# Group Theory in Quantum Mechanics Lecture 30 (5.10.17)

# Symmetry product analysis U(m)\*Sn tensors

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

## Review : 2-D at a algebra of U(2) representations

Spin-spin (1/2)<sup>2</sup> product states: Hydrogen hyperfine structure Kronecker product states and operators

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

Clebsch-Gordan Coefficients

Hydrogen hyperfine structure: Fermi-contact interaction plus B-field gives avoided crossing

Higher-J product states

 $(J=1)\otimes(J=1)=2\oplus 1\oplus 0$  case

General U(2) case

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

Magic squares - Intro to Young Tableaus

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

#### Multi-Lecture Selections

5.02.17 Lecture 27

Asymm-rotor RES&clusters

O-SymmSF<sub>6</sub> RES&clusters

T<sub>d</sub>-SymmCF<sub>4</sub>

5.03.17 Lecture 28 *Gyro-rotor REES&levels*(Lect.30  $C_{n_1n_2q}^{j_1j_2k}$  coupling intro.)

5.04.17 Lecture 29
SiF₄ and SF₆ Spin Tableau
& hyperfine effects
C₆₀ "Buckyball"

Lecture 30  $R(3)\sim U(2)$  Tensors and CG/Wigner coefficients

More Tableau theory

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

rank-0 (scalar)

$$\frac{2-by-2 \ case: \mathbf{H} = \begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix}}{\left( \begin{array}{c} A+D \\ B+iC & D \end{array} \right)} = \frac{A+D}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + C \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{A-D}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
= \frac{A+D}{2} \quad \mathbf{1} + B \mathbf{\sigma}_{x} + C \mathbf{\sigma}_{y} + \frac{A-D}{2} \mathbf{\sigma}_{z} \\
= \frac{A+D}{2} \mathbf{T}_{0} + (B-iC) \mathbf{T}_{1} + (B+iC) \mathbf{T}_{-1} + \frac{A-D}{2} \mathbf{T}_{0} \\
= \frac{A+D}{2} \mathbf{T}_{0} + (B-iC) \mathbf{T}_{1} + (B+iC) \mathbf{T}_{-1} + \frac{A-D}{2} \mathbf{T}_{0} \\
= \frac{A+D}{2} \mathbf{T}_{0} + (B-iC) \mathbf{T}_{1} + (B+iC) \mathbf{T}_{-1} + \frac{A-D}{2} \mathbf{T}_{0}$$

3-by-3 case: 
$$\mathbf{H} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

 $\mathbf{u}_{0}^{0} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{12}^{1}$ 

$$\mathbf{u}_{+2}^{2} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \mathbf{u}_{+1}^{2} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{0}^{2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{6}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-2}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \text{(vector)}$$

$$\mathbf{u}_{0}^{0} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{3}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{2}^{l} \quad \mathbf{u}_{-1}^{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 &$$

Mutually commuting diagonal operators

Wigner-Clebsch-Gordan expressions for Tensor  $\left\langle \mathbf{T}_{q}^{k} \right
angle$ 

$$\left\langle {}_{M'}^{J'} \middle| \mathbf{T}_{q}^{k} \middle| {}_{M}^{J} \right\rangle = \left( {}_{M'}^{J'} \middle| {}_{q-M}^{k} \right) (J' || k || J) = C_{qMM'}^{kJJ'} \left\langle J' || k || J \right\rangle$$

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

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..

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

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

$$\begin{pmatrix}
\cos\frac{\beta_{p}}{2} & -\sin\frac{\beta_{p}}{2} \\
\sin\frac{\beta_{p}}{2} & \cos\frac{\beta_{e}}{2}
\end{pmatrix} \otimes \begin{pmatrix}
\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{e}}{2} \\
\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{e}}{2}
\end{pmatrix} = \begin{pmatrix}
\cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\
\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2}
\end{pmatrix} - \sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} - \sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2}$$

$$\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2}$$

$$\sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2}$$

$$\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2}$$

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$$\cos\frac{\beta_{p}}{2}\cos\frac$$

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$$\begin{pmatrix} \cos\frac{\beta_{p}}{2} & -\sin\frac{\beta_{p}}{2} \\ \sin\frac{\beta_{p}}{2} & \cos\frac{\beta_{e}}{2} \end{pmatrix} \otimes \begin{pmatrix} \cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{e}}{2} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} \\ \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \end{pmatrix}$$

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  $U(2)^{e+p}$ 

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

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

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

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

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

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

$$\begin{pmatrix} \cos\frac{\beta_{p}}{2} & -\sin\frac{\beta_{p}}{2} \\ \sin\frac{\beta_{p}}{2} & \cos\frac{\beta_{e}}{2} \end{pmatrix} \otimes \begin{pmatrix} \cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{e}}{2} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & \cos\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\cos\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \sin\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} \\ \cos\frac{\beta_{p}}{2}\sin\frac{\beta_{e}}{2} & -\cos\frac{\beta_{p}}{2}\sin\frac{$$

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  $U(2)^{e+p}$ 

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

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..

$$|\uparrow\rangle|\uparrow\rangle = \begin{vmatrix} \frac{1}{2} \\ \frac{1}{2} \end{vmatrix}^{proton} \begin{vmatrix} \frac{1}{2} \\ \frac{1}{2} \end{vmatrix}^{electron}, |\uparrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}^{proton} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}^{electron}, |\downarrow\rangle|\uparrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}^{proton} \begin{vmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}^{electron} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}^{electron} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron} \begin{vmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{vmatrix}^{electron}, |\downarrow\rangle|\downarrow\rangle = \begin{vmatrix} \frac{1}{2} \\ -$$

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

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

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

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

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

$$\begin{vmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\
0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\
0 & 0 & 1 & 0
\end{vmatrix} = \begin{vmatrix}
\sin^2 \frac{\beta}{2} & -\sin \beta & \sin^2 \frac{\beta}{2} & 0 \\
\frac{\sin \beta}{\sqrt{2}} & \cos \beta & \frac{-\sin \beta}{\sqrt{2}} & 0 \\
\frac{\sin^2 \frac{\beta}{2}}{\sqrt{2}} & \frac{\sin \beta}{\sqrt{2}} & \cos^2 \frac{\beta}{2} & 0 \\
0 & 0 & 0 & 1
\end{vmatrix} = \begin{pmatrix}
D_{(0\beta 0)}^{J=1} \\
D^{J=0}
\end{pmatrix}$$

$$\sum_{m_1m_1'm_2m_2'} C_{m_1\ m_1'\ M}^{\frac{1}{2}\ \frac{1}{2}\ J} D_{m_1m_2}^{\frac{1}{2}} D_{m_1'm_2'}^{\frac{1}{2}} C_{m_2\ m_2'\ M'}^{\frac{1}{2}\ \frac{1}{2}\ J'} = \delta^{JJ'} D_{M\ M'}^{J}$$

$$\left| \frac{J}{M} \right|^{(1/2 \otimes 1/2)} = \sum_{m_1, m_2} C_{m_1 \ m_2 \ M}^{1/2 \ 1/2 \ J} \left| \frac{1/2}{m_1} \right\rangle \left| \frac{1/2}{m_2} \right\rangle$$

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

$$\uparrow^{p} \uparrow^{e} \downarrow \downarrow^{p} \uparrow^{e} \downarrow \downarrow^{p} \uparrow^{e} \downarrow^{e} \downarrow^{p} \downarrow^{p} \downarrow^{e} \downarrow^{p} \downarrow^{p} \downarrow^{e} \downarrow^{p} \downarrow^$$

$$\begin{vmatrix} 1 \\ +1 \end{vmatrix} = \begin{vmatrix} \uparrow^{p} \uparrow^{e} \\ +1 \end{vmatrix}$$

$$= \begin{vmatrix} \uparrow^{p} \uparrow^{e} \\ \downarrow^{p} \\ \downarrow^{p} \uparrow^{e} \end{vmatrix}$$

$$\begin{vmatrix} 1 \\ 0 \\ 0 \end{vmatrix} = \left( \begin{vmatrix} \uparrow^{p} \downarrow^{e} \\ \downarrow^{e} \end{vmatrix} + \left| \downarrow^{p} \uparrow^{e} \\ \downarrow^{p} \end{pmatrix} / \sqrt{2}$$

$$\begin{vmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 1 \end{vmatrix} = \begin{vmatrix} \downarrow^{p} \downarrow^{e} \\ \downarrow^{p} \end{pmatrix}$$

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

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

# Hydrogen hyperfine structure: Fermi-contact interaction

Racah's trick for energy eigenvalues

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

$$\left\langle {}_{M}^{J (1/2 \otimes 1/2)} \middle| H_{contact} \middle| {}_{M}^{J (1/2 \otimes 1/2)} \right\rangle = \frac{a_{ep}}{2} \left[ J(J+1) - \frac{1}{2} \left( \frac{1}{2} + 1 \right) - \frac{1}{2} \left( \frac{1}{2} + 1 \right) \right]$$

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

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

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

# *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}

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

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

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

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

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

`	$\left \uparrow^{p}\uparrow^{e}\right\rangle$	$\left \uparrow^{p}\downarrow^{e}\right\rangle$	$\left \downarrow^{p}\uparrow^{e}\right\rangle$	$\left  \downarrow^p \downarrow^e \right\rangle$
$\langle \uparrow^p \uparrow^e  $	$\frac{1}{2}(a_e - a_p)B_z$		•	·
$\langle \uparrow^p \downarrow^e  $	•	$\frac{-1}{2}(a_e + a_p)B_z$	0	•
$\langle \downarrow^p \uparrow^e  $		0	$\frac{1}{2}(a_e + a_p)B_z$	٠
$\langle \downarrow^p \downarrow^e  $	•		•	$\frac{-1}{2}(a_e - a_p)B_z$

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

	$\begin{vmatrix} 1 \\ 1 \end{vmatrix}$	$\begin{vmatrix} 1 \\ 0 \end{vmatrix}$	$\left  \begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \right>$	$\begin{vmatrix} 1 \\ -1 \end{vmatrix}$
$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{a_{ep}}{4}$	•	•	•
$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	•	$\frac{a_{ep}}{4}$	0	•
$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$	•	0	$\frac{-3a_{ep}}{4}$	•
$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	•	•	•	$\frac{a_{ep}}{4}$

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proton	= 5.585	$= 5.05078 \cdot 10^{-27} \frac{J}{T}$	$= 2.8209 \cdot 10^{-26} \frac{J}{T}$

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

	$\frac{1}{2} \bigotimes_{\underline{1}} \underline{1}$	<i>J</i> =1 <i>M</i> =1	1 0	1 -1	0	
_	$\frac{1}{2}, \frac{1}{2}$	1	0	0	0	
	$\frac{1}{2}, \frac{-1}{2}$	0	$\frac{1}{\sqrt{2}}$		$\frac{1}{\sqrt{2}}$	$= \left\langle C_{m_p m_e}^{\frac{1}{2} \frac{1}{2}} \left  \frac{J}{M} \right\rangle \right.$
	$\frac{-1}{2}, \frac{1}{2}$	0	$\frac{1}{\sqrt{2}}$		$-\frac{1}{\sqrt{2}}$	
	$\frac{-1}{2}, \frac{-1}{2}$	0	0	1	0	

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

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

	g – factor	Bohr – magneton	gyromagnetic factor
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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 · 10 <sup>-26</sup> $\frac{J}{T}$

Fermi – contact factor
$$a_{ep} = \mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} a_e a_p = 9.427 \cdot 10^{-25} J$$

$$\mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} \frac{a_e a_p}{h} = 1.4227 \cdot 10^9 Hz$$

$$\mu_0 \frac{2}{3} \frac{1}{\pi a_0^3} \frac{a_e a_p}{hc} = 4.746 m^{-1}$$

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

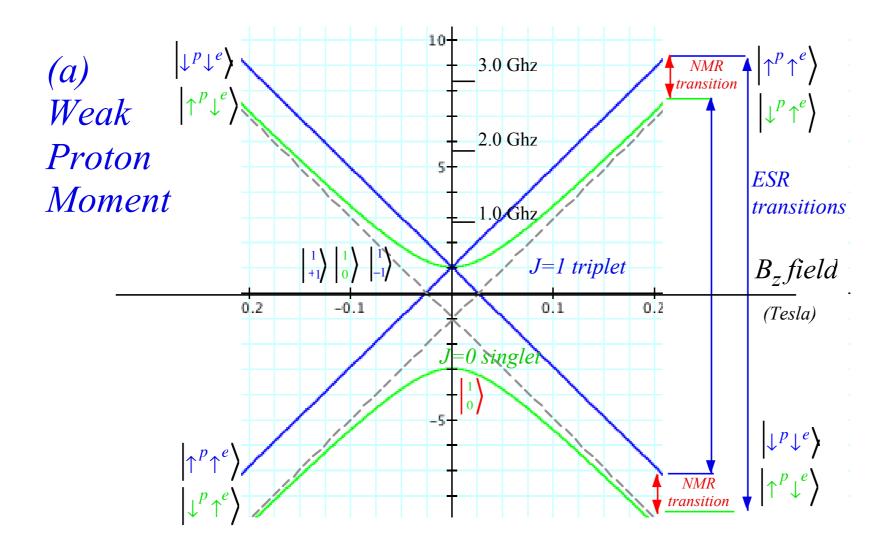
$\frac{1}{2} \otimes \frac{1}{2}$	<i>J</i> =1 <i>M</i> =1	1 0	1 -1	0	
$\frac{1}{2}, \frac{1}{2}$	1	0	0	0	
$\frac{1}{2}, \frac{-1}{2}$	0	$\frac{1}{\sqrt{2}}$		$\frac{1}{\sqrt{2}}$	$= \left\langle C_{m_p \ m_e}^{\frac{1}{2} \ \frac{1}{2}} \left  \begin{smallmatrix} J \\ M \end{smallmatrix} \right\rangle$
$\frac{-1}{2}, \frac{1}{2}$	0	$\frac{1}{\sqrt{2}}$		$-\frac{1}{\sqrt{2}}$	
$\frac{-1}{2}$ , $\frac{-1}{2}$	0	0	1	0	

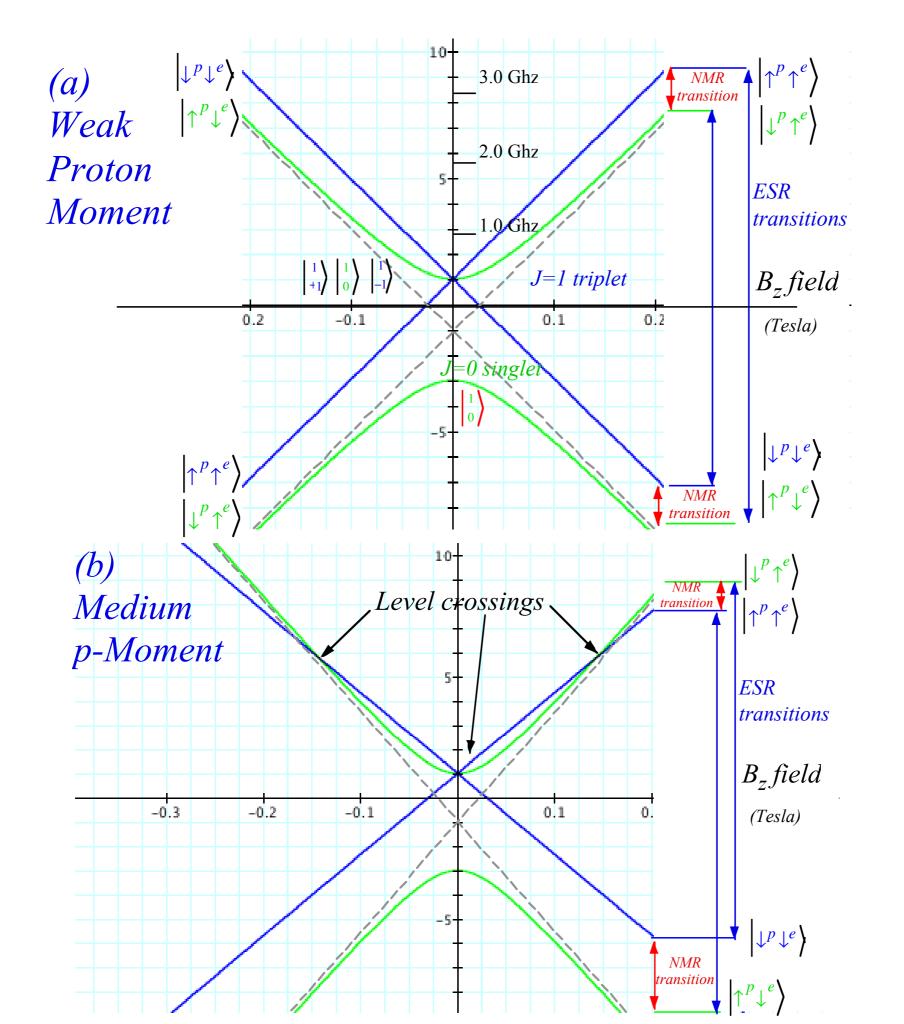
Magnetic constant :  $\mu_0 / 4\pi = 10^{-7} N / A^2$ 

$$\begin{vmatrix} \langle \downarrow^{p} \uparrow^{e} | & \cdot & \frac{a_{ep}}{2} & \frac{-a_{ep}}{4} & \cdot \\ \langle \downarrow^{p} \downarrow^{e} | & \cdot & \cdot & \frac{a_{ep}}{4} \end{vmatrix}$$

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

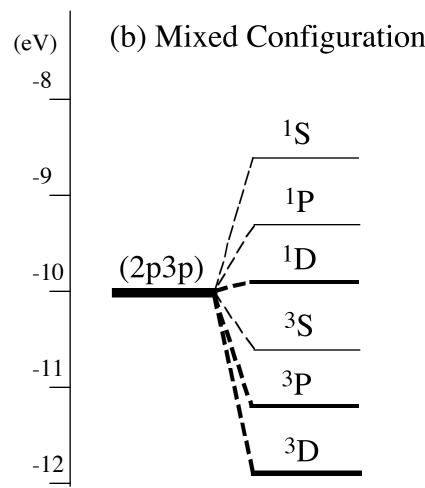
	$\begin{vmatrix} 1 \\ 1 \end{vmatrix}$	$\begin{vmatrix} 1 \\ 0 \end{vmatrix}$	$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$	$\begin{vmatrix} 1 \\ -1 \end{vmatrix}$
$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{a_{ep}}{4}$	•	٠	
$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$		$\frac{a_{ep}}{4}$	0	
$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$	•	0	$\frac{-3a_{ep}}{4}$	
$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	•	•	•	$\frac{a_{ep}}{4}$





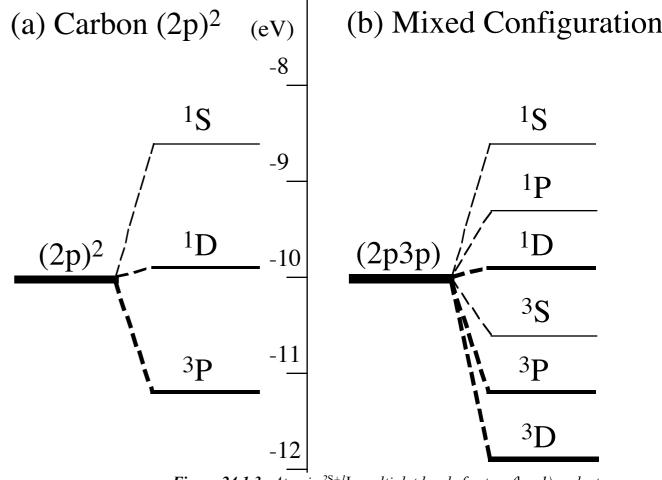
$$(J=1)\otimes (J=1)=2\oplus 1\oplus 0 \ case$$

			_	_	_	_	_	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	٠		$\frac{1}{\sqrt{6}}$	٠	•		$\frac{1}{\sqrt{2}}$	•	$\frac{1}{\sqrt{3}}$
$\left C_{m_1 m_2 M}^{1 1 L}\right\rangle =$	0	1	٠	$\frac{1}{\sqrt{2}}$		٠		$-\frac{1}{\sqrt{2}}$			٠
	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				$\frac{1}{\sqrt{2}}$				$-\frac{1}{\sqrt{2}}$	٠
	-1	-1	•	•	•	•	1	•	•		•



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

## Magher-quareduct states to Young Tableaus



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

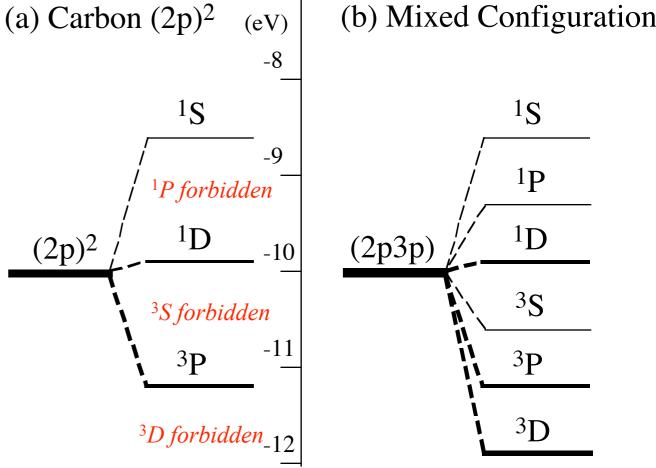
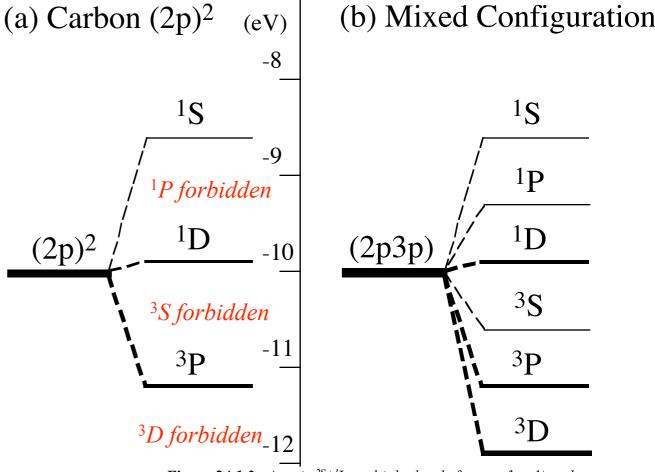


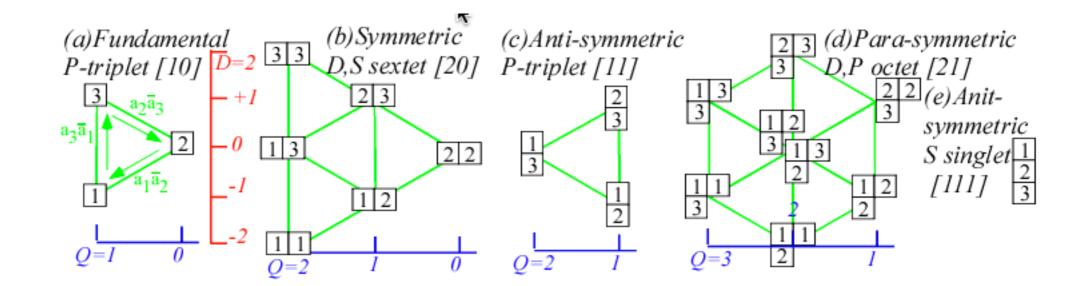
Figure 24.1.3 Atomic  ${}^{2S+1}L$  multiplet levels for two (1 = 1) p electrons.

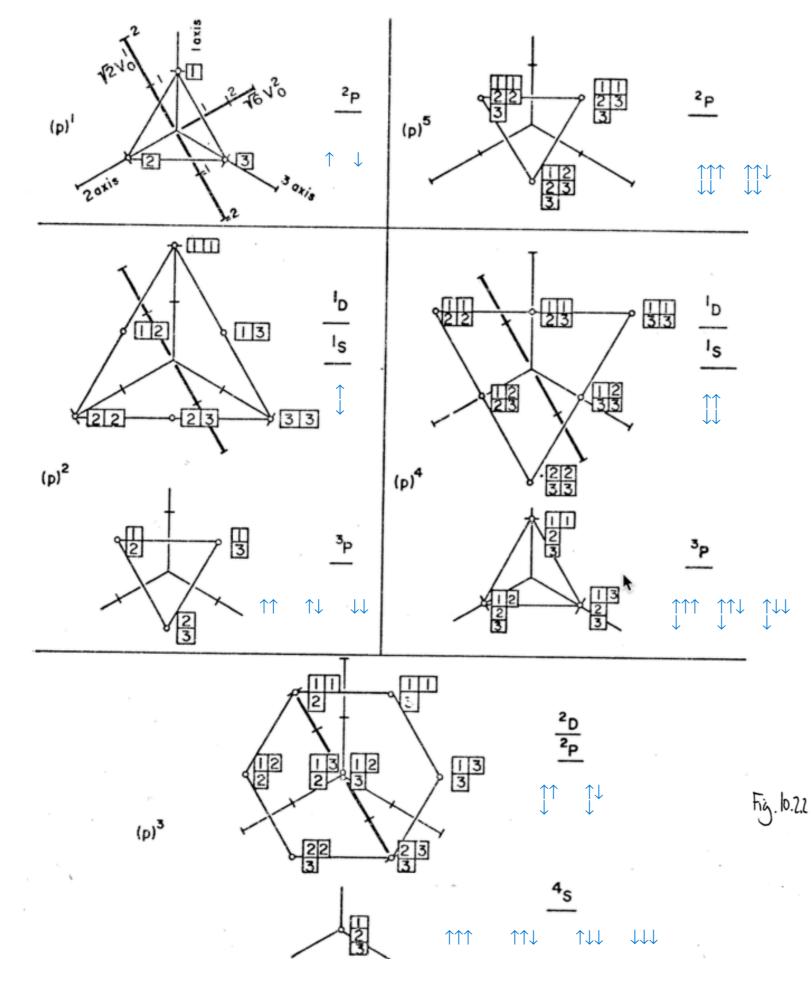
Pauli-Fermi selection rules requires total anti-symmetry



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

Pauli-Fermi selection rules requires total anti-symmetry





# From unpublished Ch.10 for Principles of Symmetry, Dynamics & Spectroscopy

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

$$(J=1)\otimes(J=1)=2\oplus 1\oplus 0$$
 case

(a) Carbon 
$$(2p)^2$$
 (eV)

-8

1S

-9

1P forbidden

(2p)<sup>2</sup>  $-10$ 

3S forbidden

3P

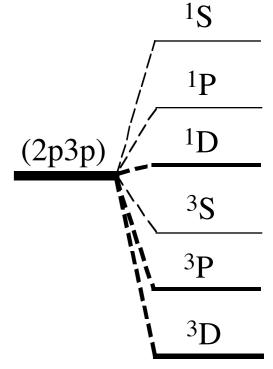
-11

3D forbidden

3D forbidden

3D forbidden

(b) Mixed Configuration



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

Pauli-Fermi selection rules requires total anti-symmetry

General U(2) case

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} C_{m_1 \ m_2 \ m_3}^{j_1 \ j_2 \ j_3} / (2j_3 + 1)^{\frac{1}{2}}$$
 Wigner 3j vs. Clebsch-Gordon (CGC)

$$|D| \otimes (J=1) = 2 \oplus 1 \oplus 0 \text{ case}$$

$$|D| \otimes (J=1) = 2 \oplus 1 \oplus 0 \text{ case}$$

$$|D| \otimes (J=1) = 2 \oplus 1 \oplus 0 \text{ case}$$

$$|D| \otimes (J=1) \otimes (J=1) = 2 \oplus 1 \oplus 0 \text{ case}$$

$$|D| \otimes (J=1) \otimes ($$

(a) Carbon 
$$(2p)^2$$
 (eV)

-8

1S

-9

1P forbidden

(2p)<sup>2</sup> / <sup>1</sup>D

-10

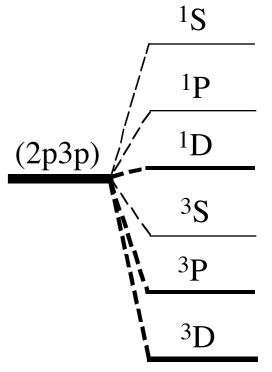
3S forbidden

3P

-11

3D forbidden<sub>-12</sub>

(b) Mixed Configuration



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

Pauli-Fermi selection rules requires total anti-symmetry

General U(2) case

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} C_{m_1 \ m_2 \ m_3}^{j_1 \ j_2 \ j_3} / (2j_3 + 1)^{\frac{1}{2}}$$
 Wigner 3j vs. Clebsch-Gordon (CGC)

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

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

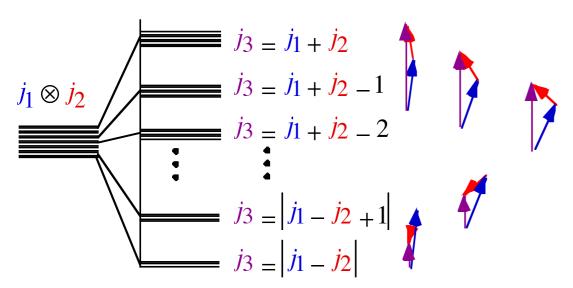


Figure 24.1.6 Level-splitting and vector-addition picture of angular-momentum coupling.

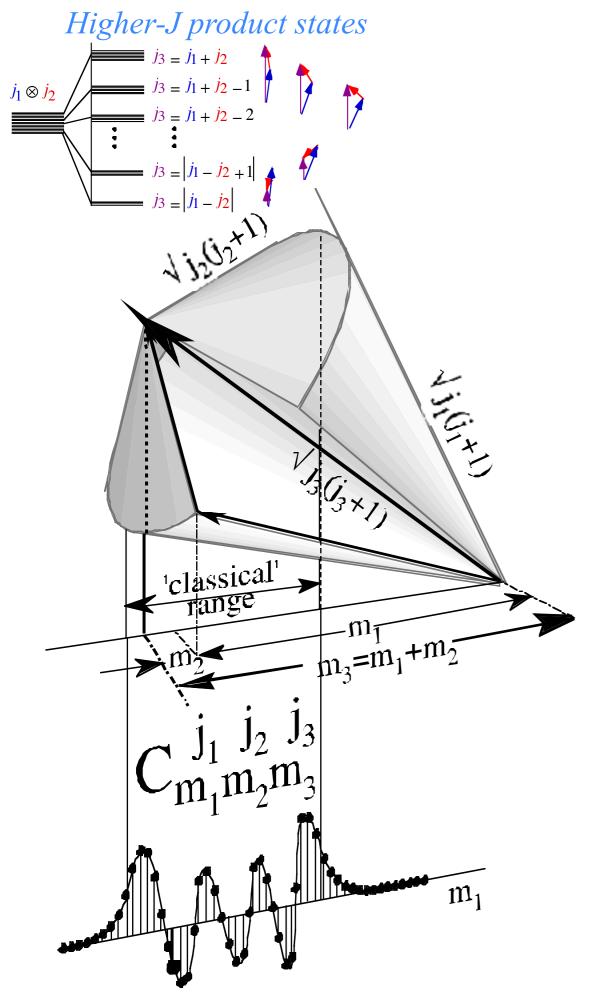


Figure 24.1.7 Angular-momentum cone picture of Clebsch-Gordan coupling amplitudes.

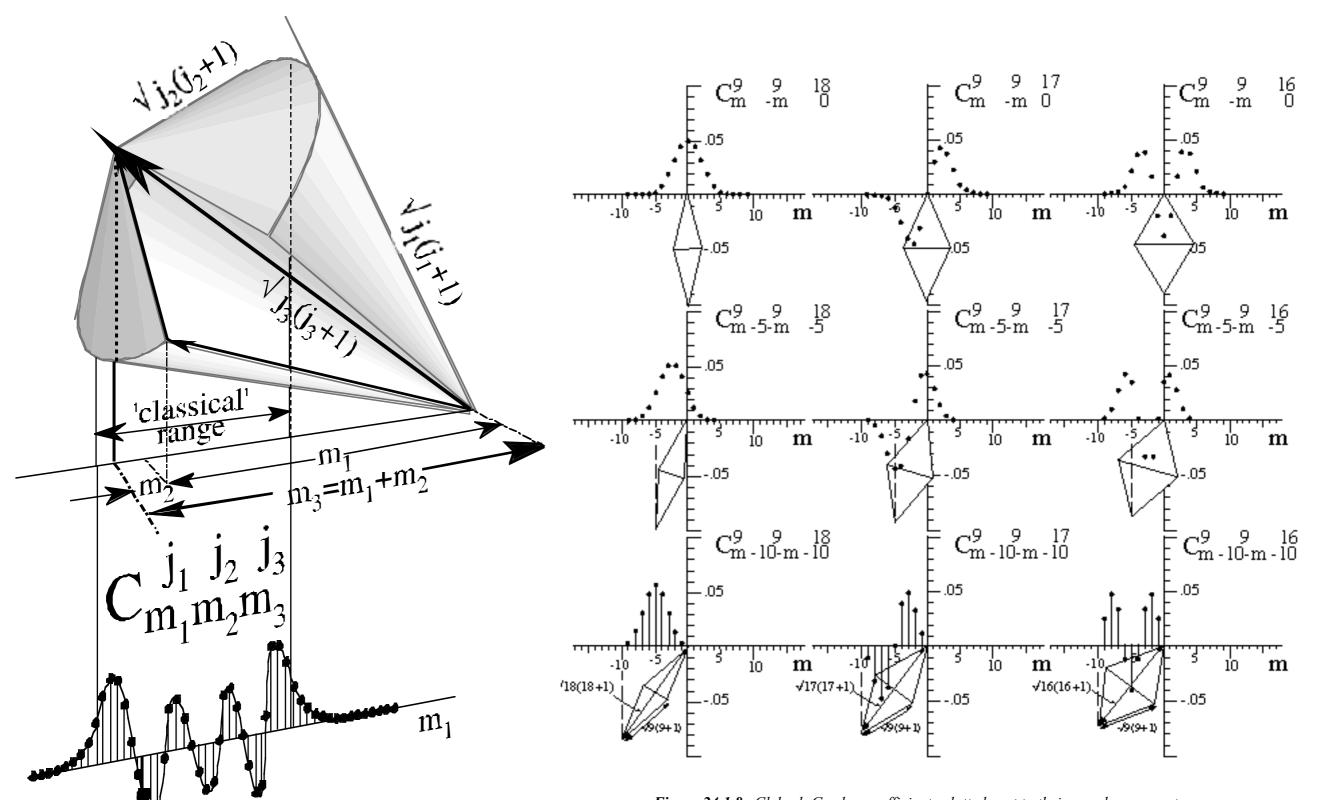


Figure 24.1.8 Clebsch-Gordan coefficients plotted next to their angular-momentum cones.

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

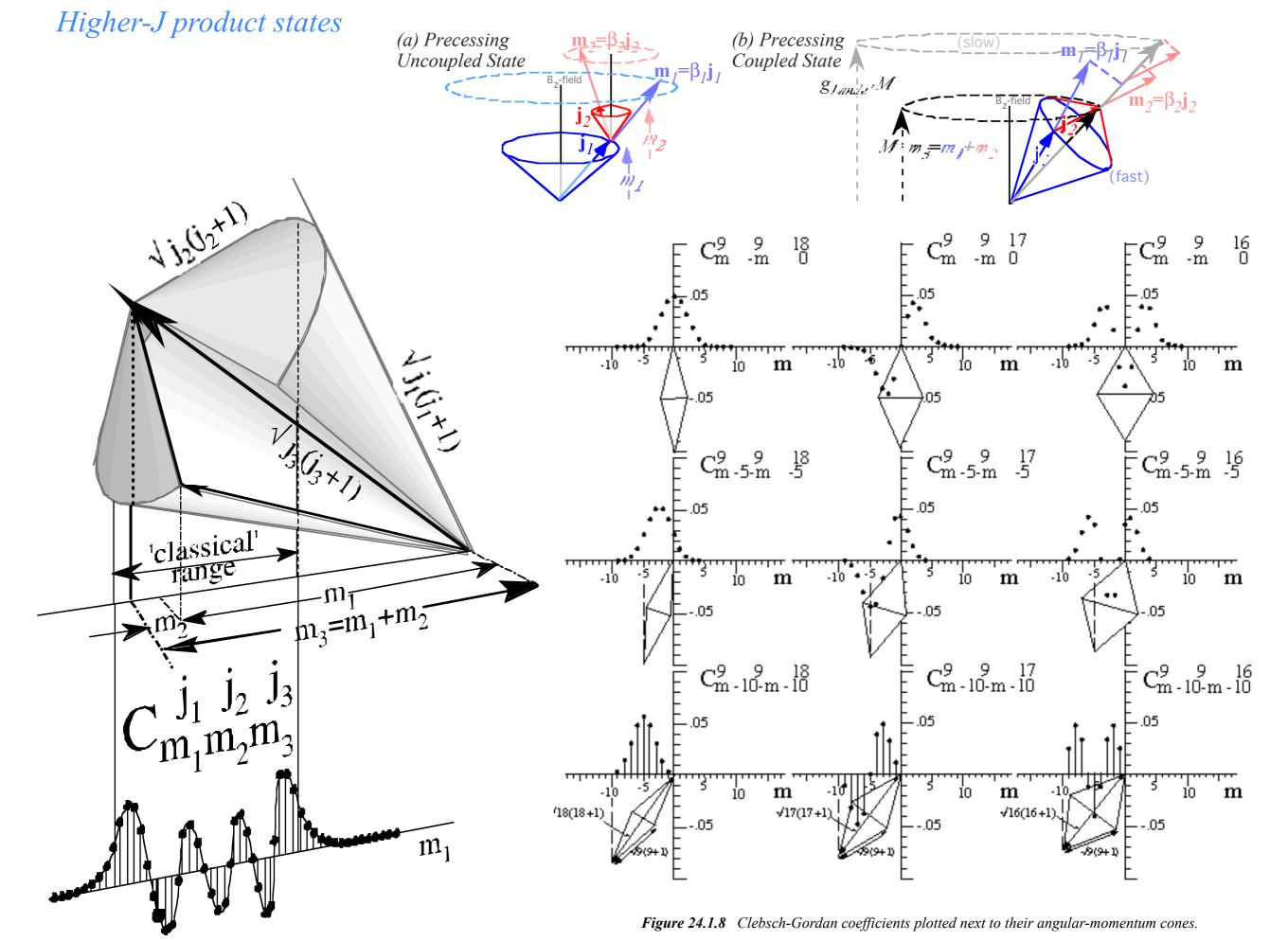


Figure 24.1.7 Angular-momentum cone picture of Clebsch-Gordan coupling amplitudes.

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

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

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

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

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right)$$

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

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right) = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}$$

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

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right) = \frac{1}{2} \oplus \frac{3}{2} = 2\left(\frac{1}{2}\right) \oplus 1\left(\frac{3}{2}\right)$$

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

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right) = \frac{1}{2} \oplus \frac{3}{2} = 2\left(\frac{1}{2}\right) \oplus 1\left(\frac{3}{2}\right)$$

$$S=5/2$$

$$S=3/2$$

$$Spin S$$

$$S=1$$

$$\ell[2,0] \uparrow \downarrow \downarrow$$

$$=1$$

$$S=1/2$$

$$N=1$$

$$N=1$$

$$N=1$$

$$N=1$$

$$N=2$$

$$N=1$$

$$N=2$$

$$N=1$$

$$N=2$$

$$N=1$$

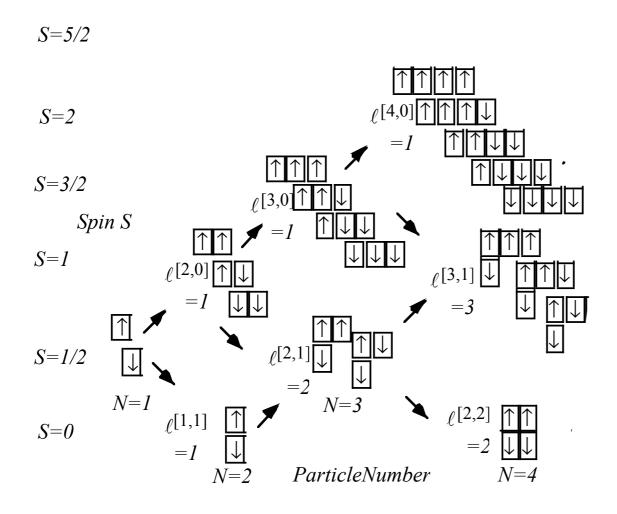
$$N=2$$

$$N=3$$

$$ParticleNumber$$

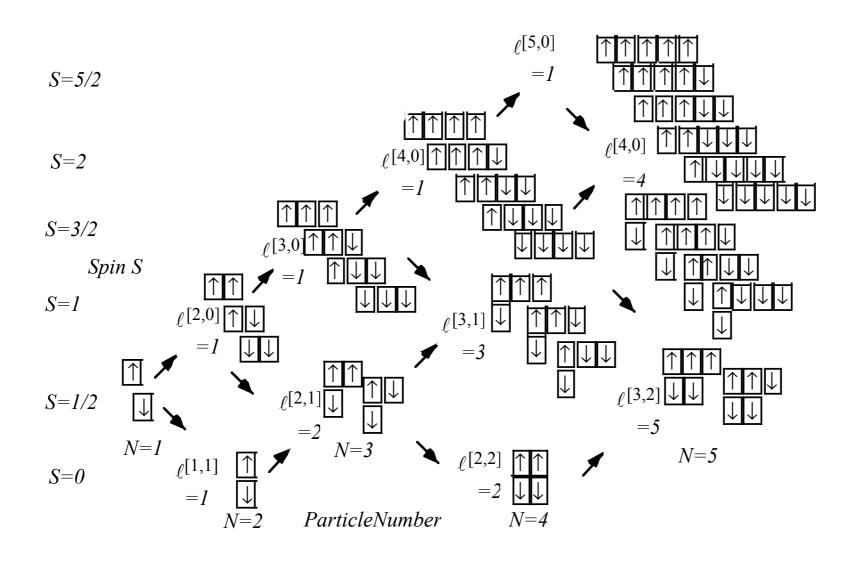
$$\left(\frac{1}{2} \otimes \frac{1}{2}\right) \otimes \frac{1}{2} = (0 \oplus 1) \otimes \frac{1}{2} = \left(0 \otimes \frac{1}{2}\right) \oplus \left(1 \otimes \frac{1}{2}\right)$$

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right) = \frac{1}{2} \oplus \frac{3}{2} = 2\left(\frac{1}{2}\right) \oplus 1\left(\frac{3}{2}\right)$$



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

$$= \left(\frac{1}{2}\right) \oplus \left(\left(\frac{1}{2}\right) \oplus \left(\frac{3}{2}\right)\right) = \frac{1}{2} \oplus \frac{3}{2} = 2\left(\frac{1}{2}\right) \oplus 1\left(\frac{3}{2}\right)$$



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

$$\uparrow \uparrow \uparrow \uparrow \downarrow \downarrow S = 2$$

$$\downarrow \downarrow \downarrow \downarrow \downarrow$$

$$+C_{1/2 \ 1/2 \ 1}^{3/2 \ 1/2 \ 2} \downarrow \downarrow \downarrow \downarrow$$

$$+C_{1/2 \ 1/2 \ 1}^{3/2 \ 1/2 \ 2} \downarrow \downarrow \downarrow \downarrow$$

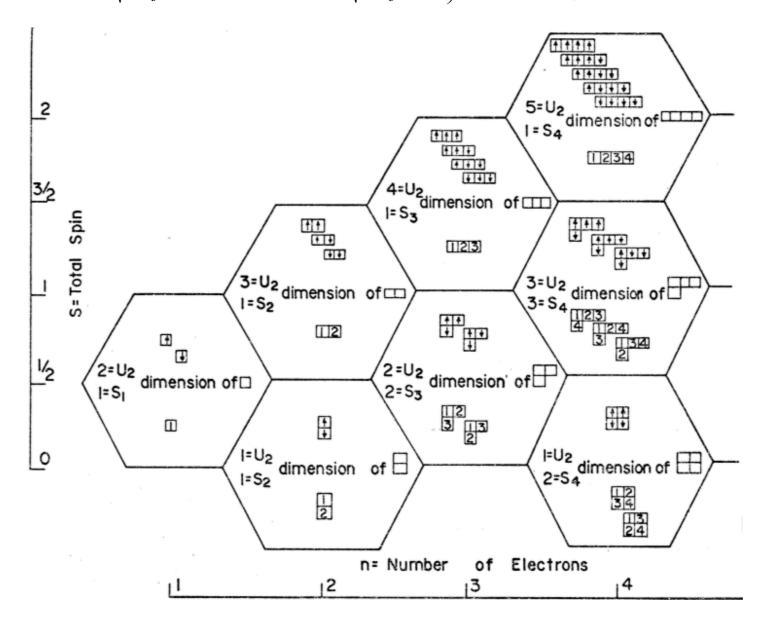
$$\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow$$

$$+C_{3/2 \ -1/2 \ 1}^{3/2 \ 1/2 \ 2} \downarrow \downarrow \downarrow \downarrow \downarrow$$

$$+C_{3/2 \ -1/2 \ 1}^{3/2 \ 1/2 \ 2} \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow$$

$$+C_{3/2 \ -1/2 \ 1}^{3/2 \ 1/2 \ 2} \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow$$

$$\begin{pmatrix} C_{m \; 1/2 \; j+1/2}^{j\; 1/2 \; j+1/2} = \sqrt{\frac{j+m+1}{2j+1}} & C_{m+1\; -1/2 \; m+1/2}^{j\; 1/2 \; j+1/2} = \sqrt{\frac{j-m}{2j+1}} \\ C_{m \; 1/2 \; m+1/2}^{j\; 1/2 \; j+1/2} = -\sqrt{\frac{j-m+1}{2j+3}} & C_{m+1\; -1/2 \; m+1/2}^{j\; 1/2 \; j+1/2} = \sqrt{\frac{j+m+2}{2j+3}} \end{pmatrix} \text{ example: } \begin{pmatrix} C_{1/2 \; 1/2 \; 1}^{3/2 \; 1/2 \; 2} = \sqrt{\frac{2}{3}} & C_{1/2 \; 1/2 \; 1}^{3/2 \; 1/2 \; 2} = \sqrt{\frac{1}{3}} \\ C_{1/2 \; 1/2 \; 1}^{5/2 \; 1/2 \; 2} = -\sqrt{\frac{1}{3}} & C_{1/2 \; 1/2 \; 1}^{5/2 \; 1/2 \; 2} = \sqrt{\frac{2}{3}} \end{pmatrix}$$



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

$$\begin{vmatrix} \bigcap_{i} \bigcap_{i} \bigcap_{i} \bigcap_{i} \bigcap_{i} \bigcap_{i} \bigcap_{i} \bigcup_{i} \bigcup_{i} S = 2 \\ M_{N} = 1 \end{vmatrix} = C_{1/2/2/2}^{1/2/2/2} \begin{vmatrix} \bigcap_{i} \bigcap_{$$

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

## Magic squares - Intro to Young Tableaus

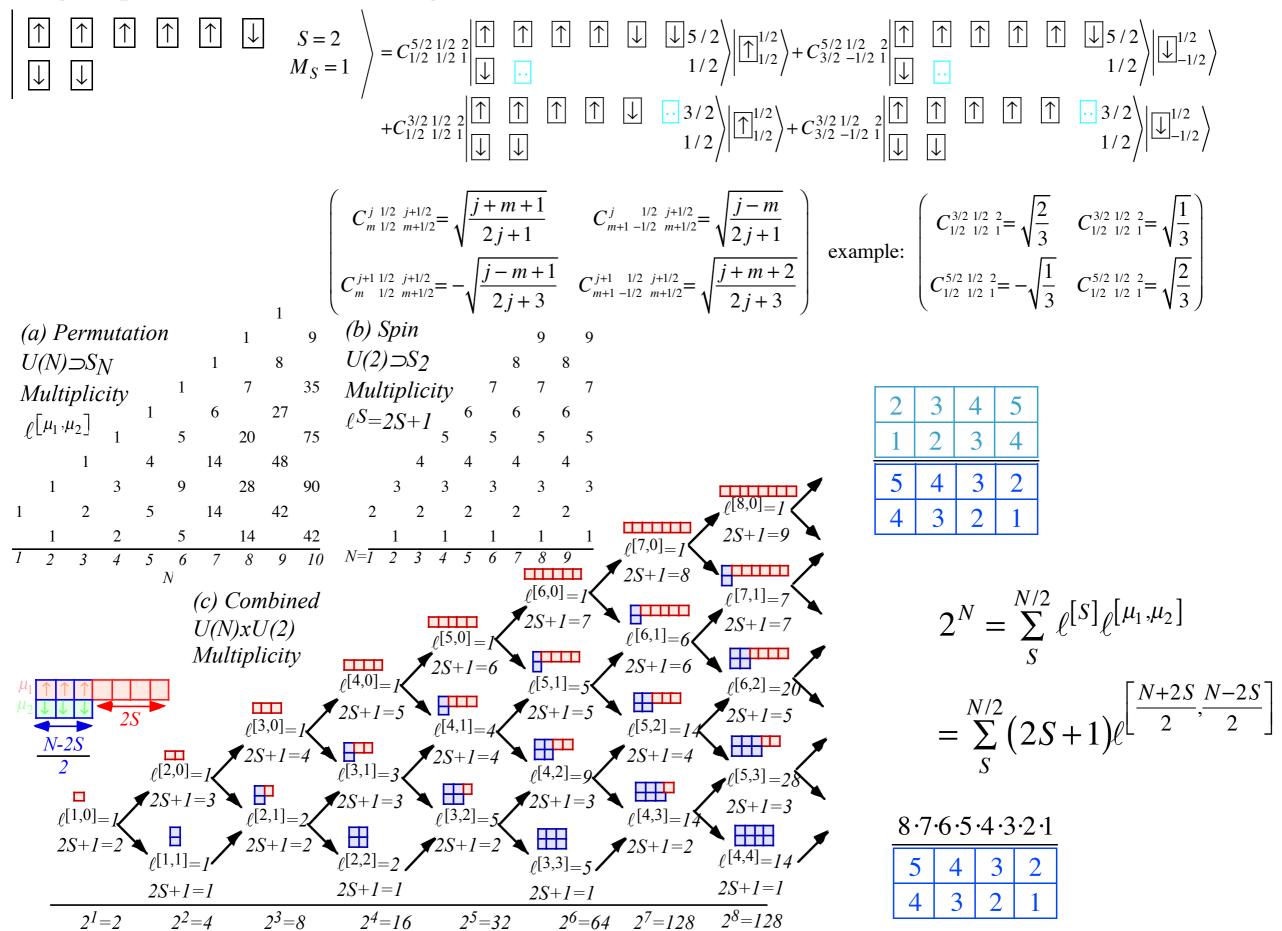


Fig. 23.3.2 Spin-1/2 and U(2) Tableau branching diagrams

# Magic squares - Intro to Young Tableaus

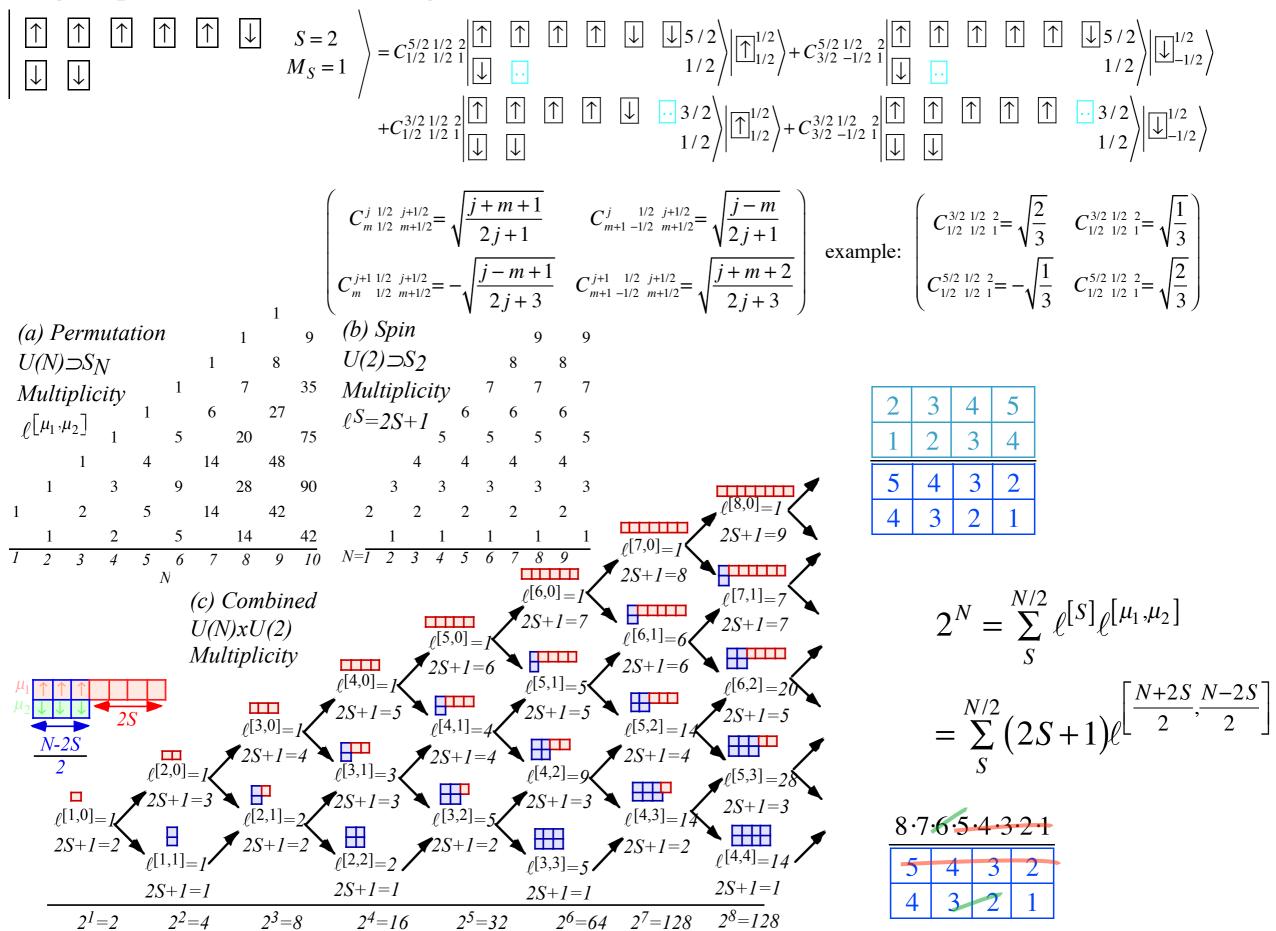


Fig. 23.3.2 Spin-1/2 and U(2) Tableau branching diagrams

## Magic squares - Intro to Young Tableaus

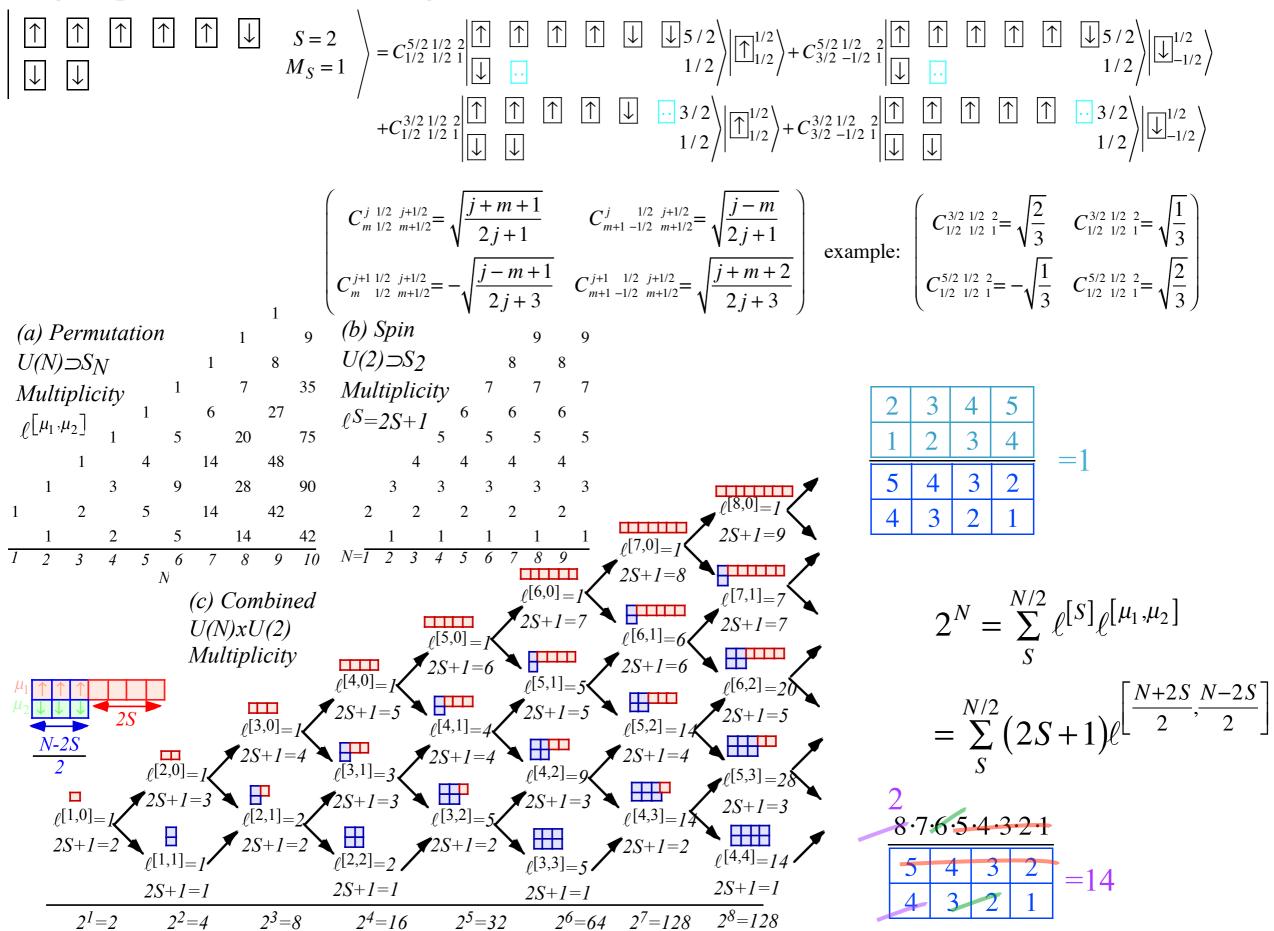


Fig. 23.3.2 Spin-1/2 and U(2) Tableau branching diagrams

# *Introducing U(N)*

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

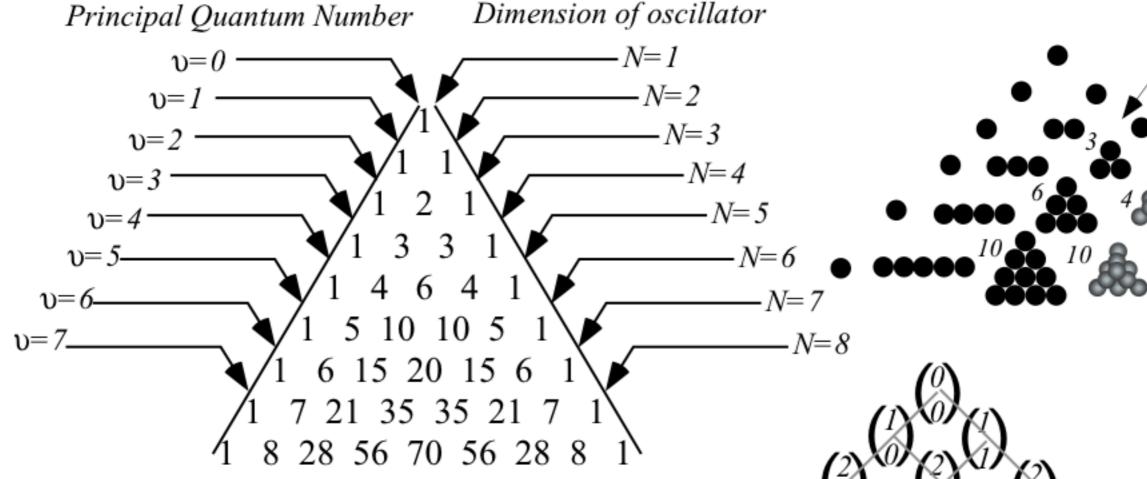
(b) Stacking numbers

triangular

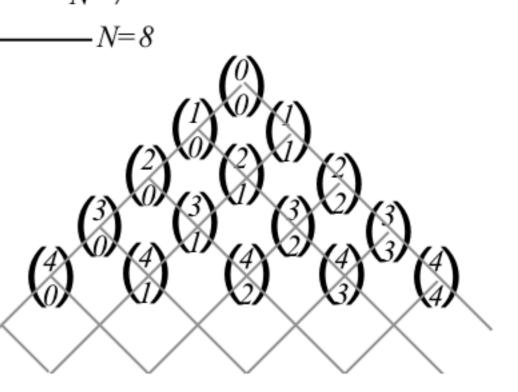
numbers

tetrahedral

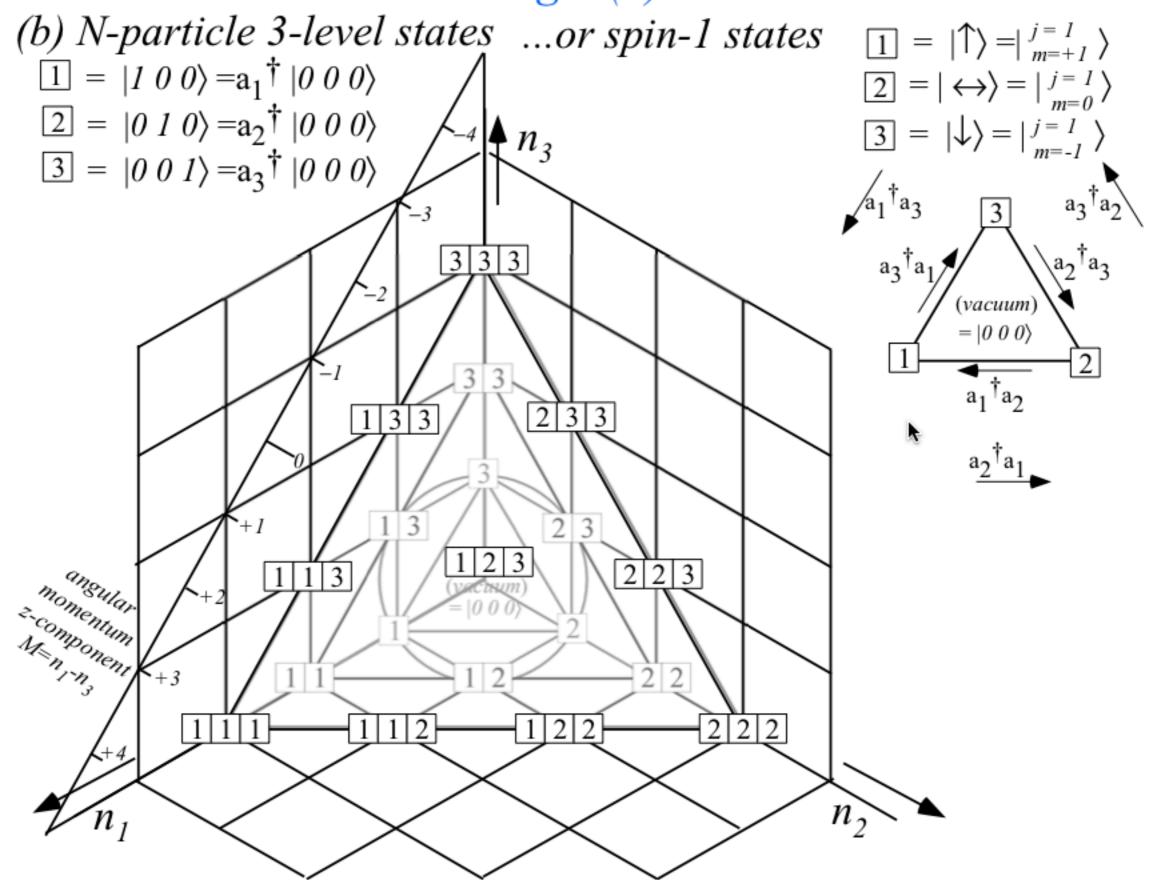
numbers

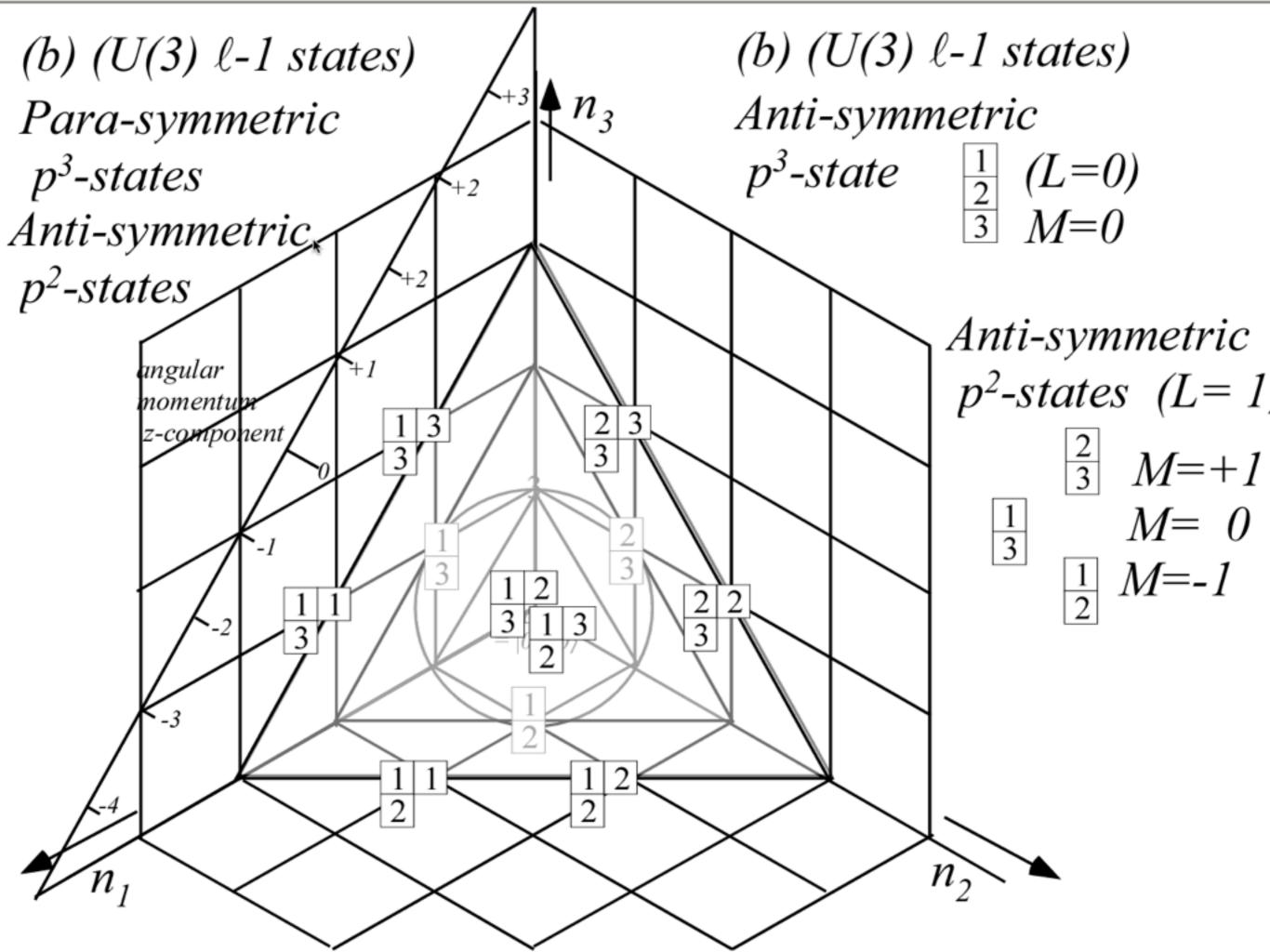


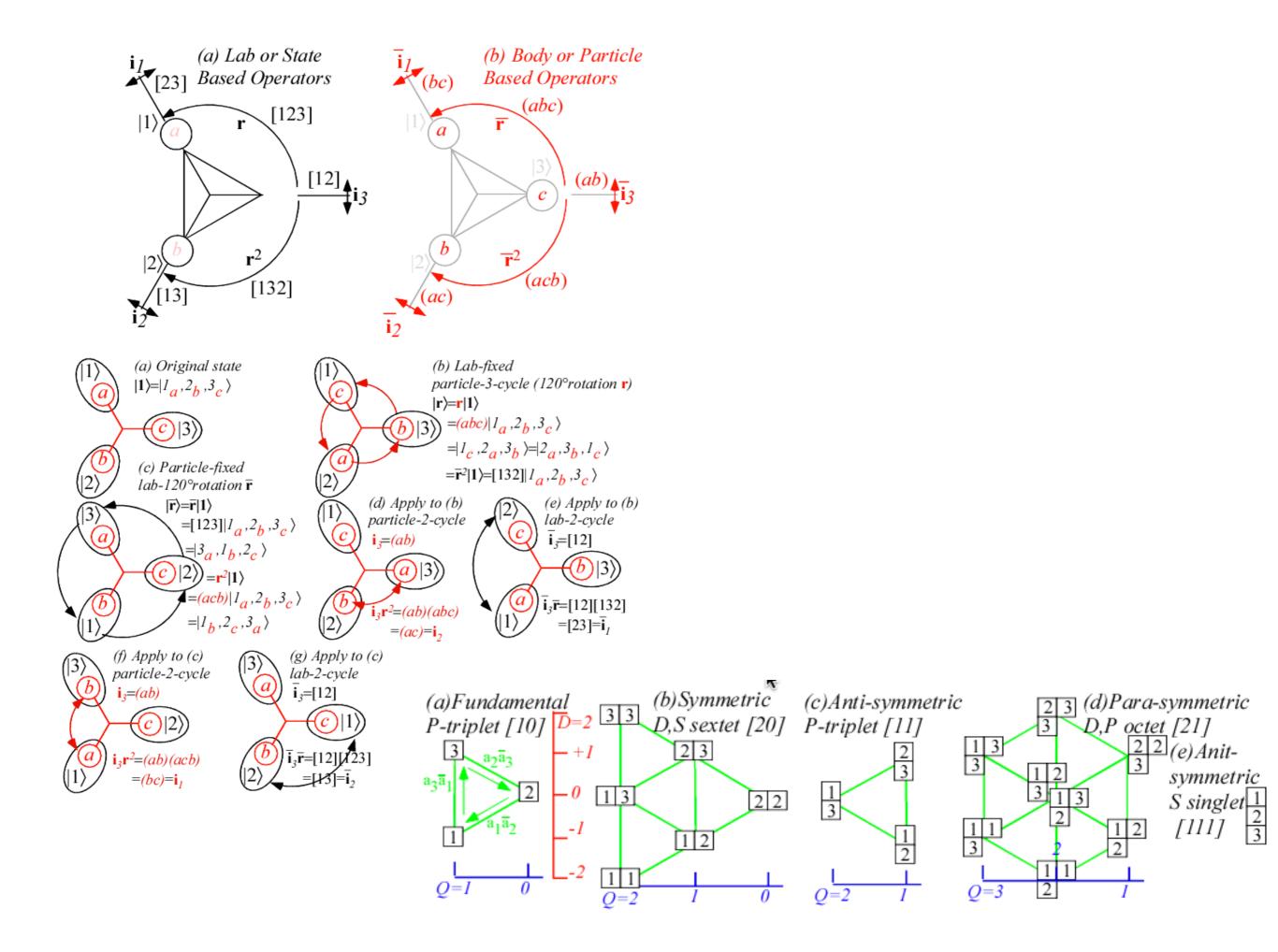
(c) Binomial coefficients
$$\frac{(N-1+\upsilon)!}{(N-1)!\upsilon!} = \begin{pmatrix} N-1+\upsilon \\ \upsilon \end{pmatrix} = \begin{pmatrix} N-1+\upsilon \\ N-1 \end{pmatrix}$$



# *Introducing U(3)*







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

CG-Products of spin- $\frac{1}{2}$  ket-bras  $\binom{1}{2}$ ,  $\binom{1}{2}$   $\binom{1}{2}$  give scalar/vector operators analogous to: ket-kets

$$T_{q}^{k} = \sum_{m_{1}, m_{2}} C_{m_{1}}^{1/2 | 1/2 | k} \begin{vmatrix} 1/2 \\ -m_{2} \end{vmatrix} \begin{pmatrix} -1 \\ 0 \end{vmatrix} \begin{pmatrix} 0 \\ -1 \end{vmatrix} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \end{pmatrix} \qquad \begin{cases} T_{-1}^{l} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \\ -1/2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 1/2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 1/2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad T_{-1}^{l} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/$$

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

$$\begin{split} T_x &\equiv -\frac{T_{-1}^1 - T_1^1}{\sqrt{2}} &\qquad T_y \equiv -i\frac{T_{-1}^1 + T_1^1}{\sqrt{2}} &\qquad T_z \equiv -T_0^1 \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} &\qquad = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} &\qquad = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &\equiv \frac{1}{\sqrt{2}} \sigma_x &\qquad \equiv \frac{1}{\sqrt{2}} \sigma_y &\qquad \equiv \frac{1}{\sqrt{2}} \sigma_z \\ &\equiv \sqrt{2}J_x &\qquad \equiv \sqrt{2}J_y &\qquad \equiv \sqrt{2}J_z \end{split}$$

Spherical vs. Cartesian operators

$$T_{-1}^1 = J_-/2 = \left(J_x - iJ_y\right)/\sqrt{2}$$
,  $T_0^1 = J_z/\sqrt{2}$ ,  $T_{-1}^1 = J_+/2 = \left(J_x + iJ_y\right)/2$ .

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

CG-Products of spin- $\frac{1}{2}$  ket-bras  $\binom{1/2}{m_1}$ ,  $\binom{1/2}{m_2}$  } give scalar/vector operators analogous to: ket-kets

$$T_{q}^{k} = \sum_{m_{1}, m_{2}} C_{m_{1}}^{1/2 | 1/2 | k} \begin{vmatrix} 1/2 \\ -m_{2} \end{vmatrix} \begin{pmatrix} -1 \\ 0 \end{vmatrix} \begin{pmatrix} 0 \\ -1 \end{vmatrix} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \end{pmatrix} \qquad \begin{cases} T_{-1}^{1} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \\ T_{-1/2}^{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{cases} \qquad \begin{cases} T_{-1/2}^{1/2 | 1/2 | k} \begin{pmatrix} 1/2 \\ 0 & 1 \end{pmatrix} \\ T_{-1/2}^{1/2} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2$$

1st three operators are a vector set that transform like a vector set

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

CG-Products of spin- $\frac{1}{2}$  ket-bras  $\binom{1}{2}$ ,  $\binom{1}{2}$   $\binom{1}{2}$  give scalar/vector operators analogous to: ket-kets

$$T_{q}^{k} = \sum_{m_{1}} C_{m_{1}}^{1/2} \frac{1/2}{m_{2}} \frac{1}{q} \frac{1/2}{m_{1}} \left\langle -1\right)^{\frac{1}{2}-m_{2}}$$
 analogous to: 
$$\left\{ \begin{array}{c} \left| \int_{M} (1/2 \otimes 1/2) \right\rangle = \sum_{m_{1}, m_{2}} C_{m_{1}}^{1/2} \frac{1/2}{m_{2}} \int \frac{1/2}{m_{1}} \left\langle -1\right\rangle \frac{1}{m_{2}} \right\rangle$$
 
$$T_{-1}^{1} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \qquad T_{0}^{1} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad T_{1}^{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
 
$$T_{1}^{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad T_{1}^{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad T_{1}^{1/2} \left\langle -1/2 \right\rangle \left$$

1st three operators are a vector set that transform like a vector set

 $R(0\beta0) \qquad T_0^1 \qquad R^{\dagger}(0\beta0) \qquad = T_0' \qquad \text{values}$   $\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$   $\left(\cos\frac{\beta}{2} - \sin\frac{\beta}{2}\right) \qquad \left(-1/\sqrt{2} \quad 0\right) \qquad \left(\cos\frac{\beta}{2} \quad \sin\frac{\beta}{2}\right) = -\frac{1}{\sqrt{2}} \left(\cos\beta \quad \sin\beta \right) \qquad \left(\frac{\cos\beta}{2} \quad \sin\beta\right) \qquad \left(\frac{\cos\beta}{2} \quad \cos\beta\right) \qquad \left(\frac{\beta}{2}\right) \qquad \left(\frac{$ 

so do

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

*CGC* definition:

Wigner 3jm definition:

$$\mathbf{v}_{q}^{k} = \sum_{m,m'} C_{m-m'}^{j \ j} \mathbf{v}_{q}^{k} \left(-1\right)^{j-m'} \begin{vmatrix} j \\ m \end{vmatrix} \left\langle \frac{j}{m'} \right| = \left(-1\right)^{2j} T_{q}^{k}. \qquad \mathbf{v}_{q}^{k} = \sum_{m,m'} \left(-1\right)^{j-m} \sqrt{2k+1} \begin{pmatrix} k & j & j \\ q & m' & -m \end{pmatrix} \begin{vmatrix} j \\ m \end{vmatrix} \left\langle \frac{j}{m'} \right|$$

$$\begin{split} \frac{T_{-2}^2 = \begin{vmatrix} 1 \\ -1 \end{vmatrix} \sqrt{\frac{1}{1}}, \quad T_{-1}^2 = \frac{\begin{vmatrix} 1 \\ 0 \end{vmatrix} \sqrt{\frac{1}{1}} - \begin{vmatrix} -1 \\ -1 \end{vmatrix} \sqrt{\frac{1}{0}}, \quad T_0^2 = \frac{\begin{vmatrix} 1 \\ 1 \end{vmatrix} \sqrt{\frac{1}{1}} - 2\begin{vmatrix} 0 \\ 0 \end{vmatrix} \sqrt{\frac{1}{0}} + \begin{vmatrix} 1 \\ -1 \end{vmatrix}}{\sqrt{6}}, \quad T_1^2 = \frac{-\begin{vmatrix} 1 \\ 1 \end{vmatrix} \sqrt{\frac{1}{0}} + \begin{vmatrix} 1 \\ 0 \end{vmatrix} \sqrt{\frac{1}{1}}}{\sqrt{2}}, \quad T_2^2 = \begin{vmatrix} 1 \\ 1 \end{vmatrix} \sqrt{\frac{1}{1}} - \begin{vmatrix} 1 \\ 0 \end{vmatrix} \sqrt{\frac{1}{1}} \\ 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 \end{vmatrix} \\ & T_{-1}^1 = \frac{\begin{vmatrix} 1 \\ 0 \end{vmatrix} \sqrt{\frac{1}{1}} + \begin{vmatrix} 1 \\ -1 \end{vmatrix} \sqrt{\frac{1}{0}}}{\sqrt{2}}, \quad T_0^1 = \frac{\begin{vmatrix} 1 \\ 1 \end{vmatrix} \sqrt{\frac{1}{1}} - \begin{vmatrix} 1 \\ -1 \end{vmatrix} \sqrt{\frac{1}{1}}}{\sqrt{2}}, \quad T_1^1 = \frac{-\begin{vmatrix} 1 \\ 1 \end{vmatrix} \sqrt{\frac{1}{0}} - \begin{vmatrix} 1 \\ 0 \end{vmatrix} \sqrt{\frac{1}{1}}}{\sqrt{2}} \\ & \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & -1/\sqrt{2} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & -1/\sqrt{2} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & -1/\sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & -1/\sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & -1/\sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 0 & 1/\sqrt{3} \end{pmatrix} \\ & \rightarrow \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0$$

These  $T^k_q$  operators are combinations of Elementary operators  $E_{mn}$ 

Example:  $T_1^2 = \frac{-1}{\sqrt{2}}E_{12} + \frac{1}{\sqrt{2}}E_{23}$ 

Tableau Formulas for Electronic Orbital Operators

- (a) Number operators E<sub>ii</sub> are diagonal. (The only eigenvalues for orbital states are 0,1, and 2.)
- (b) Raising and lowering operators are simply transposes of each other.
- (c-h) E<sub>i-1,i</sub> acting on a tableau state gives zero unless there is an (i) in a column of the tableau that doesn't already have an (i-1),too. Then it gives back a new state with the (i) changed to(i-1) and a factor (matrix element) that depends on where the other (i)'s and (i-1)'s are located. (Boxes not outlined in the figure contain numbers not equal to (i) or (i-1).) Cases (c) and (d) involved the "city block" distance d (See Fig.7) which is the denominator of the matrix element. The numerator is one larger (d+1) or smaller (d-1) depending on whether the involved tableaus favor the larger or smaller state number (i or i-1) with a higher position. The special cases of (d=1) shown in (f) always pick the larger (and non-zero) choice of d+1=2. All other non-zero matrix elements are equal to unity.

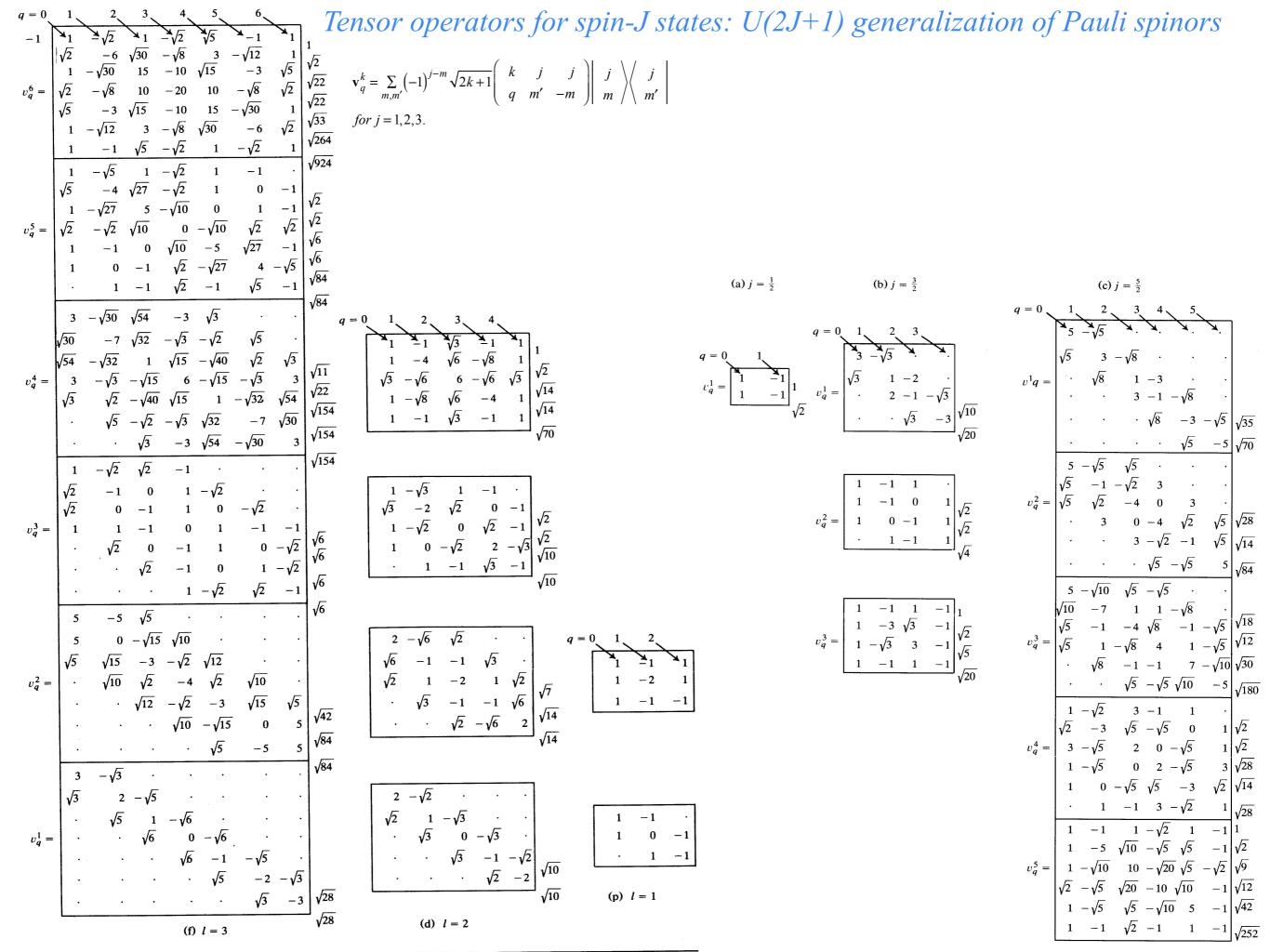
These  $T_q^k$  operators are combinations of Elementary operators  $E_{mn}$  Elementary operators have tableau hook length formula above.

Example:  

$$T_1^2 = \frac{-1}{\sqrt{2}}E_{12} + \frac{1}{\sqrt{2}}E_{23}$$

For applications of Tableaus and Tensors to Molecular physics Go back to Lect. 29 p. 50

# Tensor operators for spin-J states: U(2J+1) generalization of Pauli spinors $\mathbf{v}_{q}^{k} = \sum_{m,m'} \left(-1\right)^{j-m} \sqrt{2k+1} \begin{pmatrix} k & j & j \\ q & m' & -m \end{pmatrix} \begin{vmatrix} j \\ m \end{pmatrix} \left\langle \begin{array}{cc} j \\ m' \\ \end{pmatrix}$ for j = 1, 2, 3. (p) l = 1(d) l = 2(f) l = 3



(d) l = 2