-rank A_{1g} tensor operator $\mathrm{T}^{[6]}$*: Application to splitting* f*-orbital (l=j=3)*

$$V^{(6)} = E\left[\left(\sqrt{8}/8\right)X_0^y - \left(2\sqrt{7}/8\right)\left(X_4^6 + X_{-4}^6\right)\right]$$

$$\left(V^{(6)}\right)_{j-3} = E\begin{pmatrix} 1 & \cdot & \cdot & \cdot & -7\sqrt{15} & \cdot & \cdot \\ \cdot & -6 & \cdot & \cdot & \cdot & 42 & \cdot \\ \cdot & \cdot & 15 & \cdot & \cdot & \cdot & -7\sqrt{15} \\ \cdot & \cdot & \cdot & -20 & \cdot & \cdot & \cdot \\ -7\sqrt{15} & \cdot & \cdot & \cdot & 15 & \cdot & \cdot \\ \cdot & 42 & \cdot & \cdot & \cdot & -6 & \cdot \\ \cdot & \cdot & -7\sqrt{15} & \cdot & \cdot & \cdot & 1 \end{pmatrix}\times\langle 3\|X^6|3\rangle/\left(4\sqrt{462}\right)$$

$\mathrm{T}^{[6]}$ *eigenvalues*

$$\left\langle A_{2u}\middle|V^{(6)}\middle|A_{2u}\right\rangle = -12\delta^{(6)}$$

$$\left\langle\begin{matrix}T_{1u}\\3\end{matrix}\middle|V^{(6)}\middle|T_{1u}\right\rangle = 9\delta^{(6)}$$

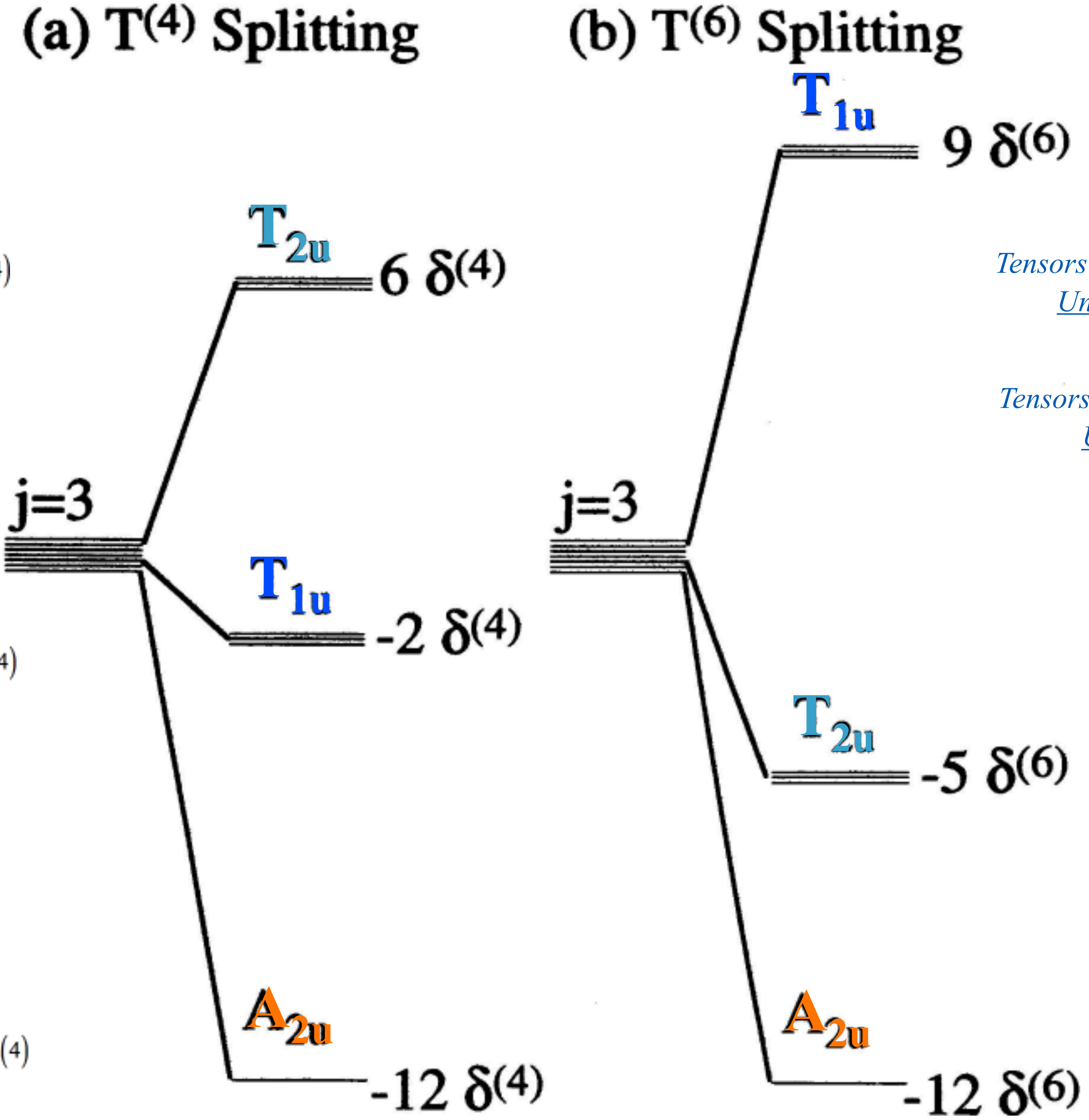
$$\left\langle\begin{matrix}T_{2u}\\3\end{matrix}\middle|V^{(6)}\middle|\begin{matrix}T_{2u}\\3\end{matrix}\right\rangle = -5\delta^{(6)}$$

A_{1g} tensor operators $\mathbf{T}^{[4]}$ *and* $\mathbf{T}^{[46]}$ split 7-fold degeneracy of a (J=3) *f-orbital level*

$$\left\langle \begin{matrix} T_{2u} \\ 3 \end{matrix} \middle| V^{(4)} \middle| \begin{matrix} T_{2u} \\ 3 \end{matrix} \right\rangle = 6\delta^{(4)}$$

$$\left\langle \begin{matrix} T_{1u} \\ 3 \end{matrix} \middle| V^{(4)} \middle| \begin{matrix} T_{1u} \\ 3 \end{matrix} \right\rangle = -2\delta^{(4)}$$

$$\left\langle A_{2u} \middle| V^{(4)} \middle| A_{2u} \right\rangle = -12\delta^{(4)}$$



$$\left\langle \begin{matrix} T_{1u} \\ 3 \end{matrix} \middle| V^{(6)} \middle| T_{1u} \right\rangle = 9\delta^{(6)}$$

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

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

$$\left\langle \begin{matrix} T_{2u} \\ 3 \end{matrix} \middle| V^{(6)} \middle| \begin{matrix} T_{2u} \\ 3 \end{matrix} \right\rangle = -5\delta^{(6)}$$

$$\left\langle A_{2u} \middle| V^{(6)} \middle| A_{2u} \right\rangle = -12\delta^{(6)}$$

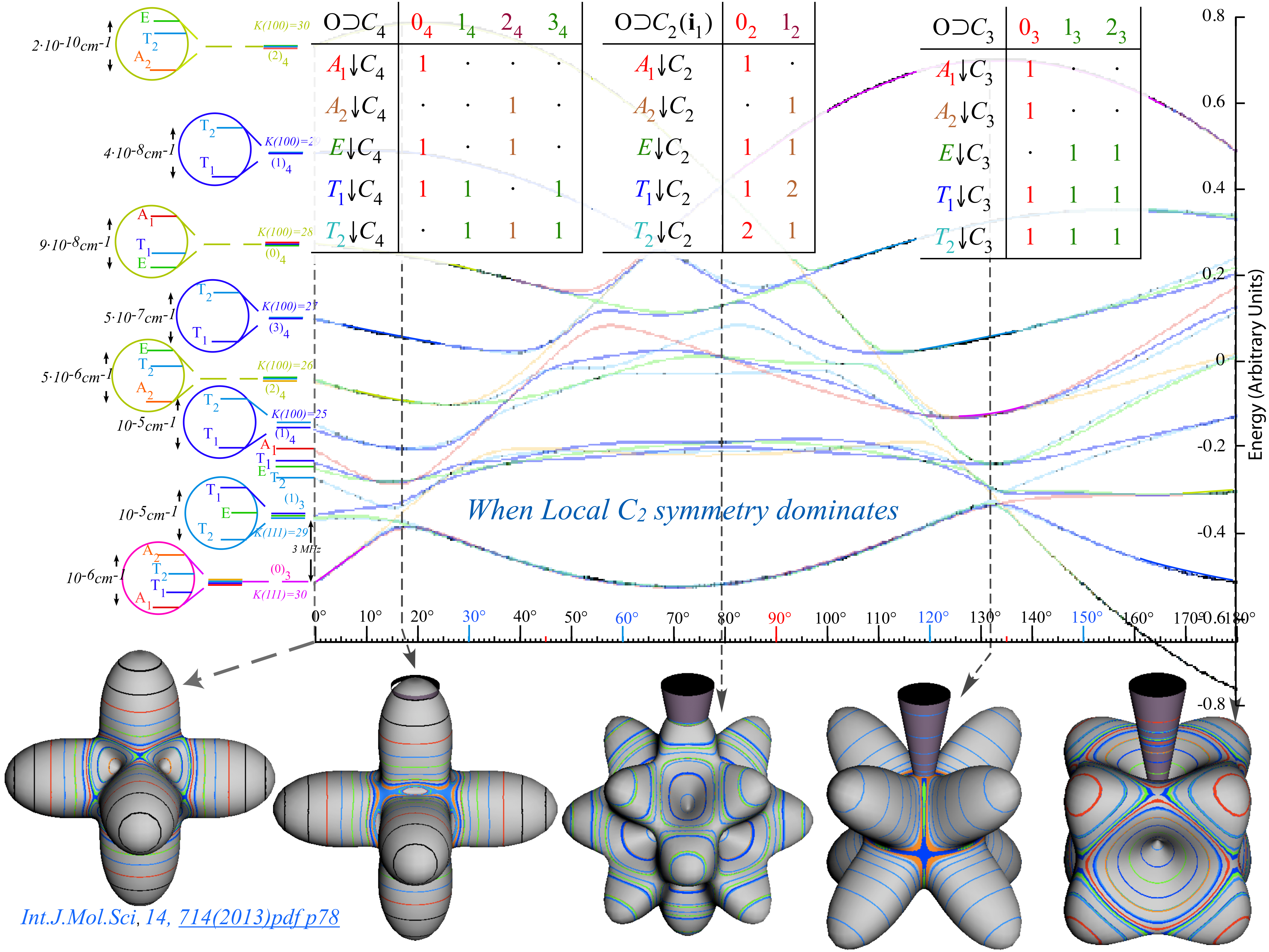
On following page:

A_{1g} *tensor operators* $\mathbf{T}^{[4]} + \mathbf{T}^{[46]}$ split *61-fold* degeneracy of a (J=30) *f-orbital level*

Compare the preceding *J=3* levels to the following pages showing curves of *J=30* levels split by combinations of 4th and 6th rank O_h symmetric tensors

J=30 $T^{[4]}+T^{[6]}$ levels
AMO Lect.17 p 102

In either case the number of linearly dependent O_h operators matches the number of parameters needed to define both the eigenvectors and the eigenvalues belonging to the symmetry.



$O\supset C_4$	0_4	1_4	2_4	3_4
$A_1\downarrow C_4$	1	·	·	·
$A_2\downarrow C_4$	·	·	1	·
$E\downarrow C_4$	1	·	1	·
$T_1\downarrow C_4$	1	1	·	1
$T_2\downarrow C_4$	·	1	1	1

$O\supset C_2(\mathbf{i}_1)$	0_2	1_2
$A_1\downarrow C_2$	1	·
$A_2\downarrow C_2$	·	1
$E\downarrow C_2$	1	1
$T_1\downarrow C_2$	1	2
$T_2\downarrow C_2$	2	1

$O\supset C_3$	0_3	1_3	2_3
$A_1\downarrow C_3$	1	·	·
$A_2\downarrow C_3$	1	·	·
$E\downarrow C_3$	·	1	1
$T_1\downarrow C_3$	1	1	1
$T_2\downarrow C_3$	1	1	1

When Local C_2 symmetry dominates

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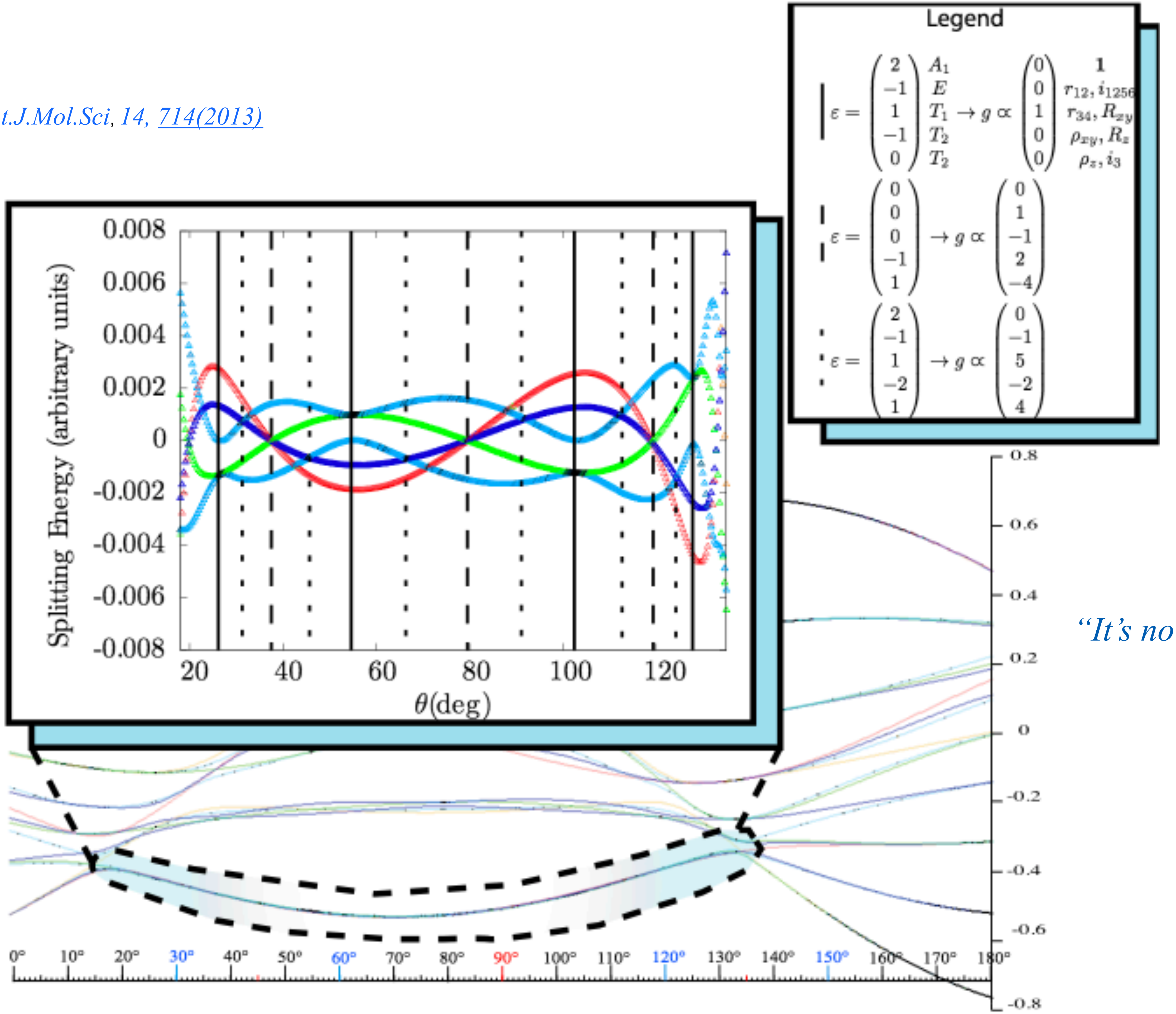

“It’s no “accident!”