4.04.18 class 21: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Characters of intertwining  $(S_n)^*(U(m))$  algebras and quantum applications

Generic U(3) $\supset$ R(3) transformations: *p*-triplet in U(3) shell model Rank-1 vector in R(3) or "quark"-triplet in U(3) Rank-2 tensor (2 particles each with U(3) state space)

U(3) tensor product states and S<sub>n</sub> permutation symmetry
2-particle U(3) transform.
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Structure of U(3) irep bases Fundamental "quark" irep. The octet "eightfold way" The p-shell in U(3) tableau plots Hooklength formulas

### 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

2014 AMOP 2017 Group Theory for QM 2018 AMOP

Classical Mechanics with a Bang!

#### Modern Physics and its Classical Foundations

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 Intro spin ½ coupling <u>Unit 8 Ch. 24 p3</u>.

*H atom hyperfine-B-level crossing* <u>Unit 8 Ch. 24 p15</u>.

Hyperf. theory Ch. 24 p48.

*Hyperf. theory Ch. 24 p48.* <u>Deeper theory ends p53</u>

> Intro 2p3p coupling <u>Unit 8 Ch. 24 p17</u>.

Intro LS-jj coupling <u>Unit 8 Ch. 24 p22</u>.

CG coupling derived (start) <u>Unit 8 Ch. 24 p39</u>. CG coupling derived (formula) <u>Unit 8 Ch. 24 p44</u>.

> Lande'g-factor <u>Unit 8 Ch. 24 p26</u>.

Irrep Tensor building <u>Unit 8 Ch. 25 p5</u>.

Irrep Tensor Tables <u>Unit 8 Ch. 25 p12</u>.

*Wigner-Eckart tensor Theorem.* <u>Unit 8 Ch. 25 p17</u>.

*Tensors Applied to d,f-levels.* <u>Unit 8 Ch. 25 p21</u>.

*Tensors Applied to high J levels.* <u>Unit 8 Ch. 25 p63</u>. *Intro 3-particle coupling.* <u>Unit 8 Ch. 25 p28</u>.

Intro 3,4-particle Young Tableaus <u>GrpThLect29 p42</u>.

Young Tableau Magic Formulae <u>GrpThLect29 p46-48</u>.

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

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### Characters of intertwining $(S_n)^*(U(m))$ algebras and quantum applications

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U(3) tensor product states and  $S_n$  permutation symmetry Generic U(3)  $\supset$  R(3) transformations (Just like  $\ell = 1$  vector basis  $\{1 = x, 2 = y, 3 = z\}$ )  $\operatorname{uark}^{*}\operatorname{triplet} \operatorname{in} \operatorname{U}(5) \quad \operatorname{ur} \quad r$ where:  $D_{jk} = (\phi_j^*, \phi_k') = (\phi_j^*, \mathbf{u}\phi_k)$   $|1\rangle = \phi_1 = \begin{pmatrix} 1 \\ \cdot \\ \cdot \end{pmatrix}$   $|3\rangle = \phi_3 = \begin{pmatrix} \cdot \\ \cdot \\ 1 \end{pmatrix}$   $(2) = \phi_2 = \begin{pmatrix} \cdot \\ 1 \\ \cdot \end{pmatrix}$   $(2) = \phi_2 = \begin{pmatrix} \cdot \\ 1 \\ \cdot \end{pmatrix}$ Rank-1 vector in R(3) or "quark"-triplet in U(3) or *p*-triplet in U(3) shell model  $\phi_1' = \mathbf{u}\phi_1 = \phi_1 D_{11} + \phi_2 D_{21} + \phi_3 D_{31}$  $\phi'_{2} = \mathbf{u}\phi_{2} = \phi_{1}D_{12} + \phi_{2}D_{22} + \phi_{3}D_{32}$  $\phi'_{3} = \mathbf{u}\phi_{3} = \phi_{1}D_{13} + \phi_{2}D_{23} + \phi_{3}D_{33}$ **Dirac notation:** where:  $D_{jk}(\mathbf{u}) = \langle j | k' \rangle = \langle j | \mathbf{u} | k \rangle$  $|1'\rangle = \mathbf{u}|1\rangle = |1\rangle D_{11} + |2\rangle D_{21} + |3\rangle D_{31}$  $D_{jk}(\mathbf{u}) = \left(\begin{array}{ccc} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{21} & D_{22} & D_{33} \end{array}\right)$  $|2'\rangle = \mathbf{u}|2\rangle = |1\rangle D_{12} + |2\rangle D_{22} + |3\rangle D_{32}$  $|3'\rangle = \mathbf{u}|3\rangle = |1\rangle D_{13} + |2\rangle D_{23} + |3\rangle D_{33}$ 

U(3) tensor product states and  $S_n$  permutation symmetry Typical U(3) $\supset$ R(3) transformations (Just like  $\ell = 1$  vector basis  $\{1=x, 2=y, 3=z\}$ ) where:  $D_{jk} = (\phi_j^*, \phi_k') = (\phi_j^*, \mathbf{u}\phi_k)$   $|1\rangle = \phi_1 = \begin{pmatrix} 1 \\ \cdot \\ \cdot \end{pmatrix}$  $|3\rangle = \phi_3 = \begin{pmatrix} \cdot \\ \cdot \\ 1 \end{pmatrix}$  $|2\rangle = \phi_2 = \begin{pmatrix} \cdot \\ 1 \\ \cdot \end{pmatrix}$ Rank-1 vector in R(3) or "quark"-triplet in U(3) or *p*-triplet in U(3) shell model  $\phi_1' = \mathbf{u}\phi_1 = \phi_1 D_{11} + \phi_2 D_{21} + \phi_3 D_{31}$  $\phi'_{2} = \mathbf{u}\phi_{2} = \phi_{1}D_{12} + \phi_{2}D_{22} + \phi_{3}D_{32}$  $\phi'_{3} = \mathbf{u}\phi_{3} = \phi_{1}D_{13} + \phi_{2}D_{23} + \phi_{3}D_{33}$ **Dirac notation:** where:  $D_{jk}(\mathbf{u}) = \langle j | k' \rangle = \langle j | \mathbf{u} | k \rangle$  $|1'\rangle = \mathbf{u}|1\rangle = |1\rangle D_{11} + |2\rangle D_{21} + |3\rangle D_{31}$  $D_{jk}(\mathbf{u}) = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{pmatrix}$  $|2'\rangle = \mathbf{u}|2\rangle = |1\rangle D_{12} + |2\rangle D_{22} + |3\rangle D_{32}$  $|3'\rangle = \mathbf{u}|3\rangle = |1\rangle D_{13} + |2\rangle D_{23} + |3\rangle D_{33}$ 

Rank-2 tensor (2 particles each with U(3) state space)

$$\begin{aligned} \left| j' \right\rangle \left| k' \right\rangle &= \mathbf{u} \left| j \right\rangle \mathbf{u} \left| k \right\rangle \\ &= \sum_{j,k} \left| j \right\rangle \left| k \right\rangle D_{jj'} D_{kk'} \\ &= \sum_{j,k} \left| j \right\rangle \left| k \right\rangle D \otimes D_{jk:j'k'} \end{aligned}$$

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Rank-2 tensor (2 particles each with U(3) state space)

 $|3'\rangle = \mathbf{u}|3\rangle = |1\rangle D_{13} + |2\rangle D_{23} + |3\rangle D_{33}$ 

$$\begin{aligned} \left| j' \right\rangle \left| k' \right\rangle &= \mathbf{u} \left| j \right\rangle \mathbf{u} \left| k \right\rangle \\ &= \sum_{j,k} \left| j \right\rangle \left| k \right\rangle D_{jj'} D_{kk'} \\ &= \sum_{j,k} \left| j \right\rangle \left| k \right\rangle D \otimes D_{jk:j'k'} \end{aligned}$$

 $= \begin{pmatrix} D_{11}D_{11} & D_{11}D_{12} & D_{11}D_{13} & D_{12}D_{11} & D_{12}D_{12} & D_{12}D_{13} & \cdots \\ D_{11}D_{21} & D_{11}D_{22} & D_{11}D_{23} & D_{12}D_{21} & D_{12}D_{22} & D_{12}D_{23} & \cdots \\ D_{11}D_{31} & D_{11}D_{32} & D_{11}D_{33} & D_{12}D_{21} & D_{12}D_{22} & D_{12}D_{23} & \cdots \\ D_{21}D_{11} & D_{21}D_{12} & \vdots & D_{22}D_{11} & D_{22}D_{12} & \vdots & \cdots \\ \vdots & \ddots \end{pmatrix}$ 

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U(3) tensor product states and  $S_n$  permutation symmetry 2-particle U(3) transform and outer-product U(3) transform matrix  $D_{jj'}D_{kk'} = D \otimes D_{jk;j'k'} =$  $D_{11}D_{11} \quad D_{11}D_{12} \quad D_{11}D_{13} \quad D_{12}D_{11} \quad D_{12}D_{12} \quad D_{12}D_{13} \quad D_{13}D_{11} \quad D_{13}D_{12} \quad D_{13}D_{13}$  $D_{11}D_{21}$   $D_{11}D_{22}$   $D_{11}D_{23}$   $D_{12}D_{21}$   $D_{12}D_{22}$   $D_{12}D_{23}$   $D_{13}D_{21}$   $D_{13}D_{22}$   $D_{13}D_{23}$  $D_{11}D_{31}$   $D_{11}D_{32}$   $D_{11}D_{33}$   $D_{12}D_{31}$   $D_{12}D_{22}$   $D_{12}D_{33}$   $D_{13}D_{31}$   $D_{13}D_{23}$   $D_{13}D_{33}$  $D_{21}D_{11} \quad D_{21}D_{12} \quad D_{21}D_{13} \quad D_{22}D_{11} \quad D_{22}D_{12} \quad D_{22}D_{13} \quad D_{23}D_{11} \quad D_{23}D_{12} \quad D_{23}D_{13}$  $= \begin{bmatrix} D_{21}D_{21} & D_{21}D_{22} & D_{21}D_{23} & D_{22}D_{21} & D_{22}D_{22} & D_{22}D_{23} & D_{23}D_{21} & D_{23}D_{22} & D_{23}D_{23} \end{bmatrix}$  $D_{21}D_{31} \quad D_{21}D_{32} \quad D_{21}D_{33} \quad D_{22}D_{31} \quad D_{22}D_{32} \quad D_{22}D_{33} \quad D_{23}D_{31} \quad D_{23}D_{23} \quad D_{23}D_{33} \quad D_{2$  $D_{31}D_{11}$   $D_{31}D_{12}$   $D_{31}D_{13}$   $D_{32}D_{11}$   $D_{32}D_{12}$   $D_{32}D_{13}$   $D_{33}D_{11}$   $D_{33}D_{12}$   $D_{33}D_{13}$  $D_{31}D_{21} \quad D_{31}D_{22} \quad D_{31}D_{23} \quad D_{32}D_{21} \quad D_{32}D_{22} \quad D_{32}D_{23} \quad D_{33}D_{21} \quad D_{33}D_{22} \quad D_{33}D_{23}$  $D_{31}D_{31} \quad D_{31}D_{23} \quad D_{31}D_{33} \quad D_{32}D_{31} \quad D_{32}D_{32} \quad D_{32}D_{33} \quad D_{33}D_{31} \quad D_{33}D_{23} \quad D_{33}D_{33} \quad D_{$ 

U(3) tensor product states and  $S_2=S_n$  permutation symmetry 2-particle U(3) transform and outer-product U(3) transform matrix  $D_{ii'}D_{kk'} = D \otimes D_{ik;i'k'} =$  $D_{11}D_{11}$   $D_{11}D_{12}$   $D_{11}D_{13}$   $D_{12}D_{11}$   $D_{12}D_{12}$   $D_{12}D_{13}$   $D_{13}D_{11}$   $D_{13}D_{12}$   $D_{13}D_{13}$  $D_{11}D_{22}$   $D_{11}D_{23}$   $D_{12}D_{21}$   $D_{12}D_{22}$   $D_{12}D_{23}$   $D_{13}D_{21}$   $D_{13}D_{22}$   $D_{13}D_{23}$  $D_{11}D_{21}$  $D_{11}D_{31}$   $D_{11}D_{32}$   $D_{11}D_{33}$   $D_{12}D_{31}$   $D_{12}D_{22}$   $D_{12}D_{33}$   $D_{13}D_{31}$   $D_{13}D_{23}$   $D_{13}D_{33}$  $D_{21}D_{11}$   $D_{21}D_{12}$   $D_{21}D_{13}$   $D_{22}D_{11}$   $D_{22}D_{12}$   $D_{22}D_{13}$   $D_{23}D_{11}$   $D_{23}D_{12}$   $D_{23}D_{13}$  $D_{21}D_{22}$   $D_{21}D_{23}$   $D_{22}D_{21}$   $D_{22}D_{22}$   $D_{22}D_{23}$   $D_{23}D_{21}$   $D_{23}D_{22}$   $D_{23}D_{23}$  $D_{21}D_{21}$ = $D_{21}D_{31} \quad D_{21}D_{32} \quad D_{21}D_{33} \quad D_{22}D_{31} \quad D_{22}D_{32} \quad D_{22}D_{33} \quad D_{23}D_{31} \quad D_{23}D_{23} \quad D_{23}D_{33}$  $D_{31}D_{11}$   $D_{31}D_{12}$   $D_{31}D_{13}$   $D_{32}D_{11}$   $D_{32}D_{12}$   $D_{32}D_{13}$   $D_{33}D_{11}$   $D_{33}D_{12}$   $D_{33}D_{12}$  $D_{31}D_{21}$  $D_{31}D_{22}$   $D_{31}D_{23}$   $D_{32}D_{21}$   $D_{32}D_{22}$   $D_{32}D_{23}$   $D_{33}D_{21}$   $D_{33}D_{22}$   $D_{33}D_{23}$  $D_{31}D_{31} \quad D_{31}D_{23} \quad D_{31}D_{33} \quad D_{32}D_{31} \quad D_{32}D_{32} \quad D_{32}D_{33} \quad D_{33}D_{31} \quad D_{33}D_{23} \quad D_{33}D_{33}$  $\mathbf{s}(a)(b) | j \rangle_a | k \rangle_b = | j \rangle_a | k \rangle_b$ ,  $\mathbf{s}(ab) | j \rangle_a | k \rangle_b = | k \rangle_a | j \rangle_b$ 2-particle permutation operations: Represented by matrices: 12 13 21 22 23 31 32 13 21 22 23 31 32 33 11 12 33 11 11 11 12 12 13 13 . . 1 . . 21 21  $\mathbf{s}(a)(b) =$  $\mathbf{s}(ab) =$ 22 22 23 23 31 31 32 32 33 33

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| S <sub>2</sub> syn  | nm       | etr  | <i>y</i> 0    | fU            | (3)           | : Aj | ppl           | yin           | $g S_{2}$     | 2 pr | ojection         |      |      |                |                 |                |                |                |                |                |     |         |
|---|----------|------|---------------|---------------|---------------|------|---------------|---------------|---------------|------|------------------|------|------|----------------|-----------------|----------------|----------------|----------------|----------------|----------------|-----|---------|
| $S_2$ matr  | ix e     | eige | n-se          | olut          | tion          | fou  | ndl           | by p          | oroj          | ecto | rs: Minir        | nale | eq.  | (ab)           | <sup>2</sup> -1 | =0=            | =( <b>(a</b>   | <b>b)</b> +:   | 1)((           | ab)-           | +1) | yields: |
| Symmetric ( $\square$ ): $\mathbf{P}^{\square} = \frac{1}{2} [1 + (\mathbf{ab})]$ |          |      |               |               |               |      | )]            |               | 1             | Ant  | i-Sy             | mn   | netr | ic (           | )               | : P            | $=\frac{1}{2}$ | [1-            | (ab)]          |                |     |         |
|   |          | 11   | 12            | 13            | 21            | 22   | 23            | 31            | 32            | 33   | ₽ <sup>□</sup> = |      | 11   | 12             | 13              | 21             | 22             | 23             | 31             | 32             | 33  |         |
|   | 11       | 1    | •             | •             | •             | •    | •             | •             | •             | •    |                  | 11   | 0    | •              | •               | •              | •              | •              | •              | •              | •   |         |
|   | 12       | •    | $\frac{1}{2}$ | •             | $\frac{1}{2}$ | •    | •             | •             | •             | •    |                  | 12   | •    | $\frac{1}{2}$  | •               | $\frac{-1}{2}$ | •              | •              | •              | •              | •   |         |
|   | 13       | •    | •             | $\frac{1}{2}$ | •             | •    | •             | $\frac{1}{2}$ | •             | •    |                  | 13   | •    | •              | $\frac{1}{2}$   | •              | •              | •              | $\frac{-1}{2}$ | •              | •   |         |
|   | 21       | •    | $\frac{1}{2}$ | •             | $\frac{1}{2}$ | •    | •             | •             | •             | •    |                  | 21   | •    | $\frac{-1}{2}$ | •               | $\frac{1}{2}$  | •              | •              | •              | •              | •   |         |
| <b>I I</b>  | 22       | •    | •             | •             | •             | 1    | •             | •             | •             | •    |                  | 22   | •    | •              | •               | •              | 0              | •              | •              | •              | •   |         |
|   | 23       | •    | •             | •             | •             | •    | $\frac{1}{2}$ | •             | $\frac{1}{2}$ | •    |                  | 23   | •    | •              | •               | •              |                | $\frac{1}{2}$  | •              | $\frac{-1}{2}$ | •   |         |
| -   | 31       | •    | •             | $\frac{1}{2}$ | •             | •    | •             | $\frac{1}{2}$ | •             | •    |                  | 31   | •    | •              | $\frac{-1}{2}$  | •              | •              | •              | $\frac{1}{2}$  | •              | •   |         |
|   | 32       | •    | •             | •             | •             | •    | $\frac{1}{2}$ | •             | $\frac{1}{2}$ | •    |                  | 32   | •    | •              | •               | •              | •              | $\frac{-1}{2}$ | •              | $\frac{1}{2}$  |     |         |
|   | 33       | •    | •             | •             | •             | •    | •             | •             | •             | 1    |                  | 33   | •    | •              | •               | •              |                | •              | •              | •              | 0   |         |
|   |          | 11   | 12            | 13            | 21            | 22   | 23            | 31            | 32            | 33   |                  |      | 11   | 12             | 13              | 21             | 22             | 23             | 31             | 32             | 33  |         |
| -   | 11       | 1    | •             | •             | •             | •    | •             | •             | •             | •    |                  | 11   | 1    | •              | •               | •              | •              | •              | •              | •              | •   |         |
|   | 12       | •    | 1             | •             | •             | •    | •             | •             | •             |      |                  | 12   | •    |                | •               | 1              | •              | •              | •              | •              |     |         |
|   | 13       | •    | •             | 1             | •             | •    | •             | •             | •             | •    |                  | 13   | •    | •              | •               | •              | •              | •              | 1              | •              | •   |         |
| (a)(b) =  | 21       | •    | •             | •             | 1             | •    | •             | •             | •             |      | (ab) =           | 21   | •    | 1              | •               | •              | •              | •              | •              | •              |     |         |
|   | 22       | ٠    | •             | •             | •             | 1    | •             | •             | •             |      | ()               | 22   | •    | •              | •               | •              | 1              | •              | •              | •              | •   |         |
|   | 23       | •    | •             | •             | •             | •    | <u> </u>      | •             | •             | •    |                  | 23   | •    | •              | •               | •              | •              | •              | •              | 1              | •   |         |
|   | 31       | •    | •             | •             | •             | •    | •             | 1             | •             | •    |                  | 31   | •    | •              | 1               | •              | •              | •              | •              | •              |     |         |
|   | 32<br>22 | •    | •             | •             | ·             | •    | •             | ·             | 1             | •    |                  | 32   | •    | •              | •               | •              | •              | 1              | •              | •              | •   |         |
|   | 33       | •    | •             | •             | •             | •    | •             | •             | •             | 1    |                  | 33   | •    | •              | •               | •              | •              | •              | •              | •              | 1   |         |

Matrix representation of *Diagonalizing Transform* (DTran T) is made by excerpting P-columns



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### S<sub>2</sub> matrix:

#### $T^{\dagger}S(\mathbf{p}_{ab})T = 6D_{\text{dim}=1}^{\square}(\mathbf{p}) \oplus 3D_{\text{dim}=1}^{\square}(\mathbf{p})$ $D^{\square\square}(\mathbf{p})$ *D* (**p**) *D* (**p**) *D* (**p**) *D* (**p**) *D* (**p**) $D^{\square}(\mathbf{p})$ $D^{\square}(\mathbf{p})$ $D^{\square}(\mathbf{p})$ +1 Diagonalized +1 $S_2$ bicycle +1 matrix: +1 $T^{\dagger}(\mathbf{ab})T =$ +1 +1 Unicycle -1 **(a)(b)** is unit matrix -1

-1

$$T^{\dagger}D \otimes D(\mathbf{u})T = 1D_{\dim=6}^{\square}(\mathbf{p}) \oplus 1D_{\dim=3}^{\square}(\mathbf{p})$$

| $D_{11}^{\square\square}(\mathbf{u})$ | $D_{12}(\mathbf{u})$ | $D_{13}({f u})$      | $D_{14}(\mathbf{u})$ | $D_{15}(\mathbf{u})$ | $D_{16}(\mathbf{u})$ |                                |                      |                 |
|---------------------------------------|----------------------|----------------------|----------------------|----------------------|----------------------|--------------------------------|----------------------|-----------------|
| $D_{21}({f u})$                       | $D_{22}(\mathbf{u})$ | $D_{23}({f u})$      | $D_{24}({f u})$      | $D_{25}(\mathbf{u})$ | $D_{26}(\mathbf{u})$ |                                |                      |                 |
| $D_{31}({f u})$                       | $D_{32}({f u})$      | $D_{33}({f u})$      | $D_{34}({f u})$      | $D_{35}(\mathbf{u})$ | $D_{36}({f u})$      |                                |                      |                 |
| $D_{41}({f u})$                       | $D_{42}(\mathbf{u})$ | $D_{43}(\mathbf{u})$ | $D_{44}(\mathbf{u})$ | $D_{45}(\mathbf{u})$ | $D_{46}(\mathbf{u})$ |                                |                      |                 |
| $D_{51}(\mathbf{u})$                  | $D_{52}(\mathbf{u})$ | $D_{53}(\mathbf{u})$ | $D_{54}(\mathbf{u})$ | $D_{55}(\mathbf{u})$ | $D_{56}(\mathbf{u})$ |                                |                      |                 |
| $D_{61}(\mathbf{u})$                  | $D_{62}(\mathbf{u})$ | $D_{63}(\mathbf{u})$ | $D_{64}(\mathbf{u})$ | $D_{65}(\mathbf{u})$ | $D_{66}(\mathbf{u})$ |                                |                      |                 |
|                                       |                      |                      |                      |                      |                      | $D_{11}^{\square}(\mathbf{u})$ | $D_{12}({f u})$      | $D_{13}({f u})$ |
|                                       |                      |                      |                      |                      |                      | $D_{21}({f u})$                | $D_{22}(\mathbf{u})$ | $D_{23}({f u})$ |
|                                       |                      |                      |                      |                      |                      | $D_{31}({\bf u})$              | $D_{32}({f u})$      | $D_{33}({f u})$ |

U(3) matrices:

 $S_2$  symmetry of U(3): Effect of  $S_2$  DTran T on intertwining  $S_2$  - U(3) irep matrices

### S<sub>2</sub> matrix:

U(3) matrices:



$$T^{\dagger}D \otimes D(\mathbf{u})T = 1D_{\dim=6}^{\square}(\mathbf{p}) \oplus 1D_{\dim=3}^{\square}(\mathbf{p})$$

| $D_{11}^{\square\square}(\mathbf{u})$ | $D_{12}(\mathbf{u})$ | $D_{13}({f u})$      | $D_{14}(\mathbf{u})$ | $D_{15}(\mathbf{u})$ | $D_{16}(\mathbf{u})$ |                                |                      |                 |
|---------------------------------------|----------------------|----------------------|----------------------|----------------------|----------------------|--------------------------------|----------------------|-----------------|
| $D_{21}({f u})$                       | $D_{22}(\mathbf{u})$ | $D_{23}(\mathbf{u})$ | $D_{24}(\mathbf{u})$ | $D_{25}(\mathbf{u})$ | $D_{26}(\mathbf{u})$ |                                |                      |                 |
| $D_{31}({f u})$                       | $D_{32}({f u})$      | $D_{33}({f u})$      | $D_{34}({f u})$      | $D_{35}(\mathbf{u})$ | $D_{36}({f u})$      |                                |                      |                 |
| $D_{41}(\mathbf{u})$                  | $D_{42}(\mathbf{u})$ | $D_{43}(\mathbf{u})$ | $D_{44}(\mathbf{u})$ | $D_{45}(\mathbf{u})$ | $D_{46}(\mathbf{u})$ |                                |                      |                 |
| $D_{51}(\mathbf{u})$                  | $D_{52}(\mathbf{u})$ | $D_{53}(\mathbf{u})$ | $D_{54}(\mathbf{u})$ | $D_{55}(\mathbf{u})$ | $D_{56}(\mathbf{u})$ |                                |                      |                 |
| $D_{61}(\mathbf{u})$                  | $D_{62}(\mathbf{u})$ | $D_{63}(\mathbf{u})$ | $D_{64}(\mathbf{u})$ | $D_{65}(\mathbf{u})$ | $D_{66}(\mathbf{u})$ |                                |                      |                 |
|                                       |                      |                      |                      |                      |                      | $D_{11}^{\square}(\mathbf{u})$ | $D_{12}({f u})$      | $D_{13}({f u})$ |
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 $S_2$  group hook formula







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S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> projection

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(3) state space) has dimension  $3^3=27$ 

S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> projection



S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> projection



Whoa! That's pretty big. So let's solve by *S*<sub>3</sub> *character theory*. Only need traces that are sums of diagonal elements (just one per-class)

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Whoa! That's pretty big. So let's solve by S<sub>3</sub> *character theory*. Only need traces that are sums of diagonal elements (just one per-class) Bicycle character :

Trace s((ab)) counts states like  $|j_a j_b k_c\rangle$ 

S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> character theory



Whoa! That's pretty big. So let's solve by S<sub>3</sub> *character theory*. Only need traces that are sums of diagonal elements (just one per-class) Bicycle character : Trace s((ab)) counts

*Trace s*((**ab**)) counts states like  $|j_a j_b k_c\rangle$ result: *Tr*(**ab**)=9

S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> character theory





Whoa! That's pretty big. So let's solve by  $S_3$ character theory. Only need traces that are sums of diagonal elements (just one per-class) Bicycle character : *Trace s*((**ab**)) counts states like  $|j_a j_b k_c\rangle$ result: Tr(ab)=9 Tricycle character : *Trace s*((abc)) counts states like  $|j_a j_b j_c\rangle$ result: Tr(abc)=3

### S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> character theory

Rank-3 tensor basis  $|i_a j_b k_c\rangle$  (3 particles each with U(3) state space) has dimension  $3^3=27$ 





Whoa! That's pretty big. So let's solve by  $S_3$ character theory. Only need traces that are sums of diagonal elements (just one per-class) Bicycle character : *Trace s*((**ab**)) counts states like  $|j_a j_b k_c\rangle$ result: Tr(ab)=9

Tricycle character : *Trace s*((abc)) counts states like |j<sub>a</sub> j<sub>b</sub> j<sub>c</sub> > result: *Tr*(abc)=3

Unicycle character : result: *Tr*(a)(b)(c)=27

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S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> character theory Rank-3 tensor basis  $|i_a j_b k_c\rangle$  (3 particles each with U(3) state space) has dimension 3<sup>3</sup>=27 Frequency formula for D<sup>[µ]</sup>:  $f^{[µ]} = \frac{1}{{}^o S_n} \sum_{classes(k)} {order of \ class(k)} \chi_k^{[µ]} Trace(\mathbf{p}_k)$ 

Tensor traces: Tr(a)(b)(c)=27, Tr(abc)=3, Tr(ab)=9,









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### $S_n$ Young Tableaus and spin-symmetry for $X_n$ and $XY_n$ molecules Tableau dimension formulae $3\cdot 2\cdot 1$ Examples:



FIG. 28. Robinson formula for statistical weights. The "hooklength" of a box in the tableau is the number of boxes in a "hook" which includes that box and all boxes in the line to the right and in the column below it.





Irep.freq.formula GrpThLect.15p.48.





U(3) group hook formula



=10

3 2



 $n!=n\cdot(n-1)\cdot(n-2)\cdots 3\cdot 2\cdot 1$ = • hook-length product

 $S_3$  group hook formula



S<sub>3</sub> symmetry of U(3): Effect of S<sub>3</sub> DTran T on intertwining S<sub>3</sub> - U(3) irep matrices S<sub>3</sub> matrices: U(3) matrices:





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Each tableau has 3D Cartesian integer coordinates  $(n_1, n_2, n_3)$  determined by number operators  $(a_1\overline{a}_1, a_2\overline{a}_2, a_3\overline{a}_3)$ Tableaus with the same total number  $N = n_1 + n_2 + n_3$  lie in the same plane normal to (1, 1, 1). Plane has orthogonal *D* and *Q* axes for *dipole-sum D* of z-component momentum  $D = \langle L_z \rangle = n_3 - n_1 = M_L$ and the *quadrupole-sum Q* of squared-z-component momentum.  $Q = \langle L_z^2 \rangle = n_3 + n_1 = N - n_2$ 



*Structure of* U(3) *irep bases* (c)Anti-symmetri D.S sextet [20] P-triplet [11] Fundamental  $\ell^{[]} = 3$  "anti-quark" -0 13 S single Each tableau has 3D Cartesian integer coordinates  $(n_1, n_2, n_3)$  determined by number operators  $(a_1\overline{a_1}, a_2\overline{a_2}, a_3\overline{a_3})$  $(\mathbf{a}_1^{\mathsf{T}}\mathbf{a}_1, \mathbf{a}_2^{\mathsf{T}}\mathbf{a}_2, \mathbf{a}_3^{\mathsf{T}}\mathbf{a}_3)$ Tableaus with the same total number  $N = n_1 + n_2 + n_3$  lie in the same plane normal to (1,1,1).  $\boldsymbol{D} = \left\langle L_z \right\rangle = n_3 - n_1 = M_L$ Plane has orthogonal D and Q axes for *dipole-sum* D of z-component momentum and the *quadrupole-sum Q* of squared-*z*-component momentum.  $\boldsymbol{Q} = \left\langle L_z^2 \right\rangle = n_3 + n_1 = N - n_2$ (*b*) (*U*(3) *l*-1 states) (b) (U(3)  $\ell$ -1 states)



Structure of U(3) irep bases Fundamental  $\ell^{\Box\Box} = 6$  "di-quark"



Each tableau has 3D Cartesian integer coordinates  $(n_1, n_2, n_3)$  determined by number operators  $(a_1\overline{a}_1, a_2\overline{a}_2, a_3\overline{a}_3)$ Tableaus with the same total number  $N = n_1 + n_2 + n_3$  lie in the same plane normal to (1,1,1). Plane has orthogonal *D* and *Q* axes for *dipole-sum D* of z-component momentum  $D = \langle L_z \rangle = n_3 - n_1 = M_L$ and the *quadrupole-sum Q* of squared-z-component momentum.  $Q = \langle L_z^2 \rangle = n_3 + n_1 = N - n_2$ 



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"anti-quark". "di-quark". The decapalet and \Omega^{-}
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Each tableau has 3D Cartesian integer coordinates  $(n_1, n_2, n_3)$  determined by number operators  $(a_1\overline{a}_1, a_2\overline{a}_2, a_3\overline{a}_3)$ Tableaus with the same total number  $N = n_1 + n_2 + n_3$  lie in the same plane normal to (1, 1, 1). Plane has orthogonal D and Q axes for *dipole-sum* D of z-component momentum  $D = \langle L_z \rangle = n_3 - n_1 = M_L$ and the *quadrupole-sum* Q of squared-z-component momentum.  $Q = \langle L_z^2 \rangle = n_3 + n_1 = N - n_2$ 





Each tableau has 3D Cartesian integer coordinates  $(n_1, n_2, n_3)$  determined by number operators  $(a_1\overline{a}_1, a_2\overline{a}_2, a_3\overline{a}_3)$ Tableaus with the same total number  $N = n_1 + n_2 + n_3$  lie in the same plane normal to (1, 1, 1). Plane has orthogonal *D* and *Q* axes for *dipole-sum D* of z-component momentum  $D = \langle L_z \rangle = n_3 - n_1 = M_L$ and the *quadrupole-sum Q* of squared-z-component momentum.  $Q = \langle L_z^2 \rangle = n_3 + n_1 = N - n_2$ 



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Fig.8 Weight or Moment Diagrams of Atomic  $(p)^n$  States Each tableau is located at point  $(x_1 \ x_2 \ x_3)$  in a cartesian co-ordinate system for which  $x_n$  is the number of n's in the tableau. An alternative co-ordinate system is  $(v_0^2, v_0^1, v_0^0)$ defined by Eq.16 which gives the 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.

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    S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> projection
    Applying S<sub>3</sub> character theory
    Frequency formula for D<sup>[µ]</sup> with tensor trace values
    Effect of S<sub>3</sub> DTran T on intertwining S<sub>3</sub> - U(3) irep matrices
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Structure of U(3) irep bases
Fundamental "quark" irep.
The octet "eightfold way"
The p-shell in U(3) tableau plots
Hooklength formulas

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"anti-quark". "di-quark". The decapalet and \Omega^{-}
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Dimension of representations of (a)  $S_n$  and (b)  $U_m$  labeled by a single tableau are given by the formulas. A <u>hooklength</u> of a tableau box is simply the number of boxes in a "hook" consisting of all the boxes below it, to the right of it, and itself. Unitary raising and lowering operators E<sub>jk</sub>

$$\mathbf{a}_{j}^{\dagger}\mathbf{a}_{k} + \mathbf{b}_{j}^{\dagger}\mathbf{b}_{k} + \ldots = E_{jk} = a_{j}\overline{a}_{k} + b_{j}\overline{b}_{k} + \ldots$$

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

Hooklength formulas for  $E_{jk}$  on atomic tableau states



*Multi-spin (1/2)*<sup>N</sup> *product states* 



*Multi-spin (1/2)*<sup>N</sup> *product states* 





$$= \frac{3!}{6!} \begin{bmatrix} (2ass(1)) & \chi_{13} & \Pi & (a)(0)(0) + (2ass(3)) & \chi_{(3)} & \Pi & (abc) + (2ass(1)(2)) & \chi_{(1)(2)} & \Pi & (ab) \end{bmatrix}$$
$$= \frac{1}{6!} \begin{bmatrix} (1) & 1 & 27 & + (2) & 1 & 3 & + (3) & (-1) & 9 \end{bmatrix} = 1$$

### S<sub>3</sub> symmetry of U(3): Applying S<sub>3</sub> projection

Rank-3 tensor basis  $|ijk\rangle$  (3 particles each with U(3) state space) has dimension  $3^3=27$ 



|   | g =  | 1 = (1)(2)(3)                         | r = (123)   | $r^2 = (132)$        | $i_1 = (23)$  | <b>i</b> <sub>2</sub> = (13)  | $i_3 = (12)$                                       |   |                       |
|---|--|---------------------------------------|---|----------------------|---|---|--|---|-----------------------|
|   | $D^{\Box\Box\Box}(\mathbf{g}) =$               |                                       |   |                      |   |   |  |   |                       |
|   | E C  | 1                                     | 1   | 1                    | 1   | 1   | 1  |   |                       |
|   | $D^{\square}(\mathbf{g}) =$                    | 1                                     | 1   | 1                    | -1  | -1  | -1   |   |                       |
|   |  | $\begin{pmatrix} 1 & 0 \end{pmatrix}$ | $-1/2 - \sqrt{3}/2$   | $-1/2  \sqrt{3}/2$   | $\begin{pmatrix} -1/2 & \sqrt{3}/2 \end{pmatrix}$   | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 \end{pmatrix}$  | $\begin{pmatrix} 1 & 0 \end{pmatrix}$              |   |                       |
|   | $D_{x_2y_2}^{[\bot]}\left(\mathbf{g}\right) =$ |                                       | $\sqrt{3}/2$ $-1/2$   | $-\sqrt{3}/2$ $-1/2$ | $\sqrt{3/2}$ $\sqrt{3}/2$   | $\left( -\sqrt{3}/2 + 1/2 \right)$  | ( 0 -1 )   |   |                       |
| 111 112 121 122 211 212 221 222   | 111 112 121 12                                 | 2 211 212 221 222                     | 111 112 121 122   | 211 212 221 222      | <u>1 111 112 121 122 211 2</u>  | 212 221 222 111 1   | 12 121 122 211 212 221 222                         | 111 112 121 12  | 22 211 212 221 222    |
|   | 1 1  |                                       | 111 1   |                      | 111 1   | 111 1   |  | 111 1   |                       |
|   | 2 1  |                                       | 112   | 1                    | 112 1   | 112   | 1  | 112   | 1                     |
|   | 1  | 1                                     | 121 1   |                      | 121 1   | 121   | 1  | 121 1   |                       |
|   | 2  | 1                                     | 122   | 1                    | 122 1   | 122   | 1  | 122   | 1                     |
| 211 1 21  | 1 1  |                                       | 211 1   |                      | 211 1   | 211   |  | 211 1   |                       |
|   | 2 1  |                                       | 212   | 1                    | 212   | 1 212   |  | 212   | 1                     |
|   | 1  |                                       | 221 1   |                      | 221   | 1 221   |  |   |                       |
|   | 2  |                                       |   |                      |   |   |  |   |                       |
| [1][2][3]   | [12]   |                                       | [13]  |                      | [23]  | [125]   |  | [152]   |                       |
| 111     112     122     211     212     221       111     112     121     111       112     121     121       121     121     121       122     121     121       211     121     121       212     121     211 | 111       112       121       122         2    | 2 211 212 221 222                     | 111     112     122       111     112     122       112     121     121       121     122     121       122     121     121       211     122     121 |                      | 111     112     122     211     2       111     112     1     1       112     1     1     1       121     1     1     1       122     1     1     1       211     1     1     1 | 221     222     111     111       111     111     111       111     112       121     121       122     211       212     212 | 12     121     122     211     212     221     222 | 111     112     121       111     112     121       112     121       121     122       211     212 | 2 211 212 221 222<br> |
| 221 221   |  |                                       | 221   |                      | 221   | 221   |  | 221   |                       |
| 222         222   | 2  |                                       | 222   |                      | 222   | 222   |  | 222   |                       |
| 111 112 121 122 211 212 221 222   | 111 112 121 12:                                | 2 211 212 221 222                     | 111 112 121 122   | 211 212 221 222      | 111 112 121 122 211 2   | 12 221 222  | 12 121 122 211 212 221 222                         |   | 2211212221222         |
|   | ,  |                                       |   |                      | 111   | 111   |  | 111   |                       |
|   | ۲<br>  |                                       | 112   |                      | 112   | 112   |  | 112   |                       |
|   |  |                                       | 121   |                      |   | 121   |  |   |                       |
|   |  |                                       | 211   |                      |   |   |  | 122   |                       |
|   |  | +                                     |   |                      | 211   |   |  |   |                       |
|   | 4  | - <u>+</u> +                          | 212   |                      | 212   |   |  |   |                       |
|   |  |                                       |   |                      |   |   | +  |   | -+                    |
|   | 4  | <u> </u>                              | 222   |                      | 222   |   |  | 222   |                       |